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## Electronic Supplementary Information

# Analytical nuclear gradients for the range-separated many-body dispersion model of noncovalent interactions

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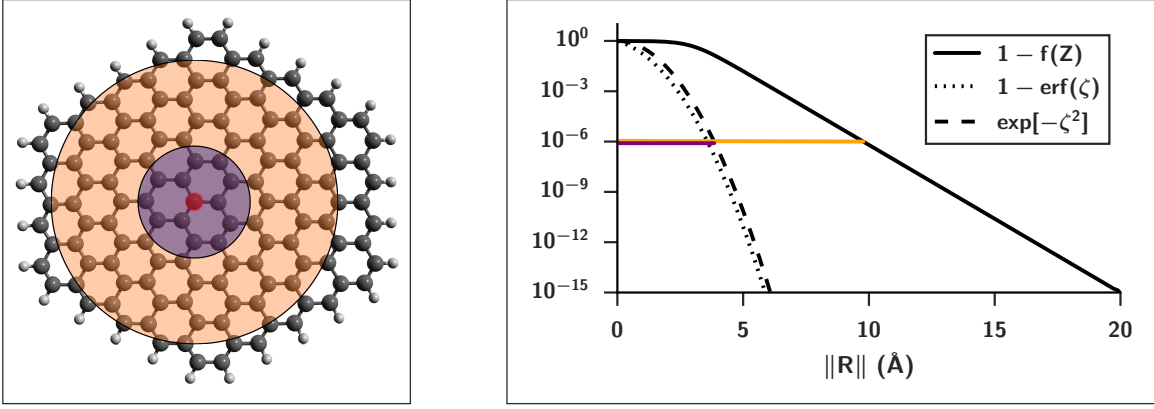
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# 1 Symbol glossary

Symbol	Description
$\alpha_a^{\text{free}}(0)$	static free-atom polarizability formed with $\alpha_a^{\text{free}}(0)$ scalars on the diagonal
$\alpha_a(0)$	Eq. (5): static bare polarizability, related to $\alpha_a^{\text{free}}(0)$ by the ratio $V_a/V_a^{\text{free}}$
$\alpha_a(i\omega)$	Eq. (7): frequency-dependent bare polarizability tensor, calculated by Padé approximant Eq. (4)
$\alpha_a(i\omega)$	'isotropized' bare dipole polarizability scalar, calculated as $\alpha_a = \frac{1}{3}\text{Tr}[\alpha_a]$
$\mathbf{A}(i\omega)$	Eq. (9): bare system polarizability tensor, $3N \times 3N$ block diagonal matrix of $\alpha_a(i\omega)$
$\bar{\mathbf{A}}(i\omega)$	Eq. (11): screened system polarizability tensor, solved at complex frequency $i\omega$ using $[\mathbf{A}^{-1} + \mathbf{T}_{SR}]^{-1}$
$\bar{\alpha}_a(0)$	Eq. (13): screened static polarizability calculated by partial contraction of $\bar{\mathbf{A}}(0)$
$\bar{\alpha}_a(i\omega)$	Eq. (12): screened frequency-dependent polarizability, calculated by partial contraction of $\bar{\mathbf{A}}(i\omega)$
$\omega_a^{\text{free}}$	free-atom QHO excitation frequency, computed as $\omega_a^{\text{free}} = 4/3 \left( C_{6,aa}^{\text{free}} / [\alpha_a^{\text{free}}(0)]^2 \right)$
$C_{6,aa}^{\text{free}}$	free-atom $C_6$ coefficient (also called Hamaker constant)
$C_{6,aa}$	bare effective atomic $C_6$ coefficient computed by weighting $C_{6,aa}^{\text{free}}$ with $(V_a/V_a^{\text{free}})^2$
$\bar{C}_{6,aa}$	Eq. (14): screened effective atomic $C_6$ coefficient
$\omega_a$	bare QHO excitation frequency, equals $\omega_a^{\text{free}}$ due to cancellation of $V_a/V_a^{\text{free}}$ factors
$\bar{\omega}_a$	Eq. (15): screened QHO excitation frequency
$y_p$	frequency grid for numerical integration
$g_p$	weights for numerical integration
$\sigma_a(i\omega)$	Eq. (24): QHO width, calculated from the bare polarizability scalar
$\Lambda_a(i\omega)$	Eq. (25): multiplicative prefactor to $V_a$ in defining $\alpha_a$
$V_a^{\text{free}}$	free-atom effective volume
$V_a$	Eq. (S.2): Hirshfeld effective atomic volume
$\Sigma_{ab}(i\omega)$	Eq. (23): effective correlation length of the interaction potential, defined from QHO widths of atoms $a$ and $b$
$\mathcal{R}_a$	nuclear position of atom $a$
$R_{ab}$	internuclear distance between atoms $a$ and $b$
$\mathbf{R}_{ab}$	internuclear vector ( $\mathcal{R}_a - \mathcal{R}_b$ ) between atoms $a$ and $b$
$R_{ab}^i$	$i^{\text{th}}$ Cartesian component of the internuclear vector
$\mathbf{r}$	spatial position such as the argument of the electron density
$\zeta$	ratio between interatomic separation $R$ and correlation length $\Sigma$
$h(\zeta)$	Eq. (58): function of $\zeta$ appearing in $\mathbf{T}$
$v(R, i\omega)$	Eq. (21): Coulomb interaction between two QHO Gaussian charge densities separated by $R$ with frequency-dependent interaction
$\mathbf{T}$	Eq. (57): dipole interaction tensor between QHO Gaussian charge densities
$\mathbf{T}_{\text{dip}}$	Eq. (27): dipole interaction tensor between point dipoles
$\mathbf{T}_{SR}$	Eq. (35): short-range component of $\mathbf{T}$ , evaluated using $f(Z^{\text{TS}})$
$\bar{\mathbf{T}}_{LR}$	Eq. (37): long-range component of $\mathbf{T}$ , evaluated using $f(\bar{Z}_{\text{vdW}})$
$f(Z)$	Eq. (28): damping function for range-separation of the dipole interaction tensor
$S_{ab}$	sum of effective vdW radii scaled by $\beta$
$Z_{ab}$	ratio of interatomic separation $R_{ab}$ and $S_{ab}$
$\mathcal{R}_a^{\text{vdW, TS}}$	Eq. (34): effective vdW radii at the TS level
$\bar{\mathcal{R}}_a^{\text{vdW}}$	Eq. (36): screened effective vdW radii
$\rho$	total electronic charge density
$\rho_a^{\text{eff}}$	Eq. (S.1): Hirshfeld effective electron density assigned to atom $a$
$\rho_{\text{sad}}$	sum of spherical free-atom densities $\sum_b \rho_b^{\text{free}}$
$\mathcal{H}^{\text{MBD}}$	Eq. (17): MBD model Hamiltonian
$\mathbf{C}^{\text{MBD}}$	Eq. (18): MBD interaction matrix
$\mathcal{X}$	matrix of eigenvectors of $\mathbf{C}^{\text{MBD}}$
$\boldsymbol{\lambda}$	vector of eigenvalues of $\mathbf{C}^{\text{MBD}}$
$\partial_c$	gradient with respect to nuclear position of atom $c$ , equivalent to $\nabla_{\mathcal{R}_c}$
$E_{\text{MBD}}$	MBD correlation energy
$\mathbf{F}_c^{\text{MBD}}$	MBD ionic forces: $-\nabla_{\mathcal{R}_c} E_{\text{MBD}}$

## 2 Length Scale of Damping



**Fig. S1 Left:** Contours at  $10^{-6}$  for damping functions  $\exp[-\zeta^2]$  (purple) and  $(1-f[Z])$  (orange), with  $\|\mathbf{R}\|$  relative to the atom marked in red. Damping parameters  $\Sigma \simeq 1.03$  and  $S \simeq 2.96$  (cf. Eqs. (23) and (30)) were computed for a graphene nanoflake with the PBE functional. **Right:** Comparison of the three damping functions with the same  $10^{-6}$  contour indicated. The rapid decay of  $\exp[-\zeta^2]$  relative to the Fermi damping function demonstrates that the short-range dipole-dipole interaction tensor  $\mathbf{T}_{SR}$  reduces to the frequency-independent  $\mathbf{T}_{dip}$  well before the long-range tensor  $\overline{\mathbf{T}}_{LR}$  has been fully “turned on” by the Fermi damping function (cf. Eqs. (26, 27, 35, 37)).

## 3 Computation of $\partial V$

Nuclear coordinate forces within a fully self-consistent  $\mathcal{O}(N)$  implementation of the Tkatchenko-Scheffler (TS) scheme<sup>3</sup> were previously developed in QUANTUM ESPRESSO (QE)<sup>4</sup> by R. A. DiStasio Jr.<sup>5</sup> A subroutine of the TSVDW module computes the Hirshfeld partitioning into effective atomic volumes,  $V_a$ , and the derivatives of that volume,  $\partial V_a$ . The Hirshfeld effective charge density of atom  $a$  is:

$$\rho_a^{\text{eff}}(\mathbf{r}) = w_a(\mathbf{r})\rho(\mathbf{r}) = \frac{\rho_a^{\text{free}}(\|\mathbf{r}-\mathcal{R}_a\|)}{\rho_{\text{sad}}(\mathbf{r})}\rho(\mathbf{r}), \quad (\text{S.1})$$

where  $\rho(\mathbf{r})$  is the total molecular charge density and  $\rho_{\text{sad}}(\mathbf{r}) = \sum_b \rho_b^{\text{free}}(\|\mathbf{r}-\mathcal{R}_b\|)$  is the sum of free-atom densities. The effective volume is then:

$$V_a = \int d\mathbf{r} \|\mathbf{r}-\mathcal{R}_a\|^3 \rho_a^{\text{eff}}(\mathbf{r}). \quad (\text{S.2})$$

Integrations on spherical atomic domains, such as in Eq. S.2, are computed on subsets of the real-space mesh. Using reference data for the free atom volumes, the radial grid cutoff value is determined for each species such that the free atom volume obtained by numerical integration up to this cutoff does not deviate from the reference value by more than 1.0%. The effective volume derivative is evaluated as

$$\partial_c V_a = \int d\mathbf{r} \|\mathbf{r}-\mathcal{R}_a\|^3 \partial_c \rho_a^{\text{eff}}(\mathbf{r}) - 3 \delta_{ca} \int d\mathbf{r} (\mathbf{r}-\mathcal{R}_a) \|\mathbf{r}-\mathcal{R}_a\| \rho_a^{\text{eff}}(\mathbf{r}) \quad (\text{S.3})$$

$$\partial_c \rho_a^{\text{eff}}(\mathbf{r}) = \left[ \frac{\rho_a^{\text{free}}(\|\mathbf{r}-\mathcal{R}_a\|)\rho(\mathbf{r})}{[\rho_{\text{sad}}(\mathbf{r})]^2} - \frac{\rho(\mathbf{r})}{\rho_{\text{sad}}(\mathbf{r})} \delta_{ca} \right] \left[ \frac{\mathbf{r}-\mathcal{R}_c}{\|\mathbf{r}-\mathcal{R}_c\|} \right] \frac{\partial \rho_c^{\text{free}}(r)}{\partial r} \quad (\text{S.4})$$

Note that the free-atom density is spherically symmetric, which is why we reduce  $\partial_c \rho_c^{\text{free}}(\|\mathbf{r}-\mathcal{R}_c\|)$  to a spherical coordinate derivative  $\partial \rho_c^{\text{free}}/\partial r$ . Likewise, Eq. (S.2) is evaluated by mapping the radial form of  $\rho_a^{\text{eff}}$  to an linear/equispaced grid, which is then interpolated using cubic splines. After interpolation, the derivative  $\partial_c \rho_a^{\text{eff}}$  at each grid point is evaluated by numerical differentiation using Bickley’s 7-point formula.<sup>6</sup>

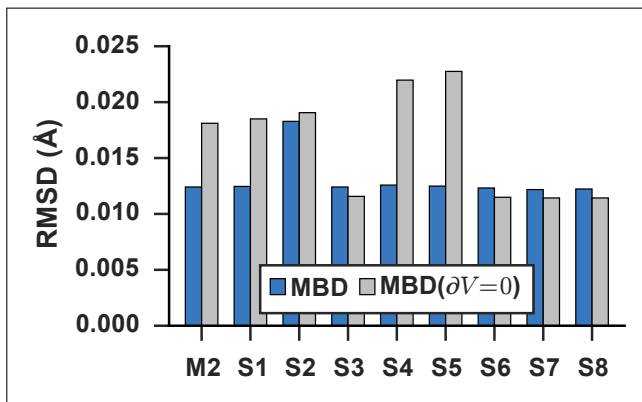
## 4 Repeated Eigenvalues of $C^{MBD}$

In considering the derivative of  $\lambda_p$ , in Eq. (41) we assumed that  $C^{MBD}$  had  $3N$  distinct eigenvalues. Due to numerical perturbations it is somewhat unlikely for  $C^{MBD}$  to have repeated eigenvalues, but we cannot assume this *a priori*. The procedure for taking derivatives of repeated eigenvalues of a real, symmetric matrix, like  $C^{MBD}$ , is essentially first order perturbation theory where the perturbation is the action of the derivative operator  $\partial_c$ . Eigenvalue degeneracies are lifted by diagonalizing the perturbation in the degenerate subspace. See Friswell<sup>7</sup> or Andrew *et al.*<sup>8</sup> for a more algorithmic discussion of repeated eigenvalue derivatives. Since  $C^{MBD}$  is real and symmetric, it is guaranteed to be diagonalizable with orthogonal eigenvectors.

## 5 Importance of $\partial V$

### 5.1 Benzene dimer

To analyze the importance of  $\partial V$ , we re-optimized the benzene dimer structures with  $\partial V$  terms set explicitly to zero. As shown in Fig. S2, setting  $\partial V = 0$  slightly degrades the consistency of the PBE+MBD optimized geometries, but the final RMSDs are still quite good (all  $< 0.025$  Å). The optimization of M1 with  $\partial V = 0$  proved numerically unstable, and was unable to converge, so M1 is not included in the figure. The fact that the Hirshfeld gradients have a negligible impact on the benzene dimer optimizations is expected since the Hirshfeld effective atomic volumes only change when nearest neighbor atoms are moved. In addition to being quite rigid, the benzene monomer is small enough that the range-separated MBD correction is largely turned off within the length scale of the monomer, which is where the Hirshfeld gradients could matter.



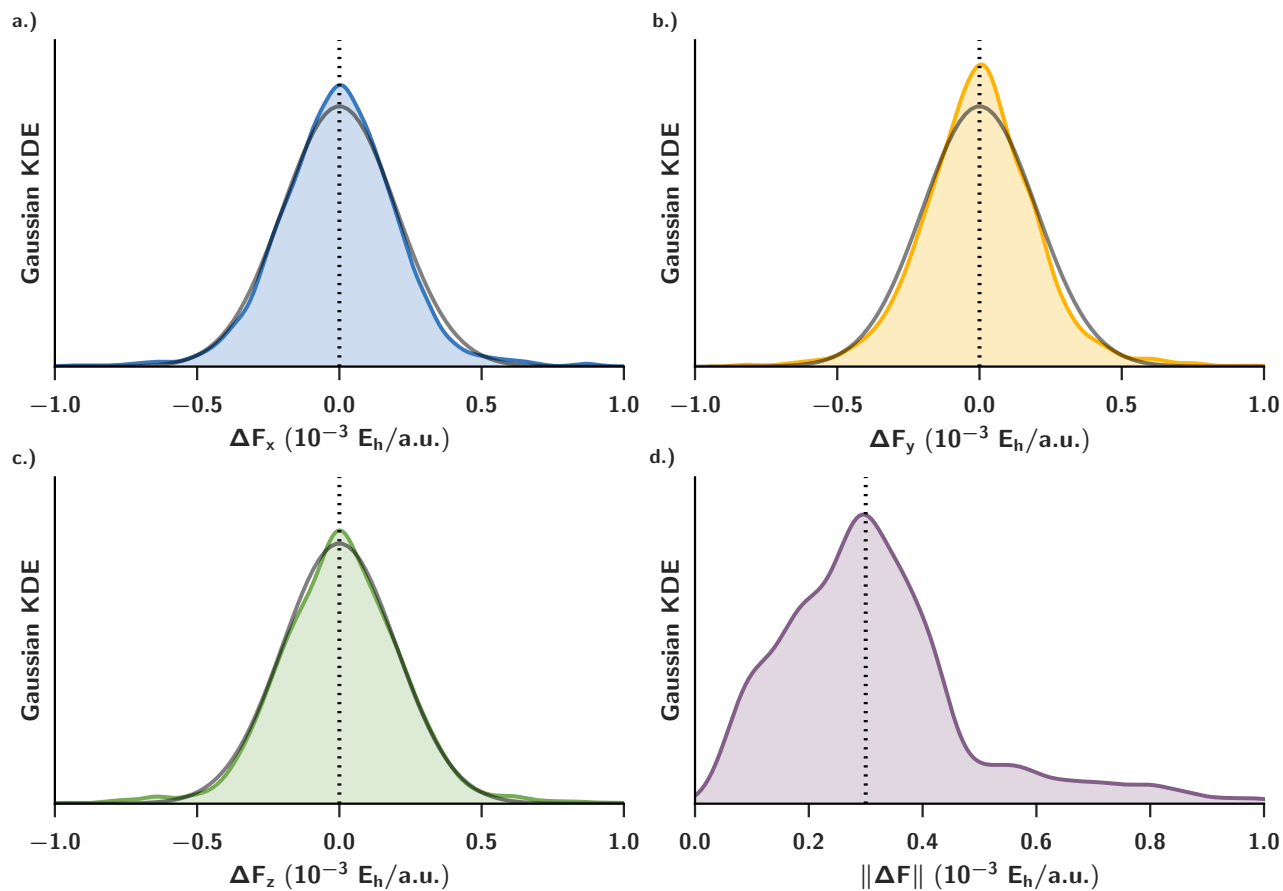
**Fig. S2** Root-mean-square-deviations (RMSD) in Å between the PBE+MBD and PBE/CCSD(T)<sup>1</sup> optimized geometries of 9 benzene dimer configurations using the full MBD gradient (shown in blue), and the approximation where  $\partial V$  contributions are set explicitly to zero (shown in grey).

### 5.2 Polypeptides

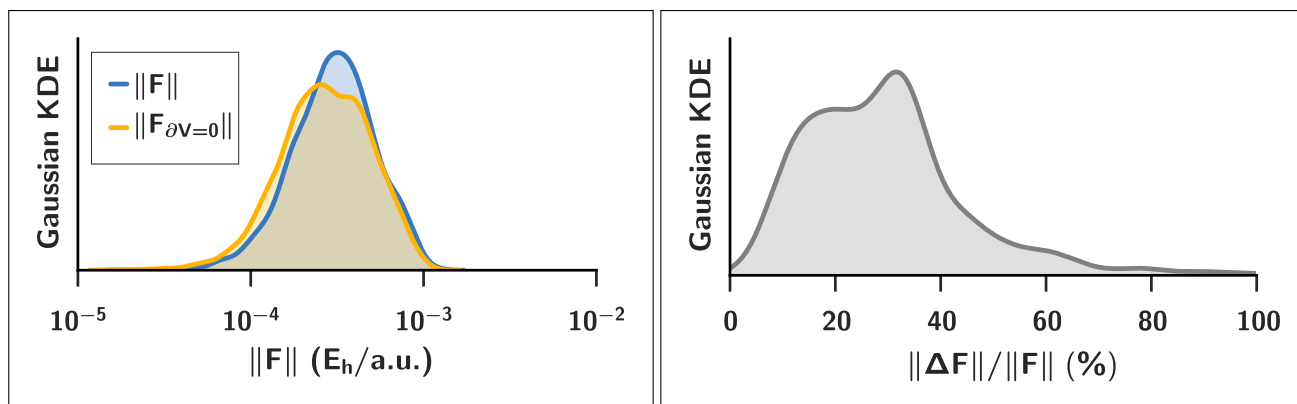
We also performed single-point calculations on the optimized geometries of all 76 polypeptide structures to compare the MBD forces computed with and without the  $\partial V$  contributions. The peptide structures are much more flexible than the benzene monomer and also have the opportunity for cooperative addition of the Hirshfeld volume gradients along the chain, *i.e.* the local Hirshfeld volume gradients acting at the nearest neighbor level can propagate along the peptide chain and result in a larger change. In Fig. S3 we visualize the deviation between the forces computed with full Hirshfeld volume gradients and those computed with  $\partial V = 0$  in several ways: difference of individual force components  $\Delta F_i = F_i - F_{i,\partial V=0}$ , norm of the difference of forces  $\|F - F_{\partial V=0}\|$ , relative percentage error  $\|\Delta F\|/\|F\|$ , and distributions of the norms of forces  $\|F\|$  vs.  $\|F_{\partial V=0}\|$ .

## 6 Structure of the $C_{60}@C_{60}H_{28}$ Buckyball Catcher Host-Guest Complex

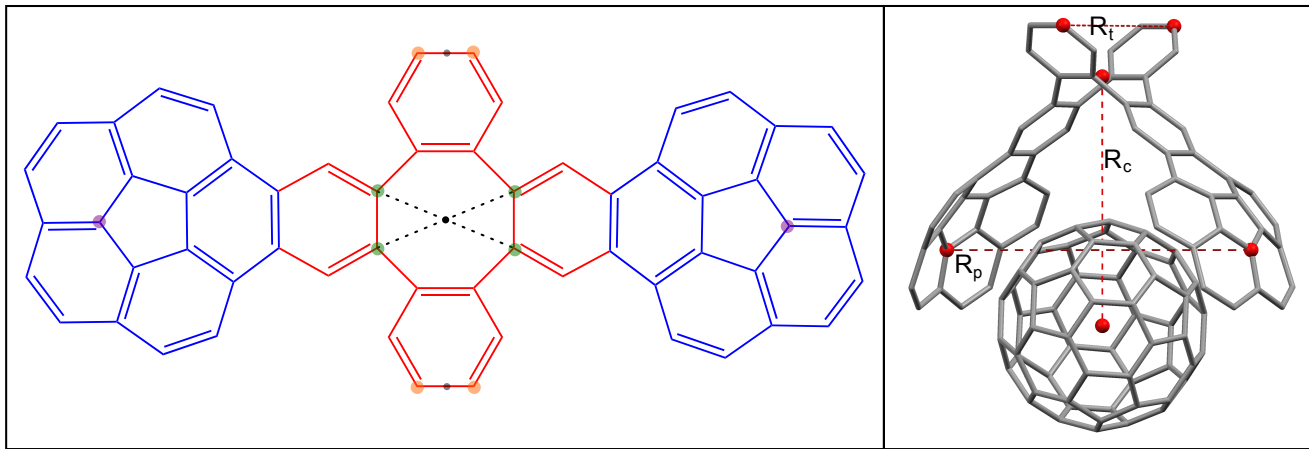
In Fig. S5 the 2D molecular structure of the buckyball catcher host and the 3D structure of the  $C_{60}@C_{60}H_{28}$  host-guest complex with the three distances  $R_c$ ,  $R_p$ , and  $R_t$  are highlighted. For each DFT-vdW optimized structure of the host, we report the  $R_p$  and  $R_t$  distances. All geometry optimizations of the  $C_{60}@C_{60}H_{28}$  buckyball catcher host-guest complex started from the TPSS+D3/def2-TZVP structures in the S12L set.<sup>9</sup> We optimized the complex, guest  $C_{60}$ , and conformers **a** and **b** of the host. Structures of the complex, guest  $C_{60}$ , and host optimized with other functionals and vdW correction schemes can be found in the supplemental information of the following references: Ref. 9: TPSS+D3/def2-TZVP, Ref. 10: B97-D/TZVP, Ref. 11: M06-2L/MIDI!.



**Fig. S3** Gaussian kernel density estimates of the distributions of MBD forces acting on each atom at the optimized geometries of 76 polypeptide structures. a.)-c.) Difference of the force components  $\Delta F_i = \mathbf{F}_i - \mathbf{F}_{i,\partial V=0}$ , with a normal distribution  $\mathcal{N}(0,0.2)$  and dotted line indicating zero mean superposed for reference. d.) Norm of the difference of forces,  $\|\Delta \mathbf{F}\| = \|\mathbf{F} - \mathbf{F}_{\partial V=0}\|$ , with the dotted line indicating that the peak occurs at  $\sim 0.3 \times 10^{-3} E_h/a.u.$



**Fig. S4** Left: Gaussian kernel density estimate of the distributions of the norm  $\|\cdot\|$  of TS forces  $\mathbf{F}_{TS}$  acting on each atom at the optimized geometries of 76 polypeptide structures. In blue, the TS forces were computed with full Hirshfeld gradients ( $\|\mathbf{F}\|$ ); in yellow, the forces were computed with the Hirshfeld gradients  $\partial V$  set to zero ( $\|\mathbf{F}_{\partial V=0}\|$ ). Right: Gaussian kernel density estimate of the distribution of relative percentage error  $\|\Delta \mathbf{F}\|/\|\mathbf{F}\|$  where  $\Delta \mathbf{F} \equiv \mathbf{F} - \mathbf{F}_{\partial V=0}$  is the error incurred by setting the Hirshfeld gradients to zero. The distribution is peaked at approximately 32% but extends to values near 100%.



**Fig. S5 Left:** 2D structure of the 'buckyball catcher'  $C_{60}H_{28}$ . The central tetrabenzocyclooctatetraene (TBCOT) tether (red) links the two corannulene bowls (blue). The orange circles mark the four atoms used to define the  $R_t$  distance between the back ends of the TBCOT tether. The green circles mark the four atoms used to define the plane from which the distance to the  $C_{60}$  centroid,  $R_c$ , is measured. The purple circles mark the two atoms used to define the  $R_p$  distance (C10e and C10e' in the notation of Ref. 2), which are the most separated atoms of the central five-membered rings of both corannulene subunits. **Right:** 3D structure of the  $C_{60}@C_{60}H_{28}$  complex with the three distances  $R_c$ ,  $R_p$ , and  $R_t$  highlighted.

## 7 Self-Consistent Screening

Self-consistent screening (SCS) is accomplished by solving the following non-homogeneous system of linear equations at a given complex frequency  $i\omega$  (Eq. (17) in DiStasio et al.<sup>12</sup>):

$$\bar{\alpha}_a(i\omega) = \alpha_a(i\omega) - \alpha_a(i\omega) \sum_{b \neq a}^N \mathbf{T}_{ab} \bar{\alpha}_a(i\omega). \quad (\text{S.5})$$

To accomplish a range-separated self-consistent screening (rsSCS), we replace  $\mathbf{T}$  with  $\mathbf{T}_{\text{SR}}$  (see Ref. 13). Eq. (S.5) can then be written as a matrix equation as:

$$\bar{\mathbf{A}} = \mathbf{A} - \mathbf{A} \mathbf{T}_{\text{SR}} \bar{\mathbf{A}} \quad (\text{S.6})$$

Note that  $\zeta_{pp} = 0$  so  $\mathbf{T}_{pp} = 0$  naturally (see Eq. (26)). Thus, the sum  $\sum_{b \neq a} \mathbf{T}_{ab} \bar{\alpha}_a$  is accomplished by the product  $\mathbf{T}_{\text{SR}} \bar{\mathbf{A}}$ . Rearranging Eq. (S.6) and then left multiplying by  $\mathbf{A}^{-1}$  gives:

$$\bar{\mathbf{A}} + \mathbf{A} \mathbf{T}_{\text{SR}} \bar{\mathbf{A}} = \mathbf{A} \quad (\text{S.7})$$

$$\mathbf{A}^{-1} [\mathcal{J} + \mathbf{A} \mathbf{T}_{\text{SR}}] \bar{\mathbf{A}} = \mathbf{A}^{-1} \mathbf{A} \quad (\text{S.8})$$

$$[\mathbf{A}^{-1} + \mathbf{T}_{\text{SR}}] \bar{\mathbf{A}} = \mathcal{J} \quad (\text{S.9})$$

Left multiplying by the inverse of the bracketed quantity yields:

$$\bar{\mathbf{A}} = [\mathbf{A}^{-1} + \mathbf{T}_{\text{SR}}]^{-1} \quad (\text{S.10})$$

## 8 Derivation of $\partial\mathbf{T}^{ij}$

To break the derivative of  $\mathbf{T}^{ij}$  into smaller pieces, we define some convenience functions:

$$U \equiv \text{erf}[\zeta] - \frac{2}{\sqrt{\pi}} \zeta \exp[-\zeta^2] \quad (\text{S.11})$$

$$\mathbf{W}^{ij} \equiv \left( \frac{R^i R^j}{R^5} \right) \frac{4}{\sqrt{\pi}} \zeta^3 \exp[-\zeta^2] \quad (\text{S.12})$$

$$\mathbf{T}_{\text{dip}}^{ij} \equiv -3 \left( \frac{R^i R^j}{R^5} \right) + \frac{\delta_{ij}}{R^3} \quad (\text{S.13})$$



So in terms of these functions,  $\mathbf{T}^{ij}$  is:

$$\mathbf{T}^{ij} = U\mathbf{T}_{\text{dip}}^{ij} + \mathbf{W}^{ij} \quad (\text{S.14})$$

$$\Rightarrow \partial\mathbf{T}^{ij} = U\partial\mathbf{T}_{\text{dip}}^{ij} + \mathbf{T}_{\text{dip}}\partial U + \partial\mathbf{W}^{ij} \quad (\text{S.15})$$

The derivative of  $\mathbf{T}_{\text{dip}}^{ij}$  is given in Eq. (53). Note that we can write  $\partial(R^i R^j / R^5)$  in terms of  $\partial\mathbf{T}_{\text{dip}}^{ij}$  as:

$$\partial\left(\frac{R^i R^j}{R^5}\right) = -\frac{1}{3}\partial\mathbf{T}_{\text{dip}}^{ij} - \frac{\delta_{ij}}{R^4}\partial R \quad (\text{S.16})$$

So the derivatives of  $U$  and  $\mathbf{W}^{ij}$  are:

$$\partial U = \frac{4}{\sqrt{\pi}}\zeta^2 \exp[-\zeta^2] \partial\zeta \quad (\text{S.17})$$

$$\partial\mathbf{W}^{ij} = \left(\frac{R^i R^j}{R^5}\right) [3 - 2\zeta^2] \frac{4}{\sqrt{\pi}}\zeta^2 \exp[-\zeta^2] \partial\zeta + \frac{4}{\sqrt{\pi}}\zeta^3 \exp[-\zeta^2] \left(-\frac{1}{3}\partial\mathbf{T}_{\text{dip}}^{ij} - \frac{\delta_{ij}}{R^4}\partial R\right) \quad (\text{S.18})$$

Now define  $h(\zeta) \equiv \frac{4}{\sqrt{\pi}}\zeta^2 \exp[-\zeta^2]$ .

$$\Rightarrow \partial U = h(\zeta)\partial\zeta \quad (\text{S.19})$$

$$\Rightarrow \partial\mathbf{W}^{ij} = \left(\frac{R^i R^j}{R^5}\right) [3 - 2\zeta^2] h(\zeta)\partial\zeta + \zeta h(\zeta) \left(-\frac{1}{3}\partial\mathbf{T}_{\text{dip}}^{ij} - \frac{\delta_{ij}}{R^4}\partial R\right) \quad (\text{S.20})$$

In terms of  $h(\zeta)$  we can then write  $\partial\mathbf{T}^{ij}$  as:

$$\partial\mathbf{T}^{ij} = \left[\text{erf}[\zeta] - \frac{1}{2}\frac{h(\zeta)}{\zeta}\right] \partial\mathbf{T}_{\text{dip}}^{ij} + \zeta h(\zeta) \left(-\frac{1}{3}\partial\mathbf{T}_{\text{dip}}^{ij} - \frac{\delta_{ij}}{R^4}\partial R\right) + \left[\mathbf{T}_{\text{dip}} + \left(\frac{R^i R^j}{R^5}\right) [3 - 2\zeta^2]\right] h(\zeta)\partial\zeta \quad (\text{S.21})$$

Where the derivative of  $\zeta_{ab}$  is in Eq. (59).

## 9 Scaling of Gauss-Legendre Quadrature

To transform Gauss-Legendre quadrature from the interval  $x_p \in [-1, 1]$ , to the semi-infinite interval  $y_p \in [0, \infty)$ , we map the abscissa  $x_p$  and weights  $w_p$  with an algebraic scaling:

$$y_p \in [0, \infty) \quad y_p = L\frac{(1+x_p)}{(1-x_p)} \quad x_p \in [-1, 1] \quad (\text{S.22})$$

$$g_p = -\frac{2L}{(1-x_p)^2} w_p \quad (\text{S.23})$$

There are many different possible transformations to  $[0, \infty)$ , but the algebraic mapping is quite robust for quadrature of functions  $f(x)$  that decay algebraically in  $|x|$  as  $x \rightarrow \infty$ .<sup>14</sup> Since the isolated atom dynamic polarizability is expected to decay as  $\alpha(i\omega) \propto 1/\omega^2$ ,<sup>15</sup> we found the algebraic scaling to be preferable, although other choices such as  $y_p = L \tan\left(\frac{\pi}{2}\frac{(x_p+1)}{2}\right)$  also perform well. Since the number of Gauss-Legendre quadrature points,  $n$ , determines the number of self-consistent screening computations that must be performed to determine  $\bar{\omega}_a$ , the computational cost (and numerical error) of evaluating the MBD correlation energy can be varied by adjusting the number of quadrature points. The quadrature error is also sensitive to the scale factor  $L$ .

Based on the available atomic dynamic polarizability reference data in Derevianko et al.<sup>15</sup> and the free atom reference quantities used in the TS method,<sup>3</sup> our quadrature method should be able to integrate a response function for excitation frequencies in the range of  $\omega_i \sim 0.06$  (K) to  $\omega_i \sim 1.2$  (Ne). In optimizing the number of Gauss-Legendre points,  $n$ , and the scale factor,  $L$ , we used the Casimir-Polder integral for a single excitation frequency dipole oscillator as a trial function with  $\omega_a$  varying in the range  $[10^{-2}, 10^2]$ .

$$C_6(\omega_a) = \frac{3}{\pi} \int_0^\infty \left[ \frac{f}{[\omega_a^2 - (i\omega)^2]} \right]^2 d(i\omega) = \frac{3}{4} \frac{f^2}{\omega_a^3} \quad (\text{S.24})$$

Using this trial function, we choose  $n = 20$  quadrature points and a scale factor  $L = \frac{6}{10}$ , which gives integration with a relative error less than  $10^{-6}$  for all excitation frequencies in the range  $[0.07, 5]$  and also performed well in self-consistent screening computations across a range of isolated atomic systems.

**Table S1** Convergence tolerances and unit cell sizes used in PWSCF geometry optimizations, reported in Rydberg atomic units ( $1 \text{ Ry} = \frac{1}{2} E_h$ )

	Benzene Dimer	Peptides	C <sub>60</sub> Catcher
E <sub>scf</sub> (Ry)	10 <sup>-8</sup>	10 <sup>-8</sup>	10 <sup>-8</sup>
E <sub>cut</sub> (Ry)	400	145	110
E <sub>tot</sub> (Ry)	10 <sup>-8</sup>	5 × 10 <sup>-7</sup>	5 × 10 <sup>-7</sup>
F <sub>tot</sub> (Ry/a <sub>0</sub> )	10 <sup>-4</sup>	5 × 10 <sup>-4</sup>	5 × 10 <sup>-4</sup> ,
Cell Size (a <sub>0</sub> )	30	30	50
Grid Spacing (Å)	0.04	0.07	0.12

**Table S2** Convergence tolerances used in ORCA geometry optimizations, reported in Hartree atomic units

	Benzene Dimer	Peptides	C <sub>60</sub> Catcher
E <sub>scf</sub> (E <sub>h</sub> )	10 <sup>-8</sup>	10 <sup>-8</sup>	10 <sup>-8</sup>
E <sub>tot</sub> (E <sub>h</sub> )	10 <sup>-6</sup>	5 × 10 <sup>-6</sup>	10 <sup>-6</sup>
F <sub>Max</sub> (E <sub>h</sub> /a <sub>0</sub> )	10 <sup>-4</sup>	3 × 10 <sup>-4</sup>	10 <sup>-4</sup>
F <sub>RMS</sub> (E <sub>h</sub> /a <sub>0</sub> )	3 × 10 <sup>-5</sup>	10 <sup>-4</sup>	3 × 10 <sup>-5</sup>
Max Disp. (a <sub>0</sub> )	10 <sup>-3</sup>	4 × 10 <sup>-3</sup>	10 <sup>-3</sup>
RMS Disp. (a <sub>0</sub> )	6 × 10 <sup>-4</sup>	2 × 10 <sup>-3</sup>	6 × 10 <sup>-4</sup>

## 10 Additional Computational Details

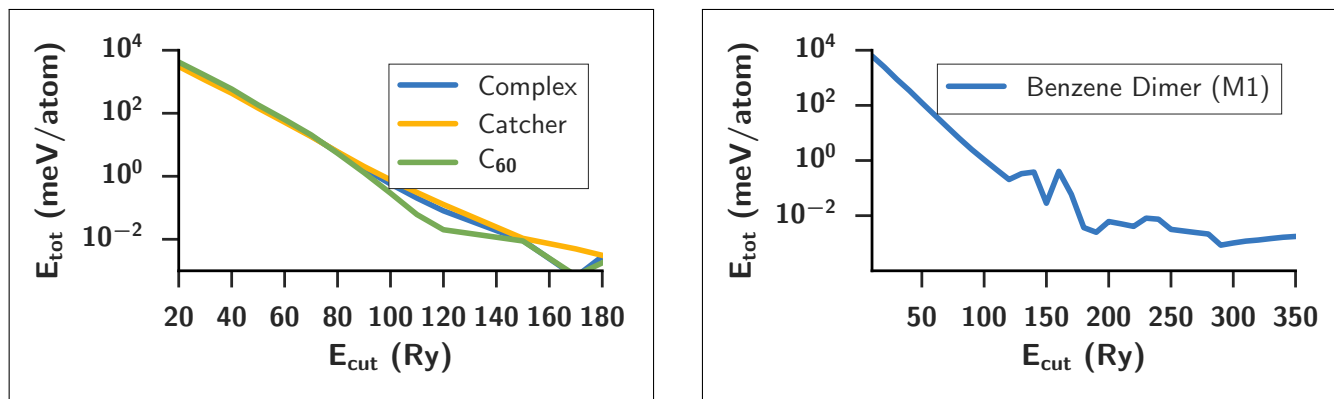
All geometry optimizations were performed using the quasi-Newton Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm,<sup>16–19</sup> with default parameters.

### 10.1 QUANTUM ESPRESSO

Cartesian coordinate geometry optimizations in QUANTUM ESPRESSO (QE)<sup>4</sup> were performed in the PWSCF module in large simple cubic unit cells. Table S1 gives details of the convergence tolerances, kinetic energy wavefunction cutoffs, and unit cell sizes used for each system. Since QE uses Rydberg energy units ( $1 \text{ Ry} = \frac{1}{2} E_h$ ), we report the tolerances in these units. The PBE functional<sup>20,21</sup> was used with Hamann-Schlüter-Chiang-Vanderbilt (HSCV) norm-conserving pseudopotentials<sup>22–24</sup> obtained from the FPMD pseudopotential repository<sup>25</sup> (and converted to UPF format using a modified version of QSO2UPF v1.2<sup>26</sup>). All QE calculations were run at the  $\Gamma$  point using a charge density cutoff of  $\rho_{\text{cut}} = 4E_{\text{cut}}$ . PBE+MBD jobs used 20 quadrature points for the Casimir-Polder integration. To ensure a fair comparison with our implementation of the MBD model, all TS calculations<sup>3</sup> were performed as *a posteriori* corrections to the solution of the non-linear Kohn-Sham equations, *i.e.* we turned off the self-consistent density updates from TS. In Fig. S6 we present the results of convergence testing with respect to the kinetic energy cutoff in the planewave basis set expansion, showing that the total energy per atom was converged to better than 0.3 meV/atom for each system.

### 10.2 Orca

Redundant internal coordinate geometry optimizations in ORCA v3.03<sup>27</sup> were performed with the PBE functional<sup>20,21</sup> with the atom-pairwise version of the D3 dispersion correction of Grimme *et al.*,<sup>28</sup> using Becke-Johnson (BJ) damping.<sup>29</sup> ORCA v3.03 implements D3 in the DFTD3 v2.1R6 software, which does not contain analytical gradients of the three-body term. The geometric counterpoise correction (gCP) of Kruse *et al.* was employed in all ORCA calculations.<sup>30</sup> We employed the Ahlrichs def2-TZVP basis set<sup>31</sup> coupled with an auxiliary Ahlrichs TZVP basis set<sup>32,33</sup> for the RI-J approximation.<sup>34–36</sup> All calculations used the G4 final integration grid. All calculations used “tight” SCF tolerances; calculations on the benzene dimer and C<sub>60</sub> catcher used “tight” optimization tolerances, while those of the peptides used default optimization tolerances. Table S2 lists the tolerances corresponding to these two settings.



**Fig. S6** Convergence of the total energy per atom with respect to kinetic energy wavefunction cutoff ( $E_{\text{cut}}$ ) of the planewave basis expansion for **Left:** simulations of the C<sub>60</sub> catcher complex, **Right:** the benzene dimer (M1 configuration).

## 11 Cartesian Coordinates of Structures

We present below the Cartesian coordinates (in Å) of all structures considered in the text.

### 11.1 Stationary points of the benzene dimer potential energy surface

We consider ten configurations of the benzene dimer, which correspond to stationary points of the SAPT(DFT)\* potential energy surface in Ref. 1. Using a fixed monomer geometry from the SDQ-MBPT(4)/cc-pVTZ results of Gauss and Stanton,<sup>37</sup> Bludský *et al.*<sup>38</sup> optimized these 10 configurations of the benzene dimer at the PBE/CCSD(T) level of theory, with an aug-cc-pVDZ basis set and counterpoise correction.

#### 11.1.1 Benzene monomer: [Gauss and Stanton *J. Phys. Chem. A.* 104, 13, 2865 (2000)]

Precisely measured ground-state rotational constants of benzene have been corrected for effects of vibration-rotation interaction using a calculated vibrational force field from SDQ-MBPT(4)/cc-pVTZ. Yielding:

$$r_{CC} = 1.3915 \pm 0.0010 \text{ \AA} \text{ and } r_{CH} = 1.0800 \pm 0.0020 \text{ \AA}.$$

```

C  1.39150  0.000000  0.000000
C  0.69575  1.205074  0.000000
C -0.69575  1.205074  0.000000
C -1.39150  0.000000  0.000000
C -0.69575 -1.205074  0.000000
C  0.69575 -1.205074  0.000000
H  2.47150  0.000000  0.000000
H  1.23575  2.140382  0.000000
H -1.23575  2.140382  0.000000
H -2.47150  0.000000  0.000000
H -1.23575 -2.140382  0.000000
H  1.23575 -2.140382  0.000000

```

#### 11.1.2 Benzene monomer: PBE

$$r_{CC} = 1.3976 \text{ \AA} \text{ and } r_{CH} = 1.0908 \text{ \AA}$$

```

C  1.397559326  0.000000000  0.000000000
C  0.698990412  1.210996311  0.000000000
C -0.698990412  1.210996311  0.000000000
C -1.397559326  0.000000000  0.000000000
C -0.698990412 -1.210996311  0.000000000
C  0.698990412 -1.210996311  0.000000000

```

\*Podeszwa *et al.* used the PBE0 functional with Fermi-Amaldi asymptotic correction and with the Tozer-Handy splicing scheme, and an aug-cc-pVTZ Dunning basis with a monomer-centered "plus" basis set scheme. Their symmetry-adapted perturbation theory procedure used density fitting. They also used the vibrationally averaged monomer geometry ( $r_{CC} = 1.3965 \text{ \AA}$  and  $r_{CH} = 1.085 \text{ \AA}$ ) from Tamagawa *et al. J. Mol. Struct.* 1976, **30**, 243.

```

H  2.488329409  0.000000000  0.000000000
H  1.244394934  2.155337592  0.000000000
H -1.244394934  2.155337592  0.000000000
H -2.488329409  0.000000000  0.000000000
H -1.244394934 -2.155337592  0.000000000
H  1.244394934 -2.155337592  0.000000000

```

**11.1.3 Benzene monomer: PBE+MBD@rsSCS**

$r_{CC} = 1.3966 \text{ \AA}$  and  $r_{CH} = 1.0905 \text{ \AA}$

```

C  1.396631096  0.000000000  0.000000000
C  0.698430765  1.210204560  0.000000000
C -0.698430765  1.210204560  0.000000000
C -1.396631096  0.000000000  0.000000000
C -0.698430765 -1.210204560  0.000000000
C  0.698430765 -1.210204560  0.000000000
H  2.487089208  0.000000000  0.000000000
H  1.243806698  2.154332980  0.000000000
H -1.243806698  2.154332980  0.000000000
H -2.487089208  0.000000000  0.000000000
H -1.243806698 -2.154332980  0.000000000
H  1.243806698 -2.154332980  0.000000000

```

**11.1.4 Benzene monomer: PBE+TS**

$r_{CC} = 1.3973 \text{ \AA}$  and  $r_{CH} = 1.0905 \text{ \AA}$

```

C  1.397268653  0.000000000  0.000000000
C  0.698819532  1.210888317  0.000000000
C -0.698819532  1.210888317  0.000000000
C -1.397268653  0.000000000  0.000000000
C -0.698819532 -1.210888317  0.000000000
C  0.698819532 -1.210888317  0.000000000
H  2.487735553  0.000000000  0.000000000
H  1.244290651  2.155045024  0.000000000
H -1.244290651  2.155045024  0.000000000
H -2.487735553  0.000000000  0.000000000
H -1.244290651 -2.155045024  0.000000000
H  1.244290651 -2.155045024  0.000000000

```

**11.1.5 Benzene monomer: PBE+D3**

$r_{CC} = 1.3975 \text{ \AA}$  and  $r_{CH} = 1.0923 \text{ \AA}$

```

C  1.397392892 -0.000000003 -0.000000001
C  0.698748952  1.210307350 -0.000000001
C -0.698748960  1.210307354  0.000000000
C -1.397392892  0.000000002  0.000000000
C -0.698748955 -1.210307350  0.000000000
C  0.698748958 -1.210307358 -0.000000001
H  2.489952054  0.000000002  0.000000003
H  1.244992126  2.156116450 -0.000000001
H -1.244992132  2.156116462  0.000000000
H -2.489952045  0.000000003  0.000000001
H -1.244992130 -2.156116456 -0.000000000
H  1.244992134 -2.156116457 -0.000000001

```

**11.1.6 Benzene dimer: PBE/CCSD(T)**

———— M1: PBE/CCSD(T) ————

C	1.205074	-0.695750	0.000000
C	0.000000	-1.391500	0.000000
C	-1.205074	-0.695750	0.000000
C	-1.205074	0.695750	0.000000
C	0.000000	1.391500	0.000000
C	1.205074	0.695750	0.000000
H	2.140382	-1.235750	0.000000
H	0.000000	-2.471500	0.000000
H	-2.140382	-1.235750	0.000000
H	-2.140382	1.235750	0.000000
H	0.000000	2.471500	0.000000
H	2.140382	1.235750	0.000000
C	-1.205074	-2.406104	3.488382
C	0.000000	-3.101854	3.488382
C	1.205074	-2.406104	3.488382
C	1.205074	-1.014604	3.488382
C	0.000000	-0.318854	3.488382
C	-1.205074	-1.014604	3.488382
H	-2.140382	-2.946104	3.488382
H	0.000000	-4.181854	3.488382
H	2.140382	-2.946104	3.488382
H	2.140382	-0.474604	3.488382
H	0.000000	0.761146	3.488382
H	-2.140382	-0.474604	3.488382

## ————— M2: PBE/CCSD(T) —————

C	1.205074	-0.695750	0.000000
C	0.000000	-1.391500	0.000000
C	-1.205074	-0.695750	0.000000
C	-1.205074	0.695750	0.000000
C	0.000000	1.391500	0.000000
C	1.205074	0.695750	0.000000
H	2.140382	-1.235750	0.000000
H	0.000000	-2.471500	0.000000
H	-2.140382	-1.235750	0.000000
H	-2.140382	1.235750	0.000000
H	0.000000	2.471500	0.000000
H	2.140382	1.235750	0.000000
C	-0.298590	0.000000	3.573827
C	0.530663	0.000000	4.691240
C	-0.022418	0.000000	5.968101
C	-1.404753	0.000000	6.127548
C	-2.234006	0.000000	5.010135
C	-1.680924	0.000000	3.733275
H	0.130679	0.000000	2.582803
H	1.603550	0.000000	4.567486
H	0.621199	0.000000	6.835371
H	-1.834022	0.000000	7.118572
H	-3.306892	0.000000	5.133889
H	-2.324541	0.000000	2.866005

## ————— S1: PBE/CCSD(T) —————

C	0.000000	-1.391500	0.000000
C	-1.205074	-0.695750	0.000000
C	-1.205074	0.695750	0.000000
C	0.000000	1.391500	0.000000

C	1.205074	0.695750	0.000000
C	1.205074	-0.695750	0.000000
H	0.000000	-2.471500	0.000000
H	-2.140382	-1.235750	0.000000
H	-2.140382	1.235750	0.000000
H	0.000000	2.471500	0.000000
H	2.140382	1.235750	0.000000
H	2.140382	-1.235750	0.000000
C	0.000000	0.280719	3.584731
C	0.000000	-0.558834	4.694426
C	0.000000	-0.017586	5.976348
C	0.000000	1.363214	6.148575
C	0.000000	2.202767	5.038880
C	0.000000	1.661520	3.756958
H	0.000000	-0.139365	2.589780
H	0.000000	-1.630530	4.560754
H	0.000000	-0.669198	6.837628
H	0.000000	1.783299	7.143527
H	0.000000	3.274463	5.172552
H	0.000000	2.313131	2.895678

## ——— S2: PBE/CCSD(T) ———

C	0.695750	-1.205074	0.000000
C	-0.695750	-1.205074	0.000000
C	1.391500	0.000000	0.000000
C	-1.391500	0.000000	0.000000
C	-0.695750	1.205074	0.000000
C	0.695750	1.205074	0.000000
H	1.235750	-2.140382	0.000000
H	-1.235750	-2.140382	0.000000
H	2.471500	0.000000	0.000000
H	-2.471500	0.000000	0.000000
H	-1.235750	2.140382	0.000000
H	1.235750	2.140382	0.000000
C	-1.205074	-2.411341	3.491220
C	0.000000	-3.107091	3.491337
C	1.205074	-2.411341	3.491220
C	1.205074	-1.019841	3.490985
C	0.000000	-0.324091	3.490868
C	-1.205074	-1.019841	3.490985
H	-2.140382	-2.951341	3.491311
H	0.000000	-4.187091	3.491519
H	2.140382	-2.951341	3.491311
H	2.140382	-0.479841	3.490894
H	0.000000	0.755909	3.490686
H	-2.140382	-0.479841	3.490894

## ——— S3: PBE/CCSD(T) ———

C	0.000000	-1.391500	0.000000
C	0.000000	1.391500	0.000000
C	-1.205074	-0.695750	0.000000
C	1.205074	-0.695750	0.000000
C	1.205074	0.695750	0.000000
C	-1.205074	0.695750	0.000000
H	0.000000	-2.471500	0.000000
H	0.000000	2.471500	0.000000

H	-2.140382	-1.235750	0.000000
H	2.140382	-1.235750	0.000000
H	2.140382	1.235750	0.000000
H	-2.140382	1.235750	0.000000
C	0.000000	0.000000	3.617700
C	1.205074	0.000000	4.313450
C	1.205074	0.000000	5.704950
C	0.000000	0.000000	6.400700
C	-1.205074	0.000000	5.704950
C	-1.205074	0.000000	4.313450
H	0.000000	0.000000	2.537700
H	2.140382	0.000000	3.773450
H	2.140382	0.000000	6.244950
H	0.000000	0.000000	7.480700
H	-2.140382	0.000000	6.244950
H	-2.140382	0.000000	3.773450

## ———— S4: PBE/CCSD(T) ————

C	0.695750	-1.205074	0.000000
C	-0.695750	-1.205074	0.000000
C	1.391500	0.000000	0.000000
C	-1.391500	0.000000	0.000000
C	-0.695750	1.205074	0.000000
C	0.695750	1.205074	0.000000
H	1.235750	-2.140382	0.000000
H	-1.235750	-2.140382	0.000000
H	2.471500	0.000000	0.000000
H	-2.471500	0.000000	0.000000
H	-1.235750	2.140382	0.000000
H	1.235750	2.140382	0.000000
C	-1.205074	-1.608886	5.131580
C	0.000000	-2.020261	5.692685
C	1.205074	-1.608886	5.131580
C	1.205074	-0.786135	4.009371
C	0.000000	-0.374760	3.448266
C	-1.205074	-0.786135	4.009371
H	-2.140382	-1.928171	5.567077
H	0.000000	-2.658831	6.563678
H	2.140382	-1.928171	5.567077
H	2.140382	-0.466850	3.573875
H	0.000000	0.263811	2.577274
H	-2.140382	-0.466850	3.573875

## ———— S5: PBE/CCSD(T) ————

C	0.000000	-1.391500	0.000000
C	0.000000	-0.695750	-1.205074
C	0.000000	0.695750	-1.205074
C	0.000000	1.391500	0.000000
C	0.000000	0.695750	1.205074
C	0.000000	-0.695750	1.205074
H	0.000000	-2.471500	0.000000
H	0.000000	-1.235750	-2.140382
H	0.000000	1.235750	-2.140382
H	0.000000	2.471500	0.000000
H	0.000000	1.235750	2.140382
H	0.000000	-1.235750	2.140382

C	6.204300	0.000000	-0.695750
C	6.204300	0.000000	0.695750
C	4.999226	0.000000	1.391500
C	3.794152	0.000000	0.695750
C	3.794152	0.000000	-0.695750
C	4.999226	0.000000	-1.391500
H	7.139608	0.000000	-1.235750
H	7.139608	0.000000	1.235750
H	4.999226	0.000000	2.471500
H	2.858844	0.000000	1.235750
H	2.858844	0.000000	-1.235750
H	4.999226	0.000000	-2.471500

———— S6: PBE/CCSD(T) ————

C	-1.205074	0.000000	0.695750
C	-1.205074	0.000000	-0.695750
C	0.000000	0.000000	-1.391500
C	1.205074	0.000000	-0.695750
C	1.205074	0.000000	0.695750
C	0.000000	0.000000	1.391500
H	-2.140382	0.000000	1.235750
H	-2.140382	0.000000	-1.235750
H	0.000000	0.000000	-2.471500
H	2.140382	0.000000	-1.235750
H	2.140382	0.000000	1.235750
H	0.000000	0.000000	2.471500
C	7.298921	-0.695750	0.000000
C	7.298921	0.695750	0.000000
C	6.093846	1.391500	0.000000
C	4.888772	0.695750	0.000000
C	4.888772	-0.695750	0.000000
C	6.093846	-1.391500	0.000000
H	8.234228	-1.235750	0.000000
H	8.234228	1.235750	0.000000
H	6.093846	2.471500	0.000000
H	3.953465	1.235750	0.000000
H	3.953465	-1.235750	0.000000
H	6.093846	-2.471500	0.000000

———— S7: PBE/CCSD(T) ————

C	1.391500	0.000000	0.000000
C	0.695750	1.205074	0.000000
C	-0.695750	1.205074	0.000000
C	-1.391500	0.000000	0.000000
C	-0.695750	-1.205074	0.000000
C	0.695750	-1.205074	0.000000
H	2.471500	0.000000	0.000000
H	1.235750	2.140382	0.000000
H	-1.235750	2.140382	0.000000
H	-2.471500	0.000000	0.000000
H	-1.235750	-2.140382	0.000000
H	1.235750	-2.140382	0.000000
C	1.205074	0.695750	3.872966
C	1.205074	-0.695750	3.872966
C	0.000000	-1.391500	3.872966
C	-1.205074	-0.695750	3.872966



```

C -1.205074  0.695750  3.872966
C  0.000000  1.391500  3.872966
H  2.140382  1.235750  3.872966
H  2.140382 -1.235750  3.872966
H  0.000000 -2.471500  3.872966
H -2.140382 -1.235750  3.872966
H -2.140382  1.235750  3.872966
H  0.000000  2.471500  3.872966

```

———— S8: PBE/CCSD(T) ————

```

C  1.391500  0.000000  0.000000
C  0.695750  1.205074  0.000000
C -0.695750  1.205074  0.000000
C -1.391500  0.000000  0.000000
C -0.695750 -1.205074  0.000000
C  0.695750 -1.205074  0.000000
H  2.471500  0.000000  0.000000
H  1.235750  2.140382  0.000000
H -1.235750  2.140382  0.000000
H -2.471500  0.000000  0.000000
H -1.235750 -2.140382  0.000000
H  1.235750 -2.140382  0.000000
C  1.391500  0.000000  3.873344
C  0.695750 -1.205074  3.873344
C -0.695750 -1.205074  3.873344
C -1.391500  0.000000  3.873344
C -0.695750  1.205074  3.873344
C  0.695750  1.205074  3.873344
H  2.471500  0.000000  3.873344
H  1.235750 -2.140382  3.873344
H -1.235750 -2.140382  3.873344
H -2.471500  0.000000  3.873344
H -1.235750  2.140382  3.873344
H  1.235750  2.140382  3.873344

```

### 11.1.7 Benzene dimer: PBE+MBD@rsSCS

———— M1: PBE+MBD@rsSCS ————

```

C  1.209054592 -0.705008318 -0.021161299
C  0.000000000 -1.403503732 -0.024348683
C -1.209054592 -0.705008318 -0.021161299
C -1.209841340  0.691910949 -0.012687262
C  0.000000000  1.390848488 -0.006805957
C  1.209841340  0.691910949 -0.012687262
H  2.152982299 -1.250842599 -0.015879535
H  0.000000000 -2.493596773 -0.013679695
H -2.152982299 -1.250842599 -0.015879535
H -2.154308295  1.237262494 -0.008085500
H  0.000000000  2.481460298  0.001008648
H  2.154308295  1.237262494 -0.008085500
C -1.209842363 -2.402308433  3.501229132
C  0.000000000 -3.101249059  3.495560058
C  1.209842363 -2.402308433  3.501229132
C  1.209039386 -1.005359989  3.509342202
C  0.000000000 -0.306862227  3.512374727
C -1.209039386 -1.005359989  3.509342202
H -2.154353761 -2.947548983  3.496838258

```

```
H 0.000000000 -4.191858082 3.488172186
H 2.154353761 -2.947548983 3.496838258
H 2.152938775 -0.459474112 3.503880009
H 0.000000000 0.783251067 3.501350711
H -2.152938775 -0.459474112 3.503880009
```

————— M2: PBE+MBD@rsSCS —————

```
C 1.209799879 -0.698799358 -0.000805912
C -0.000513903 -1.397253740 -0.000217924
C -1.210465253 -0.698590800 -0.001764288
C -1.210465253 0.698590800 -0.001764288
C -0.000513903 1.397253740 -0.000217924
C 1.209799879 0.698799358 -0.000805912
H 2.153823083 -1.244272422 0.002019676
H -0.000634539 -2.487433737 0.005180376
H -2.154217121 -1.244848515 0.001424647
H -2.154217121 1.244848515 0.001424647
H -0.000634539 2.487433737 0.005180376
H 2.153823083 1.244272422 0.002019676
C -0.295603790 0.000000000 3.566326844
C 0.535352916 0.000000000 4.689185501
C -0.018859103 0.000000000 5.972064828
C -1.406902408 0.000000000 6.132989137
C -2.239204810 0.000000000 5.010383606
C -1.683202426 0.000000000 3.728803488
H 0.133874749 0.000000000 2.564679776
H 1.618896897 0.000000000 4.564469797
H 0.630871758 0.000000000 6.847910213
H -1.839838088 0.000000000 7.133834875
H -3.322608620 0.000000000 5.136242695
H -2.328416367 0.000000000 2.849688090
```

————— S1: PBE+MBD@rsSCS —————

```
C 0.000000000 -1.396823817 -0.000436618
C -1.210338487 -0.698198871 0.000427563
C -1.210267788 0.699094264 0.000344627
C 0.000000000 1.397200023 -0.001455694
C 1.210267788 0.699094264 0.000344627
C 1.210338487 -0.698198871 0.000427563
H 0.000000000 -2.487216339 0.001071068
H -2.154594217 -1.243149802 0.004067612
H -2.154532809 1.243951244 0.005262841
H 0.000000000 2.487816219 -0.001834277
H 2.154532809 1.243951244 0.005262841
H 2.154594217 -1.243149802 0.004067612
C 0.000000000 0.277733557 3.576559136
C 0.000000000 -0.563453567 4.691894490
C 0.000000000 -0.021054032 5.979837240
C 0.000000000 1.365319494 6.153550580
C 0.000000000 2.207900053 5.038586548
C 0.000000000 1.663748010 3.751870142
H 0.000000000 -0.142693489 2.571047585
H 0.000000000 -1.645757782 4.557319409
H 0.000000000 -0.678842564 6.849711342
H 0.000000000 1.789075592 7.158401967
H 0.000000000 3.289988940 5.174606951
```

H 0.000000000 2.317266032 2.878901843

———— S2: PBE+MBD@rsSCS ————

C 0.697980413 -1.216556668 -0.022009526  
C -0.697980413 -1.216556668 -0.022009526  
C 1.396431684 -0.006718871 -0.015722560  
C -1.396431684 -0.006718871 -0.015722560  
C -0.698933903 1.203481452 -0.006694110  
C 0.698933903 1.203481452 -0.006694110  
H 1.242026830 -2.161294096 -0.014398558  
H -1.242026830 -2.161294096 -0.014398558  
H 2.487118503 -0.007114796 -0.012324630  
H -2.487118503 -0.007114796 -0.012324630  
H -1.244496745 2.147839894 -0.000760660  
H 1.244496745 2.147839894 -0.000760660  
C -1.209859107 -2.407414245 3.502635066  
C 0.000000000 -3.106567982 3.497556063  
C 1.209859107 -2.407414245 3.502635066  
C 1.209001438 -1.010405117 3.510443615  
C 0.000000000 -0.312004977 3.513209423  
C -1.209001438 -1.010405117 3.510443615  
H -2.154582751 -2.952424794 3.498789918  
H 0.000000000 -4.197153543 3.491290376  
H 2.154582751 -2.952424794 3.498789918  
H 2.152742708 -0.464170398 3.504411675  
H 0.000000000 0.778189779 3.502433677  
H -2.152742708 -0.464170398 3.504411675

———— S3: PBE+MBD@rsSCS ————

C 0.000000000 -1.397338963 0.000992416  
C -0.000000000 1.397338963 0.000992416  
C -1.210179172 -0.698695720 0.000765260  
C 1.210179172 -0.698695720 0.000765260  
C 1.210179172 0.698695720 0.000765260  
C -1.210179172 0.698695720 0.000765260  
H -0.000000000 -2.487510350 0.004590652  
H -0.000000000 2.487510350 0.004590652  
H -2.154173720 -1.244318448 0.002546001  
H 2.154173720 -1.244318448 0.002546001  
H 2.154173720 1.244318448 0.002546001  
H -2.154173720 1.244318448 0.002546001  
C 0.000000000 0.000000000 3.608519374  
C 1.208855095 0.000000000 4.308767843  
C 1.209999371 0.000000000 5.706036028  
C 0.000000000 0.000000000 6.405174693  
C -1.209999371 -0.000000000 5.706036028  
C -1.208855095 -0.000000000 4.308767843  
H 0.000000000 0.000000000 2.519069449  
H 2.152597031 0.000000000 3.761915738  
H 2.154135721 0.000000000 6.252084184  
H 0.000000000 0.000000000 7.495617718  
H -2.154135721 0.000000000 6.252084184  
H -2.152597031 -0.000000000 3.761915738

———— S4: PBE+MBD@rsSCS ————

C 0.698333423 -1.211401529 -0.003303035

```
C -0.698333423 -1.211401529 -0.003303035
C  1.397099780 -0.001699678 -0.002176395
C -1.397099780 -0.001699678 -0.002176395
C -0.698910808  1.208949175  0.000447542
C  0.698910808  1.208949175  0.000447542
H  1.242914371 -2.155741768  0.004510612
H -1.242914371 -2.155741768  0.004510612
H  2.487560785 -0.001908810  0.000376097
H -2.487560785 -0.001908810  0.000376097
H -1.243934602  2.153306109  0.004189853
H  1.243934602  2.153306109  0.004189853
C -1.210027154 -1.608904489  5.133767462
C  0.000000000 -2.023084469  5.697048849
C  1.210027154 -1.608904489  5.133767462
C  1.208788982 -0.780368240  4.008620085
C  0.000000000 -0.364465764  3.445999439
C -1.208788982 -0.780368240  4.008620085
H -2.154064696 -1.934490754  5.572220759
H  0.000000000 -2.670309321  6.574728312
H  2.154064696 -1.934490754  5.572220759
H  2.152062204 -0.460718451  3.563951515
H  0.000000000  0.273691428  2.562723407
H -2.152062204 -0.460718451  3.563951515
```

———— S5: PBE+MBD@rsSCS ————

```
C  0.001195981 -1.397362095  0.000000000
C -0.001171295 -0.698662079 -1.210013107
C -0.001171295  0.698662079 -1.210013107
C  0.001195981  1.397362095  0.000000000
C -0.001171295  0.698662079  1.210013107
C -0.001171295 -0.698662079  1.210013107
H  0.005626736 -2.487507443 -0.000000000
H  0.000163294 -1.244394592 -2.154068485
H  0.000163294  1.244394592 -2.154068485
H  0.005626736  2.487507443  0.000000000
H  0.000163294  1.244394592  2.154068485
H  0.000163294 -1.244394592  2.154068485
C  6.209332816  0.000000000 -0.698550438
C  6.209332816  0.000000000  0.698550438
C  4.998563121 -0.000000000  1.396561972
C  3.788432018  0.000000000  0.698785621
C  3.788432018  0.000000000 -0.698785621
C  4.998563121 -0.000000000 -1.396561972
H  7.153905444  0.000000000 -1.243575626
H  7.153905444  0.000000000  1.243575626
H  4.999800897  0.000000000  2.487277125
H  2.840514989  0.000000000  1.236782568
H  2.840514989  0.000000000 -1.236782568
H  4.999800897  0.000000000 -2.487277125
```

———— S6: PBE+MBD@rsSCS ————

```
C -1.209118206 -0.000000000  0.698572525
C -1.209118206  0.000000000 -0.698572525
C  0.001005087  0.000000000 -1.396919939
C  1.211277848  0.000000000 -0.698647111
C  1.211277848  0.000000000  0.698647111
```

C	0.001005087	0.000000000	1.396919939
H	-2.153456679	0.000000000	1.243963152
H	-2.153456679	0.000000000	-1.243963152
H	0.000781468	0.000000000	-2.487312466
H	2.154559693	0.000000000	-1.246769479
H	2.154559693	0.000000000	1.246769479
H	0.000781468	0.000000000	2.487312466
C	7.302842829	-0.698568543	0.000000000
C	7.302842829	0.698568543	0.000000000
C	6.092855507	1.397030121	0.000000000
C	4.882683518	0.698633498	-0.000000000
C	4.882683518	-0.698633498	0.000000000
C	6.092855507	-1.397030121	0.000000000
H	8.247234672	-1.243891655	0.000000000
H	8.247234672	1.243891655	0.000000000
H	6.093064186	2.487424151	0.000000000
H	3.939348075	1.246699667	0.000000000
H	3.939348075	-1.246699667	0.000000000
H	6.093064186	-2.487424151	0.000000000

## ——— S7: PBE+MBD@rsSCS ———

C	1.396534448	0.000000000	-0.004515414
C	0.698319863	1.209647131	-0.004509489
C	-0.698319863	1.209647131	-0.004509489
C	-1.396534448	0.000000000	-0.004515414
C	-0.698319863	-1.209647131	-0.004509489
C	0.698319863	-1.209647131	-0.004509489
H	2.487021356	0.000000000	0.002124540
H	1.243664343	2.153989008	0.002127034
H	-1.243664343	2.153989008	0.002127034
H	-2.487021356	0.000000000	0.002124540
H	-1.243664343	-2.153989008	0.002127034
H	1.243664343	-2.153989008	0.002127034
C	1.209629862	0.698320649	3.877388337
C	1.209629862	-0.698320649	3.877388337
C	-0.000000000	-1.396552606	3.877363032
C	-1.209629862	-0.698320649	3.877388337
C	-1.209629862	0.698320649	3.877388337
C	0.000000000	1.396552606	3.877363032
H	2.153982992	1.243648387	3.870940269
H	2.153982992	-1.243648387	3.870940269
H	0.000000000	-2.487045782	3.870931541
H	-2.153982992	-1.243648387	3.870940269
H	-2.153982992	1.243648387	3.870940269
H	-0.000000000	2.487045782	3.870931541

## ——— S8: PBE+MBD@rsSCS ———

C	1.396554031	0.000000000	-0.004881719
C	0.698274020	1.209641559	-0.004874773
C	-0.698274020	1.209641559	-0.004874773
C	-1.396554031	0.000000000	-0.004881719
C	-0.698274020	-1.209641559	-0.004874773
C	0.698274020	-1.209641559	-0.004874773
H	2.486984833	0.000000000	0.002198946
H	1.243658584	2.153966305	0.002202101
H	-1.243658584	2.153966305	0.002202101

H	-2.486984833	0.000000000	0.002198946
H	-1.243658584	-2.153966305	0.002202101
H	1.243658584	-2.153966305	0.002202101
C	1.396551777	0.000000000	3.878098961
C	0.698303739	-1.209626988	3.878121530
C	-0.698303739	-1.209626988	3.878121530
C	-1.396551777	0.000000000	3.878098961
C	-0.698303739	1.209626988	3.878121530
C	0.698303739	1.209626988	3.878121530
H	2.487011105	0.000000000	3.871242167
H	1.243640279	-2.153958501	3.871253964
H	-1.243640279	-2.153958501	3.871253964
H	-2.487011105	0.000000000	3.871242167
H	-1.243640279	2.153958501	3.871253964
H	1.243640279	2.153958501	3.871253964

### 11.1.8 Benzene dimer: PBE+TS

———— M1: PBE+TS ————

C	1.209053928	-0.673835868	0.021922550
C	0.000000000	-1.372054608	0.029382754
C	-1.209053928	-0.673835868	0.021922550
C	-1.210326887	0.723410992	0.014572493
C	0.000000000	1.422773857	0.015016494
C	1.210326887	0.723410992	0.014572493
H	2.151615303	-1.221081006	0.033631629
H	0.000000000	-2.461124833	0.062377415
H	-2.151615303	-1.221081006	0.033631629
H	-2.155431813	1.267471658	0.008905789
H	0.000000000	2.513298673	0.010865530
H	2.155431813	1.267471658	0.008905789
C	-1.210462689	-2.433760181	3.474379310
C	0.000000000	-3.132986597	3.474458950
C	1.210462689	-2.433760181	3.474379310
C	1.209156201	-1.036549626	3.465990108
C	0.000000000	-0.338485034	3.458019196
C	-1.209156201	-1.036549626	3.465990108
H	-2.155574211	-2.977873059	3.480102747
H	0.000000000	-4.223494883	3.478908000
H	2.155574211	-2.977873059	3.480102747
H	2.151663601	-0.489170157	3.453983551
H	0.000000000	0.750599916	3.424579304
H	-2.151663601	-0.489170157	3.453983551

———— M2: PBE+TS ————

C	1.212106519	-0.699111402	-0.074458944
C	0.001450739	-1.398250186	-0.067946279
C	-1.208947570	-0.698925966	-0.065085857
C	-1.208947570	0.698925966	-0.065085857
C	0.001450739	1.398250186	-0.067946279
C	1.212106519	0.699111402	-0.074458944
H	2.156269335	-1.244536041	-0.076594592
H	0.000966783	-2.488543421	-0.063351921
H	-2.153019665	-1.244528511	-0.062376379
H	-2.153019665	1.244528511	-0.062376379
H	0.000966783	2.488543421	-0.063351921
H	2.156269335	1.244536041	-0.076594592

C	-0.274285894	0.000000000	3.645579645
C	0.536388435	0.000000000	4.783793813
C	-0.041202315	0.000000000	6.056893809
C	-1.432256626	0.000000000	6.192952296
C	-2.244353240	0.000000000	5.054771800
C	-1.665054652	0.000000000	3.782574474
H	0.174670466	0.000000000	2.653328864
H	1.621544769	0.000000000	4.677747987
H	0.593742660	0.000000000	6.943337448
H	-1.883791448	0.000000000	7.185599446
H	-3.329726111	0.000000000	5.159410747
H	-2.293383327	0.000000000	2.891889615

## ——— S1: PBE+TS ———

C	0.000000000	-1.397585545	-0.066495203
C	-1.210939414	-0.698560653	-0.065556444
C	-1.210866518	0.699445337	-0.066180889
C	0.000000000	1.397910004	-0.068536216
C	1.210866518	0.699445337	-0.066180889
C	1.210939414	-0.698560653	-0.065556444
H	0.000000000	-2.488065980	-0.064861178
H	-2.155377721	-1.243353161	-0.062039199
H	-2.154979238	1.244772776	-0.063414355
H	0.000000000	2.488505929	-0.072102162
H	2.154979238	1.244772776	-0.063414355
H	2.155377721	-1.243353161	-0.062039199
C	0.000000000	0.255022890	3.653748364
C	0.000000000	-0.566866220	4.783928391
C	0.000000000	-0.001328001	6.062261169
C	0.000000000	1.388486572	6.211281780
C	0.000000000	2.211473716	5.081058673
C	0.000000000	1.644344851	3.803470692
H	0.000000000	-0.184146138	2.657299840
H	0.000000000	-1.651020227	4.667118297
H	0.000000000	-0.644821176	6.942454127
H	0.000000000	1.829963080	7.208336948
H	0.000000000	3.295800554	5.196445582
H	0.000000000	2.281317093	2.918809670

## ——— S2: PBE+TS ———

C	0.698053062	-1.195078618	0.017079814
C	-0.698053062	-1.195078618	0.017079814
C	1.396599108	0.015278725	0.010392228
C	-1.396599108	0.015278725	0.010392228
C	-0.699020432	1.225609978	0.012776956
C	0.699020432	1.225609978	0.012776956
H	1.242701534	-2.138761171	0.038842471
H	-1.242701534	-2.138761171	0.038842471
H	2.486958532	0.014986752	0.009031833
H	-2.486958532	0.014986752	0.009031833
H	-1.244011468	2.170100897	0.012567972
H	1.244011468	2.170100897	0.012567972
C	-1.210018714	-2.429426421	3.482914319
C	0.000000000	-3.128684278	3.480426042
C	1.210018714	-2.429426421	3.482914319
C	1.209206839	-1.032117991	3.476968914

C	0.000000000	-0.333276158	3.468661436
C	-1.209206839	-1.032117991	3.476968914
H	-2.154320431	-2.974683234	3.487698845
H	0.000000000	-4.219144430	3.479422469
H	2.154320431	-2.974683234	3.487698845
H	2.153106686	-0.486885898	3.466548353
H	0.000000000	0.755966830	3.435076643
H	-2.153106686	-0.486885898	3.466548353

## ———— S3: PBE+TS ————

C	0.000000000	-1.398054498	-0.060517300
C	0.000000000	1.398054498	-0.060517300
C	-1.210622837	-0.699005419	-0.060978737
C	1.210622837	-0.699005419	-0.060978737
C	1.210622837	0.699005419	-0.060978737
C	-1.210622837	0.699005419	-0.060978737
H	-0.000000000	-2.488178914	-0.056060943
H	0.000000000	2.488178914	-0.056060943
H	-2.154599874	-1.244491946	-0.058949979
H	2.154599874	-1.244491946	-0.058949979
H	2.154599874	1.244491946	-0.058949979
H	-2.154599874	1.244491946	-0.058949979
C	0.000000000	0.000000000	3.669694657
C	1.209599079	-0.000000000	4.369898649
C	1.210532913	-0.000000000	5.767913166
C	0.000000000	0.000000000	6.467239919
C	-1.210532913	0.000000000	5.767913166
C	-1.209599079	0.000000000	4.369898649
H	0.000000000	0.000000000	2.581210779
H	2.152671503	-0.000000000	3.822203558
H	2.154709909	0.000000000	6.313688891
H	0.000000000	0.000000000	7.557717465
H	-2.154709909	-0.000000000	6.313688891
H	-2.152671503	0.000000000	3.822203558

## ———— S4: PBE+TS ————

C	0.698627888	-1.201867557	-0.034068527
C	-0.698627888	-1.201867557	-0.034068527
C	1.397622180	0.008311036	-0.039752652
C	-1.397622180	0.008311036	-0.039752652
C	-0.699165570	1.219339882	-0.043966601
C	0.699165570	1.219339882	-0.043966601
H	1.243180441	-2.146118574	-0.024610808
H	-1.243180441	-2.146118574	-0.024610808
H	2.487983912	0.007928652	-0.040079316
H	-2.487983912	0.007928652	-0.040079316
H	-1.244216978	2.163601208	-0.047030255
H	1.244216978	2.163601208	-0.047030255
C	-1.210617399	-1.638379970	5.158359952
C	0.000000000	-2.070433907	5.708349704
C	1.210617399	-1.638379970	5.158359952
C	1.209551793	-0.773628777	4.060055062
C	0.000000000	-0.339294881	3.511384411
C	-1.209551793	-0.773628777	4.060055062
H	-2.154823070	-1.976335139	5.587016364
H	0.000000000	-2.743754504	6.566027416



H	2.154823070	-1.976335139	5.587016364
H	2.152217691	-0.437173107	3.627054454
H	0.000000000	0.332002983	2.653992127
H	-2.152217691	-0.437173107	3.627054454

## ———— S5: PBE+TS ————

C	-0.022689417	-1.397976764	0.000000000
C	-0.025826867	-0.699000609	-1.210473233
C	-0.025826867	0.699000609	-1.210473233
C	-0.022689417	1.397976764	0.000000000
C	-0.025826867	0.699000609	1.210473233
C	-0.025826867	-0.699000609	1.210473233
H	-0.018616727	-2.488212124	-0.000000000
H	-0.024263061	-1.244507760	-2.154601134
H	-0.024263061	1.244507760	-2.154601134
H	-0.018616727	2.488212124	0.000000000
H	-0.024263061	1.244507760	2.154601134
H	-0.024263061	-1.244507760	2.154601134
C	6.234188505	-0.000000000	-0.698894383
C	6.234188505	0.000000000	0.698894383
C	5.022986692	0.000000000	1.397429093
C	3.812242679	0.000000000	0.699027833
C	3.812242679	-0.000000000	-0.699027833
C	5.022986692	-0.000000000	-1.397429093
H	7.178770852	0.000000000	-1.243784618
H	7.178770852	0.000000000	1.243784618
H	5.023439021	0.000000000	2.488126060
H	2.865214251	0.000000000	1.238025876
H	2.865214251	0.000000000	-1.238025876
H	5.023439021	-0.000000000	-2.488126060

## ———— S6: PBE+TS ————

C	-1.299393959	-0.000000000	0.698899923
C	-1.299393959	-0.000000000	-0.698899923
C	-0.088859232	0.000000000	-1.397594123
C	1.122154759	0.000000000	-0.698968760
C	1.122154759	-0.000000000	0.698968760
C	-0.088859232	0.000000000	1.397594123
H	-2.243485110	0.000000000	1.244534537
H	-2.243485110	0.000000000	-1.244534537
H	-0.088519006	0.000000000	-2.487893913
H	2.064716991	0.000000000	-1.247636492
H	2.064716991	-0.000000000	1.247636492
H	-0.088519006	0.000000000	2.487893913
C	7.393157382	-0.698948482	-0.000000000
C	7.393157382	0.698948482	0.000000000
C	6.182670663	1.397662582	0.000000000
C	4.971808128	0.699000927	0.000000000
C	4.971808128	-0.699000927	-0.000000000
C	6.182670663	-1.397662582	-0.000000000
H	8.337288235	-1.244453725	-0.000000000
H	8.337288235	1.244453725	0.000000000
H	6.182365044	2.488009669	-0.000000000
H	4.029174104	1.247563945	0.000000000
H	4.029174104	-1.247563945	0.000000000
H	6.182365044	-2.488009669	0.000000000

## ———— S7: PBE+TS ————

C	1.396907134	-0.000000000	0.048229878
C	0.698466010	1.209840911	0.048219305
C	-0.698466010	1.209840911	0.048219305
C	-1.396907134	0.000000000	0.048229878
C	-0.698466010	-1.209840911	0.048219305
C	0.698466010	-1.209840911	0.048219305
H	2.487239339	-0.000000000	0.055386248
H	1.243517947	2.154138271	0.055389970
H	-1.243517947	2.154138271	0.055389970
H	-2.487239339	-0.000000000	0.055386248
H	-1.243517947	-2.154138271	0.055389970
H	1.243517947	-2.154138271	0.055389970
C	1.209813485	0.698470540	3.824765840
C	1.209813485	-0.698470540	3.824765840
C	0.000000000	-1.396909975	3.824650285
C	-1.209813485	-0.698470540	3.824765840
C	-1.209813485	0.698470540	3.824765840
C	-0.000000000	1.396909975	3.824650285
H	2.154109357	1.243548172	3.817694475
H	2.154109357	-1.243548172	3.817694475
H	-0.000000000	-2.487255797	3.817390408
H	-2.154109357	-1.243548172	3.817694475
H	-2.154109357	1.243548172	3.817694475
H	0.000000000	2.487255797	3.817390408

## ———— S8: PBE+TS ————

C	1.396948102	0.000000000	0.046778769
C	0.698489254	1.209791307	0.046782408
C	-0.698489254	1.209791307	0.046782408
C	-1.396948102	0.000000000	0.046778769
C	-0.698489254	-1.209791307	0.046782408
C	0.698489254	-1.209791307	0.046782408
H	2.487326417	0.000000000	0.054023125
H	1.243489453	2.154092114	0.054062259
H	-1.243489453	2.154092114	0.054062259
H	-2.487326417	0.000000000	0.054023125
H	-1.243489453	-2.154092114	0.054062259
H	1.243489453	-2.154092114	0.054062259
C	1.396966472	0.000000000	3.826416457
C	0.698465835	-1.209788741	3.826525685
C	-0.698465835	-1.209788741	3.826525685
C	-1.396966472	-0.000000000	3.826416457
C	-0.698465835	1.209788741	3.826525685
C	0.698465835	1.209788741	3.826525685
H	2.487307671	-0.000000000	3.819156439
H	1.243530038	-2.154076330	3.819474252
H	-1.243530038	-2.154076330	3.819474252
H	-2.487307671	0.000000000	3.819156439
H	-1.243530038	2.154076330	3.819474252
H	1.243530038	2.154076330	3.819474252

**11.1.9 Benzene dimer: PBE+D3**

## ———— M1: PBE+D3 ————

C	1.209494083	-0.691669692	-0.028079614
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C -0.000000062 -1.390065710 -0.030136784  
C -1.209494154 -0.691669588 -0.028079746  
C -1.210211303 0.705612731 -0.020694273  
C 0.000000038 1.404559367 -0.015118616  
C 1.210211317 0.705612620 -0.020694113  
H 2.154509395 -1.238924965 -0.021876324  
H -0.000000123 -2.482063486 -0.017151085  
H -2.154509514 -1.238924807 -0.021876486  
H -2.156169059 1.251981525 -0.017097777  
H 0.000000087 2.497286622 -0.008489720  
H 2.156169096 1.251981364 -0.017097567  
C -1.210211290 -2.415966717 3.509076277  
C 0.000000055 -3.114913351 3.503500802  
C 1.210211355 -2.415966635 3.509076244  
C 1.209494120 -1.018684314 3.516461511  
C -0.000000026 -0.320288287 3.518518592  
C -1.209494129 -1.018684405 3.516461619  
H -2.156169048 -2.962335502 3.505479824  
H 0.000000106 -4.207640605 3.496872078  
H 2.156169149 -2.962335379 3.505479808  
H 2.154509456 -0.471429068 3.510258209  
H -0.000000054 0.771709494 3.505532820  
H -2.154509495 -0.471429212 3.510258323

———— M2: PBE+D3 ————

C 1.213332950 -0.699039739 -0.017467798  
C 0.002866086 -1.397936188 -0.016849776  
C -1.207429460 -0.698914217 -0.018304727  
C -1.207429477 0.698914194 -0.018304733  
C 0.002866060 1.397936180 -0.016849770  
C 1.213332939 0.699039756 -0.017467772  
H 2.158924154 -1.245516674 -0.016319930  
H 0.002576904 -2.490244678 -0.014114244  
H -2.153064682 -1.245489709 -0.017678649  
H -2.153064710 1.245489677 -0.017678655  
H 0.002576869 2.490244674 -0.014114232  
H 2.158924143 1.245516702 -0.016319876  
C -0.298852008 -0.000000002 3.583353335  
C 0.532350148 -0.000000009 4.706895579  
C -0.021932880 -0.000000018 5.990242114  
C -1.410115696 0.000000008 6.150829737  
C -2.242493458 0.000000022 5.028163677  
C -1.686618944 0.000000002 3.745699164  
H 0.134250586 -0.000000004 2.581717020  
H 1.617787485 -0.000000023 4.580711120  
H 0.628791481 -0.000000038 6.867515716  
H -1.844341214 0.000000025 7.153159072  
H -3.328029815 0.000000056 5.154028388  
H -2.335262459 0.000000003 2.867407238

———— S1: PBE+D3 ————

C 0.000000024 -1.397347208 -0.000083074  
C -1.210794689 -0.698758645 -0.012838670  
C -1.210773403 0.698652102 -0.039817025  
C 0.000000001 1.396697890 -0.054879381  
C 1.210773416 0.698652121 -0.039817003

C 1.210794725 -0.698758626 -0.012838675  
H 0.000000039 -2.489603707 0.023339625  
H -2.156551274 -1.244541215 0.002926830  
H -2.156466949 1.244664036 -0.044826289  
H -0.000000017 2.489089581 -0.077330854  
H 2.156466960 1.244664062 -0.044826226  
H 2.156551315 -1.244541188 0.002926812  
C -0.000000065 0.284362385 3.600086299  
C -0.000000100 -0.562828641 4.711442921  
C 0.000000001 -0.026387989 6.002362702  
C 0.000000055 1.359488888 6.182569553  
C -0.000000041 2.207970693 5.071973707  
C -0.000000042 1.669801589 3.782184678  
H -0.000000059 -0.131213921 2.591271080  
H -0.000000102 -1.646391351 4.569984322  
H 0.000000048 -0.689190225 6.870553092  
H 0.000000155 1.779314118 7.190997240  
H 0.000000006 3.291573308 5.213343356  
H -0.000000003 2.328231942 2.911131981

———— S2: PBE+D3 ————

C 0.698154119 -1.202224898 -0.029746521  
C -0.698154233 -1.202224884 -0.029746562  
C 1.396711908 0.007916499 -0.025817558  
C -1.396711987 0.007916536 -0.025817638  
C -0.698928250 1.218253475 -0.018774166  
C 0.698928215 1.218253455 -0.018774108  
H 1.243375925 -2.148085175 -0.019421250  
H -1.243376054 -2.148085166 -0.019421345  
H 2.489305116 0.007445181 -0.021956142  
H -2.489305207 0.007445245 -0.021956253  
H -1.245289075 2.164171805 -0.013632175  
H 1.245289100 2.164171760 -0.013632145  
C -1.210111976 -2.422120828 3.513205186  
C 0.000000029 -3.121224324 3.508091164  
C 1.210112047 -2.422120836 3.513205275  
C 1.209400868 -1.024850979 3.520031215  
C 0.000000037 -0.326368869 3.522248343  
C -1.209400797 -1.024850974 3.520031122  
H -2.156133018 -2.968341428 3.509144093  
H 0.000000021 -4.213897281 3.501686508  
H 2.156133111 -2.968341430 3.509144273  
H 2.154536563 -0.477762019 3.513295684  
H 0.000000039 0.765595168 3.508547441  
H -2.154536501 -0.477762035 3.513295559

———— S3: PBE+D3 ————

C 0.000000007 -1.397760181 -0.014584311  
C 0.000000006 1.397760197 -0.014584429  
C -1.210470917 -0.698910999 -0.015211480  
C 1.210470931 -0.698910990 -0.015211438  
C 1.210470928 0.698911018 -0.015211506  
C -1.210470912 0.698911007 -0.015211538  
H 0.000000006 -2.490036928 -0.011543266  
H 0.000000007 2.490036946 -0.011543459  
H -2.156091223 -1.245264326 -0.013649473

H	2.156091237	-1.245264317	-0.013649403
H	2.156091224	1.245264359	-0.013649482
H	-2.156091209	1.245264336	-0.013649534
C	-0.000000032	0.000000002	3.624582261
C	1.209376854	-0.000000002	4.324665350
C	1.210368700	-0.000000020	5.722335425
C	0.000000013	-0.000000031	6.421346774
C	-1.210368701	-0.000000014	5.722335474
C	-1.209376897	-0.000000006	4.324665394
H	-0.000000022	0.000000007	2.533469360
H	2.154421570	0.000000005	3.776402568
H	2.156179265	-0.000000032	6.268940610
H	0.000000037	-0.000000046	7.514012769
H	-2.156179245	-0.000000012	6.268940690
H	-2.154421627	0.000000026	3.776402643

## ——— S4: PBE+D3 ———

C	0.698616614	-1.192027982	-0.059947972
C	-0.698618633	-1.192027129	-0.059951047
C	1.397436737	0.018019257	-0.040467776
C	-1.397437328	0.018020984	-0.040473713
C	-0.699052545	1.228795636	-0.020341177
C	0.699053386	1.228794786	-0.020338319
H	1.244345572	-2.137777877	-0.066262139
H	-1.244348697	-2.137776358	-0.066267994
H	2.489962659	0.017875806	-0.037989888
H	-2.489963256	0.017878922	-0.038000630
H	-1.245077360	2.174500139	-0.001534866
H	1.245079297	2.174498617	-0.001529702
C	-1.210042284	-1.609654540	5.185901613
C	0.000001549	-2.004228363	5.763239278
C	1.210044122	-1.609653304	5.185899817
C	1.209027226	-0.820161472	4.032564207
C	-0.000000956	-0.424265605	3.455074657
C	-1.209027859	-0.820162701	4.032566033
H	-2.155771644	-1.918074095	5.636626085
H	0.000002545	-2.619582316	6.665668750
H	2.155774438	-1.918071872	5.636622951
H	2.153743437	-0.513894194	3.577975619
H	-0.000001957	0.182745050	2.548696313
H	-2.153745065	-0.513896390	3.577978899

## ——— S5: PBE+D3 ———

C	-0.026987509	-1.397676272	-0.000000042
C	-0.032414099	-0.698882216	-1.210424759
C	-0.032413920	0.698882135	-1.210424756
C	-0.026987180	1.397676184	-0.000000039
C	-0.032413849	0.698882136	1.210424680
C	-0.032414005	-0.698882219	1.210424680
H	-0.020923754	-2.489978411	-0.000000041
H	-0.032842626	-1.245827798	-2.155838300
H	-0.032842327	1.245827714	-2.155838305
H	-0.020923153	2.489978316	-0.000000047
H	-0.032842178	1.245827726	2.155838218
H	-0.032842439	-1.245827808	2.155838213
C	6.240229274	0.000000062	-0.698720186

C	6.240229324	0.000000069	0.698720192
C	5.029243264	0.000000051	1.396936396
C	3.818684898	0.000000030	0.698900150
C	3.818684854	0.000000036	-0.698899974
C	5.029243172	0.000000041	-1.396936304
H	7.186137800	0.000000074	-1.245071596
H	7.186137891	0.000000058	1.245071539
H	5.029841677	0.000000032	2.489704607
H	2.869642720	0.000000012	1.238387490
H	2.869642676	0.000000014	-1.238387300
H	5.029841488	0.000000034	-2.489704518

## ——— S6: PBE+D3 ———

C	-1.259241206	-0.000000032	0.698828303
C	-1.259241208	0.000000005	-0.698828347
C	-0.049176329	0.000000047	-1.397554520
C	1.161369521	0.000000009	-0.699000195
C	1.161369504	-0.000000043	0.699000187
C	-0.049176343	-0.000000042	1.397554481
H	-2.205103492	-0.000000062	1.244945870
H	-2.205103495	0.000000009	-1.244945910
H	-0.048787627	0.000000083	-2.490037867
H	2.106352945	0.000000026	-1.247335627
H	2.106352948	-0.000000053	1.247335576
H	-0.048787652	-0.000000076	2.490037822
C	7.353087559	-0.698828309	-0.000000038
C	7.353087589	0.698828298	-0.000000078
C	6.143022660	1.397554496	-0.000000010
C	4.932476804	0.699000239	0.000000070
C	4.932476804	-0.699000191	0.000000119
C	6.143022623	-1.397554469	0.000000084
H	8.298949721	-1.244946102	-0.000000109
H	8.298949788	1.244946036	-0.000000161
H	6.142634193	2.490037846	-0.000000033
H	3.987493306	1.247335542	0.000000085
H	3.987493285	-1.247335443	0.000000168
H	6.142634100	-2.490037814	0.000000130

## ——— S7: PBE+D3 ———

C	1.396739045	-0.000007638	0.009262644
C	0.698432051	1.209846785	0.008744144
C	-0.698419150	1.209854196	0.008745567
C	-1.396739211	0.000007636	0.009265677
C	-0.698432348	-1.209846468	0.008746439
C	0.698418757	-1.209854325	0.008744919
H	2.489216816	-0.000013577	0.016689751
H	1.244878991	2.155568768	0.014940834
H	-1.244855128	2.155582422	0.014943380
H	-2.489216722	0.000013772	0.016695386
H	-1.244878774	-2.155568590	0.014945113
H	1.244855360	-2.155582258	0.014942237
C	1.209846549	0.698432156	3.864222249
C	1.209854155	-0.698419137	3.864221878
C	0.000007452	-1.396739283	3.863701596
C	-1.209846580	-0.698432229	3.864219178
C	-1.209854217	0.698418738	3.864219600

C	-0.000007807	1.396739219	3.863702151
H	2.155568810	1.244878708	3.858025796
H	2.155582462	-1.244855153	3.858025223
H	0.000013794	-2.489216881	3.856273102
H	-2.155568553	-1.244878847	3.858020026
H	-2.155582198	1.244855103	3.858020871
H	-0.000013555	2.489216885	3.856274238

———— S8: PBE+D3 ————

C	1.396791280	-0.000003716	0.000199172
C	0.698428528	1.209833692	0.000169553
C	-0.698422106	1.209837833	0.000170827
C	-1.396791322	0.000003788	0.000200798
C	-0.698428500	-1.209833978	0.000170444
C	0.698422239	-1.209837606	0.000169881
H	2.489310885	-0.000006373	0.003077022
H	1.244729976	2.155653697	0.002955327
H	-1.244719014	2.155660148	0.002956824
H	-2.489310477	0.000006398	0.003079004
H	-1.244730274	-2.155653495	0.002956334
H	1.244718771	-2.155660435	0.002955772
C	1.396791283	0.000003718	3.873144831
C	0.698428531	-1.209833689	3.873174465
C	-0.698422109	-1.209837838	3.873173196
C	-1.396791327	-0.000003791	3.873143190
C	-0.698428500	1.209833981	3.873173540
C	0.698422247	1.209837606	3.873174126
H	2.489310887	0.000006373	3.870266983
H	1.244729988	-2.155653687	3.870388667
H	-1.244719014	-2.155660160	3.870387196
H	-2.489310493	-0.000006398	3.870264989
H	-1.244730269	2.155653500	3.870387641
H	1.244718787	2.155660431	3.870388220

### 11.2 Secondary structure of isolated polypeptides

We considered 76 conformers of the following 5 isolated small peptides, GFA, FGG, GGF, WG, and WGG, containing the residues glycine (G), alanine (A), phenylalanine (F), and tryptophan (W).

Our starting geometries were taken from [www.begdb.com](http://www.begdb.com), corresponding to the RI-MP2/cc-pVTZ optimized structures given in the supplemental information of Valdes *et al.*<sup>39</sup> Table S3 gives the correspondence between the structure indexing scheme used in this work, the nomenclature of the BEGDB database and the nomenclature of Valdes *et al.*<sup>39</sup> Due to the ease of downloading structures from the BEGDB database, we only present our PBE+MBD and PBE+D3 optimized geometries below.

**Table S3** Peptide naming conventions in this work, the BEGDB database, and Ref. 39

This work	BEGDB	Ref. 39	This work	BEGDB	Ref. 39
0	252_FGG55	FGG_055	38	228_GGF08	GGF_08
1	263_FGG80	FGG_080	39	230_GGF09	GGF_09
2	253_FGG99	FGG_099	40	225_GGF10	GGF_10
3	264_FGG114	FGG_114	41	229_GGF11	GGF_11
4	257_FGG215	FGG_215	42	224_GGF12	GGF_12
5	258_FGG224	FGG_224	43	222_GGF13	GGF_13
6	255_FGG252	FGG_252	44	221_GGF14	GGF_14
7	254_FGG300	FGG_300	45	226_GGF15	GGF_15
8	265_FGG357	FGG_357	46	214_WGG01	WGG_01
9	256_FGG366	FGG_366	47	211_WGG02	WGG_02
10	259_FGG380	FGG_380	48	209_WGG03	WGG_03
11	260_FGG412	FGG_412	49	208_WGG04	WGG_04
12	261_FGG444	FGG_444	50	210_WGG05	WGG_05
13	262_FGG470	FGG_470	51	206_WGG06	WGG_06
14	266_FGG691	FGG_691	52	215_WGG07	WGG_07
15	248_GFA01	GFA_01	53	207_WGG08	WGG_08
16	239_GFA02	GFA_02	54	217_WGG09	WGG_09
17	247_GFA03	GFA_03	55	219_WGG10	WGG_10
18	251_GFA04	GFA_04	56	216_WGG11	WGG_11
19	250_GFA05	GFA_05	57	220_WGG12	WGG_12
20	245_GFA06	GFA_06	58	218_WGG13	WGG_13
21	237_GFA07	GFA_07	59	212_WGG14	WGG_14
22	242_GFA08	GFA_08	60	213_WGG15	WGG_15
23	241_GFA09	GFA_09	61	195_WG01	WG_01
24	238_GFA10	GFA_10	62	194_WG02	WG_02
25	240_GFA11	GFA_11	63	191_WG03	WG_03
26	244_GFA12	GFA_12	64	204_WG04	WG_04
27	243_GFA13	GFA_13	65	205_WG05	WG_05
28	249_GFA14	GFA_14	66	193_WG06	WG_06
29	236_GFA15	GFA_15	67	197_WG07	WG_07
30	246_GFA16	GFA_16	68	202_WG08	WG_08
31	231_GGF01	GGF_01	69	198_WG09	WG_09
32	234_GGF02	GGF_02	70	192_WG10	WG_10
33	233_GGF03	GGF_03	71	203_WG11	WG_11
34	227_GGF04	GGF_04	72	201_WG12	WG_12
35	235_GGF05	GGF_05	73	200_WG13	WG_13
36	232_GGF06	GGF_06	74	196_WG14	WG_14
37	223_GGF07	GGF_07	75	199_WG15	WG_15

#### 11.2.1 FGG: PBE+MBD@rsSCS

———— 252\_FGG55: PBE+MBD@rsSCS —————

```
O -3.134888393  0.098471760 -2.287348868
C -3.052553976 -0.061581146 -1.082298024
O -3.148508384  0.963670248 -0.208065162
H -2.955349167  0.619251201  0.725207131
C -2.857042843 -1.445827260 -0.436105142
H -2.845620869 -2.191827807 -1.235548094
```



```

H -3.715356319 -1.644723735 0.226828448
N -1.619291915 -1.573660617 0.327097559
H -0.847742851 -2.167282032 -0.018541262
C -1.404243389 -0.929313925 1.491738204
O -2.223650713 -0.129624332 2.001996631
C -0.068540549 -1.249600379 2.170419892
H -0.020078290 -2.328326302 2.380948955
H -0.041615168 -0.700602208 3.116604388
N 1.106328976 -0.883830701 1.382487765
H 1.507007068 0.042883598 1.523857238
C 1.520067458 -1.591862589 0.297380407
O 0.925237191 -2.618695828 -0.094548573
C 2.754044601 -1.050341534 -0.445130160
N 3.484447470 -2.089677756 -1.163606934
H 2.812478824 -2.653938768 -1.693484128
H 3.921060130 -2.733241473 -0.499880495
H 3.438363608 -0.596936631 0.290491679
C 2.317562836 0.055274569 -1.440563467
H 3.227888530 0.350659310 -1.983146642
H 1.629624249 -0.388010091 -2.177563844
C 1.673913003 1.240184982 -0.770095338
C 2.417834585 2.034475433 0.118837845
H 3.483146324 1.834495901 0.258758406
C 1.815613929 3.083754567 0.815764027
H 2.408919744 3.691189927 1.500086162
C 0.458311886 3.361059347 0.627341029
H -0.013972677 4.178467820 1.172449051
C -0.286542472 2.592267446 -0.268671990
H -1.345761582 2.793591141 -0.423943189
C 0.318815897 1.538781904 -0.958500319
H -0.274894753 0.939422960 -1.652255185

```

———— 253\_FGG99: PBE+MBD@rsSCS ————

```

O 1.118635171 0.029160170 -1.280438928
C 2.099324194 0.068450338 -0.558194683
O 3.247877847 -0.621698397 -0.818896398
H 3.076278315 -1.135319227 -1.635610441
C 2.239508363 0.873260517 0.730040811
H 3.124500156 1.516744938 0.626940586
H 2.429030067 0.176540897 1.556967175
N 1.074125693 1.675698497 1.004103451
H 0.263989642 1.232467799 1.448654704
C 0.823789977 2.771941422 0.214269618
O 1.681413889 3.309298506 -0.491244750
C -0.642940701 3.223694098 0.236756382
H -0.724182536 4.154412297 -0.333295119
H -0.985554474 3.388063160 1.267956678
N -1.486040663 2.199402116 -0.364951876
H -1.495489305 2.069339844 -1.380498040
C -1.910138813 1.119123271 0.338681149
O -1.774682998 1.012860731 1.573718508
C -2.588773273 0.039694277 -0.523768593
N -2.037691067 0.099532908 -1.883085563
H -1.073025611 -0.249211132 -1.894851670
H -2.592469539 -0.459835558 -2.531456616
H -3.649105168 0.340776052 -0.593007072

```

C -2.571564355 -1.341729923 0.180729715  
H -3.002277043 -1.207491485 1.182767115  
H -3.252078123 -1.998790043 -0.383090655  
C -1.219296582 -1.996517709 0.285778185  
C -0.727741205 -2.795503142 -0.756680084  
H -1.344465430 -2.958926475 -1.643150257  
C 0.527377913 -3.402616014 -0.670908077  
H 0.885912620 -4.025851271 -1.491220333  
C 1.313329526 -3.225441677 0.468917534  
H 2.290081844 -3.704341241 0.544040840  
C 0.831556684 -2.439725490 1.520083682  
H 1.431122505 -2.313434388 2.423220917  
C -0.420481694 -1.830401813 1.428323968  
H -0.796855827 -1.216626852 2.247398139

———— 254\_FGG300: PBE+MBD@rsSCS ————

O -1.214259559 -1.582913058 0.343774956  
C -2.189620294 -2.068429442 -0.206643128  
O -2.421139057 -3.412041668 -0.259234925  
H -1.679600932 -3.840490668 0.217391130  
C -3.295779256 -1.303873802 -0.925597051  
H -4.252515427 -1.588363528 -0.465216615  
H -3.323994905 -1.636224011 -1.972582947  
N -3.129238620 0.123936331 -0.843882789  
H -2.390662672 0.572999636 -1.400987960  
C -3.509210802 0.782330868 0.300659319  
O -4.261601422 0.297861061 1.150568698  
C -2.843822253 2.158247904 0.452747093  
H -3.303928069 2.674727251 1.300457692  
H -2.970157951 2.756814588 -0.460618875  
N -1.418315531 1.985096495 0.699522122  
H -1.074128118 1.747186233 1.634737956  
C -0.545404093 1.697400792 -0.298505384  
O -0.846475960 1.749783892 -1.508386401  
C 0.850174186 1.280324731 0.187940139  
N 0.757351577 0.774733035 1.566956747  
H 1.687853165 0.713091816 1.983534250  
H 0.369382542 -0.174466749 1.550225411  
H 1.464063826 2.197926381 0.216772057  
C 1.483116720 0.308520333 -0.834774256  
H 0.846402402 -0.587113667 -0.893403714  
H 1.458022140 0.790524786 -1.822057495  
C 2.884649569 -0.068054750 -0.447360342  
C 3.147873028 -1.271020413 0.222473088  
H 2.325771254 -1.964052397 0.414011527  
C 4.442055193 -1.594528761 0.636962209  
H 4.626941658 -2.536173260 1.155014594  
C 5.496961895 -0.714197587 0.390213426  
H 6.507128648 -0.961416395 0.716232333  
C 5.249403505 0.486632832 -0.280837314  
H 6.069679893 1.175875410 -0.483252669  
C 3.955429641 0.803906848 -0.694698148  
H 3.770594079 1.741438932 -1.224154728

———— 255\_FGG252: PBE+MBD@rsSCS ————

O -2.785425923 -1.279438620 -0.560134690

```

C -3.798876005 -0.699552482 -0.205934432
O -5.054453533 -1.189749133 -0.424930799
H -4.944223447 -2.036618030 -0.905506841
C -3.866133447 0.637457019 0.524165834
H -4.432950870 0.502037343 1.455939315
H -4.435052628 1.334274066 -0.108482151
N -2.560899761 1.189124227 0.781815671
H -1.953378046 0.719757546 1.468199728
C -1.913334973 1.881515646 -0.213150592
O -2.479397153 2.359945044 -1.199737890
C -0.391609547 1.931795690 -0.009466654
H -0.141860289 2.293386054 0.998763149
H 0.041644653 2.602463799 -0.757509154
N 0.157447328 0.593955851 -0.173845438
H 0.410939715 0.240446045 -1.100017815
C 0.099707192 -0.344172713 0.798276602
O -0.298996136 -0.115943602 1.960343634
C 0.578635764 -1.733342152 0.370655053
N 0.421716102 -1.882719097 -1.083987347
H -0.574149389 -1.958402061 -1.310206961
H 0.882188527 -2.733809434 -1.410613641
H -0.037987160 -2.441817054 0.952299732
C 2.051795521 -1.941081768 0.803195945
H 2.067495741 -1.976351662 1.901325256
H 2.371553272 -2.933306297 0.445162944
C 2.985045503 -0.868769318 0.308796293
C 3.554156565 -0.928634466 -0.969738186
H 3.373336186 -1.801208012 -1.599740411
C 4.338880485 0.119851326 -1.452492559
H 4.768305953 0.060412934 -2.452819389
C 4.571329780 1.244963407 -0.658356576
H 5.183197761 2.064766819 -1.035183895
C 4.021724686 1.309173928 0.624151399
H 4.202293473 2.181627044 1.252706426
C 3.237217324 0.259584662 1.102175396
H 2.795083775 0.320376449 2.098884043

```

———— 256\_FGG366: PBE+MBD@rsSCS ————

```

O -1.900197390 1.693691946 0.384857229
C -3.045088012 1.915291590 0.026803208
O -3.666417758 3.116578422 0.212719593
H -3.018766664 3.697665426 0.663292159
C -3.971278146 0.935762889 -0.686073841
H -4.197769417 1.335072695 -1.684585294
H -4.914976509 0.893848875 -0.124794765
N -3.402514699 -0.384681890 -0.781816256
H -2.637542017 -0.543074295 -1.451976935
C -3.383049782 -1.175777484 0.342124210
O -4.082959451 -0.967930256 1.337126908
C -2.335355252 -2.294471979 0.271646251
H -2.388999936 -2.825589422 -0.689098512
H -2.512187588 -2.994405368 1.093817798
N -1.007995222 -1.706894546 0.403676437
H -0.645752229 -1.442674060 1.325603722
C -0.400063238 -1.064379297 -0.625536647
O -0.813052198 -1.091205204 -1.802513979

```

C 0.859926520 -0.296299816 -0.228279493  
N 0.795636121 0.081229504 1.190214601  
H 1.714535254 0.395852781 1.511176910  
H 0.136219549 0.855166515 1.307893214  
H 0.898346546 0.571366974 -0.912337712  
C 2.100794882 -1.174422034 -0.499268781  
H 2.042725097 -2.067812494 0.141424189  
H 2.054730742 -1.505631716 -1.546805879  
C 3.378744698 -0.424706842 -0.234336097  
C 4.067629464 -0.578826355 0.977039995  
H 3.698937166 -1.295954544 1.713795203  
C 5.220700263 0.163536016 1.245440453  
H 5.746142184 0.027698843 2.191086336  
C 5.702234698 1.072367066 0.302016982  
H 6.603531326 1.649982698 0.507965420  
C 5.026161060 1.231593093 -0.911303959  
H 5.401367495 1.933983819 -1.656390497  
C 3.874548904 0.490496553 -1.174700218  
H 3.351070540 0.617570900 -2.124902954

————— 257\_FGG215: PBE+MBD@rsSCS —————

O 3.118157028 -2.143434532 0.378705927  
C 2.976869936 -0.974288087 0.060347115  
O 3.148165933 -0.543143125 -1.202947772  
H 3.062070800 0.466967494 -1.224668492  
C 2.656577767 0.117462553 1.099926846  
H 3.587230983 0.688610163 1.260974239  
H 2.398109821 -0.385114118 2.036023209  
N 1.577641209 1.046004607 0.769212955  
H 0.720465339 1.065294127 1.340850623  
C 1.666587717 1.963539075 -0.214793028  
O 2.632608515 2.027974026 -1.011246272  
C 0.492416195 2.941564855 -0.306792931  
H 0.703553037 3.630637315 -1.130335925  
H 0.426991562 3.511055105 0.633757652  
N -0.782954048 2.286103510 -0.543764320  
H -1.213931103 2.247704798 -1.471657798  
C -1.501934899 1.699627144 0.441163007  
O -1.106827245 1.626300357 1.623324973  
C -2.859097515 1.138527819 -0.015376825  
N -2.915552331 1.098600909 -1.485596563  
H -3.880293800 1.142036320 -1.814429451  
H -2.515035592 0.217470516 -1.823981453  
H -3.606272780 1.875336152 0.323962172  
C -3.167149391 -0.203788024 0.700585848  
H -3.173662246 -0.018571792 1.783293967  
H -4.183613711 -0.508374626 0.407165802  
C -2.168293600 -1.277996286 0.362022108  
C -2.279551342 -2.029127997 -0.818812151  
H -3.164744095 -1.916050254 -1.450274982  
C -1.284130383 -2.940302527 -1.185359709  
H -1.379803188 -3.502323710 -2.114934002  
C -0.170795719 -3.128125624 -0.365580386  
H 0.622130507 -3.817135304 -0.654616867  
C -0.072811419 -2.421908102 0.836354109  
H 0.793168646 -2.580020572 1.478901082

C -1.059303944 -1.504102717 1.192940334  
H -0.975954645 -0.939026449 2.122656957

———— 258\_FGG224: PBE+MBD@rsSCS ————

O 3.401170000 -1.207176000 1.557447000  
C 3.176140000 -0.431635000 0.642554000  
O 3.221900000 -0.809600000 -0.649928000  
H 2.948240000 -0.027560000 -1.235058000  
C 2.855066000 1.054180000 0.880913000  
H 3.670103000 1.652152000 0.438735000  
H 2.840432000 1.223155000 1.961475000  
N 1.580078000 1.501361000 0.330381000  
H 0.806302000 1.789279000 0.958408000  
C 1.351788000 1.620120000 -0.990709000  
O 2.171942000 1.272000000 -1.873884000  
C 0.014390000 2.267190000 -1.365730000  
H -0.042544000 2.275590000 -2.458412000  
H 0.025569000 3.308820000 -1.004664000  
N -1.169578000 1.598910000 -0.843753000  
H -1.806147000 1.095530000 -1.467118000  
C -1.562504000 1.635309000 0.448733000  
O -0.892901000 2.152552000 1.369270000  
C -2.904492000 0.954750000 0.730660000  
N -3.687350000 0.828200000 -0.510489000  
H -4.134656000 1.716580000 -0.744866000  
H -4.432138000 0.138940000 -0.396021000  
H -3.394946000 1.586424000 1.492785000  
C -2.661430000 -0.430450000 1.381439000  
H -2.208610000 -0.250874000 2.366047000  
H -3.650060000 -0.884426000 1.562949000  
C -1.785800000 -1.363235000 0.584068000  
C -0.448180000 -1.561094000 0.955925000  
H -0.059150000 -1.061770000 1.846621000  
C 0.390270000 -2.392318000 0.210887000  
H 1.425020000 -2.536719000 0.519147000  
C -0.097740000 -3.028710000 -0.931596000  
H 0.558530000 -3.667950000 -1.522402000  
C -1.430980000 -2.849930000 -1.308039000  
H -1.821580000 -3.353390000 -2.192969000  
C -2.269920000 -2.031480000 -0.550534000  
H -3.313200000 -1.914720000 -0.848277000

———— 259\_FGG380: PBE+MBD@rsSCS ————

O -2.587075141 -2.629410466 0.693909314  
C -2.765953620 -1.455607208 0.413831647  
O -3.302979021 -0.580777441 1.287123813  
H -3.420853830 0.314969664 0.827843300  
C -2.436312866 -0.885762027 -0.978417149  
H -3.396163819 -0.688287752 -1.485832131  
H -1.899024233 -1.659512870 -1.533531067  
N -1.625932307 0.329230397 -0.992178618  
H -0.660962112 0.305383526 -1.360951699  
C -2.085359182 1.523529924 -0.569902250  
O -3.217048316 1.683082938 -0.051845121  
C -1.125709625 2.702323108 -0.755300249  
H -1.635459005 3.598087538 -0.387902023

```
H -0.910678188  2.821352327 -1.829379754
N  0.132425210  2.538824898 -0.041435708
H  0.341348857  3.062349549  0.811033417
C  1.130950426  1.746463415 -0.503524702
O  1.033706009  1.067040541 -1.544221050
C  2.373425890  1.694594371  0.387196989
N  2.472642276  2.917492347  1.201362988
H  2.877342625  3.687558105  0.665686051
H  3.071808177  2.762925143  2.014128265
H  3.225302307  1.540491974 -0.298380440
C  2.289470436  0.475750263  1.339302529
H  3.234126612  0.452497658  1.909789522
H  1.479863721  0.662134279  2.062282937
C  2.074449021 -0.844939358  0.649136485
C  3.083365058 -1.406848268 -0.144742052
H  4.042313641 -0.893500617 -0.244382724
C  2.872800630 -2.608662613 -0.818600147
H  3.665264911 -3.028273450 -1.439142972
C  1.647602930 -3.271592976 -0.701776349
H  1.481722954 -4.210129561 -1.231592505
C  0.639137349 -2.731070960  0.097472703
H -0.321858967 -3.235255328  0.204745894
C  0.855738446 -1.523471212  0.766419157
H  0.064546748 -1.105989858  1.393775696
```

———— 260\_FGG412: PBE+MBD@rsSCS ————

```
O  3.536522198  0.186883871  0.491102468
C  2.464875495 -0.370026531  0.325861662
O  1.365197286 -0.121830465  1.096173136
H  1.630274476  0.605508686  1.698845703
C  2.221624845 -1.406773438 -0.764754800
H  2.902346979 -2.243781242 -0.554153465
H  2.540931571 -0.952944176 -1.711892228
N  0.874302075 -1.910174555 -0.877582610
H  0.163864286 -1.367439725 -1.379858857
C  0.430444914 -2.890920398 -0.032307272
O  1.170862086 -3.552632718  0.700962474
C -1.094723751 -3.072066608 -0.049173549
H -1.339119325 -3.910623995  0.609932740
H -1.437650223 -3.295093798 -1.069982687
N -1.783475125 -1.875442069  0.411828445
H -1.937813426 -1.702076412  1.407541097
C -2.031243846 -0.818465140 -0.397517792
O -1.754739899 -0.807693704 -1.614113565
C -2.721325502  0.364313794  0.306834619
N -2.426714613  0.323639447  1.747776882
H -1.496225172  0.715533532  1.922854592
H -3.098844964  0.885382605  2.272469686
H -3.803266356  0.174860601  0.197462453
C -2.426037209  1.702683276 -0.415584393
H -2.720756461  1.585470220 -1.467289983
H -3.085329908  2.464526779  0.029177497
C -0.993398364  2.161573131 -0.334555785
C -0.525031519  2.872714758  0.781209814
H -1.219428745  3.132999682  1.583957506
C  0.807889582  3.290526820  0.862502539
```

```

H 1.148756272 3.852396091 1.733304285
C 1.692888536 3.014486651 -0.181381136
H 2.732160182 3.337093264 -0.122310965
C 1.233970278 2.320202044 -1.304537027
H 1.917612778 2.111845345 -2.128928328
C -0.091832771 1.893172487 -1.377224445
H -0.446596661 1.341155891 -2.248645713

```

———— 261\_FGG444: PBE+MBD@rsSCS ————

```

O 2.316359249 -2.662128184 1.084322775
C 2.605287118 -1.701427443 0.389909808
O 2.558100390 -1.746304434 -0.957261598
H 2.819431370 -0.842488511 -1.329153425
C 3.067668689 -0.360331811 0.985221883
H 4.111780670 -0.189856088 0.675356992
H 3.033199854 -0.447084652 2.075049499
N 2.260981078 0.787925396 0.586878082
H 1.567238078 1.198926710 1.237721003
C 2.272990092 1.292042458 -0.663609110
O 2.940130555 0.797965776 -1.603119379
C 1.397112929 2.534019339 -0.859836884
H 1.582751788 2.912349672 -1.869463503
H 1.689797851 3.302088329 -0.126211934
N -0.024427156 2.255812017 -0.715568414
H -0.670649227 2.286417307 -1.511179259
C -0.632676005 2.065135137 0.474797443
O -0.025818780 2.013157103 1.567221829
C -2.163172491 1.944096202 0.394779718
N -2.615597179 1.948731058 -1.005913283
H -3.489009002 2.463160611 -1.111965582
H -2.781739250 0.988057044 -1.323296366
H -2.533833527 2.861296365 0.880893807
C -2.658625875 0.736094192 1.233603515
H -2.164309387 0.784560042 2.213542041
H -3.739970220 0.858827005 1.395296829
C -2.388290966 -0.582732607 0.558465172
C -3.356718129 -1.162366325 -0.276403311
H -4.336612909 -0.687522640 -0.371397287
C -3.094787199 -2.351565462 -0.962126794
H -3.861505699 -2.788691552 -1.602561325
C -1.857698293 -2.981216196 -0.817637105
H -1.650029160 -3.909931539 -1.349758857
C -0.888262033 -2.424616685 0.021143892
H 0.075297145 -2.917140489 0.152325148
C -1.153068357 -1.234429379 0.700136887
H -0.396319013 -0.809837764 1.362796093

```

———— 262\_FGG470: PBE+MBD@rsSCS ————

```

O -2.483188590 0.896916170 1.761023744
C -2.972864521 0.980229756 0.648156694
O -3.823270992 1.987841682 0.279482192
H -3.929288949 2.553148764 1.072817163
C -2.728721128 0.037293352 -0.499964431
H -2.319348868 0.618143930 -1.345969692
H -3.691190742 -0.362440573 -0.857924206
N -1.842709641 -1.028591800 -0.102285520

```

H -1.332384806 -0.966611788 0.788917562  
C -1.568469451 -2.043309448 -0.966364864  
O -2.108589841 -2.160405386 -2.073877759  
C -0.514970457 -3.034958762 -0.450671138  
H -0.449919840 -3.850924394 -1.176992588  
H -0.832670814 -3.434920691 0.524639576  
N 0.797175980 -2.427726941 -0.292360934  
H 1.524207173 -2.510372879 -1.006513054  
C 1.140242965 -1.699832648 0.795370581  
O 0.365085406 -1.473379067 1.744893697  
C 2.592121689 -1.187685349 0.786735142  
N 3.201636660 -1.374220343 -0.539564199  
H 3.024055065 -0.553071894 -1.126526745  
H 4.213425442 -1.482101291 -0.466592006  
H 3.127002947 -1.845266930 1.491966351  
C 2.660133032 0.254440902 1.354557513  
H 2.162154869 0.250128089 2.333363150  
H 3.720553489 0.502158036 1.514747826  
C 2.021229374 1.271543224 0.446540907  
C 0.667622400 1.614720651 0.591023739  
H 0.085462947 1.169979945 1.399059264  
C 0.067724026 2.519017237 -0.286274709  
H -0.979520783 2.793483769 -0.151319177  
C 0.802369462 3.088643742 -1.329537027  
H 0.329244218 3.792803175 -2.014151476  
C 2.151541505 2.764047361 -1.477964446  
H 2.738489562 3.216365621 -2.277905652  
C 2.755025381 1.868467849 -0.591198814  
H 3.820576829 1.647457928 -0.691333663

———— 263\_FGG80: PBE+MBD@rsSCS ————

O 3.871596429 -1.407219590 -0.229791918  
C 3.444352969 -0.276492332 -0.071649740  
O 3.820833605 0.758537673 -0.852179115  
H 3.358674087 1.596869804 -0.526330807  
C 2.459373453 0.091882035 1.049886276  
H 2.966040581 0.792861070 1.733066746  
H 2.204857956 -0.819365523 1.595497111  
N 1.223512753 0.709242650 0.578008909  
H 0.362695944 0.161256989 0.604479443  
C 1.187658842 1.994237556 0.170379760  
O 2.225823903 2.685169321 0.043460063  
C -0.177254767 2.611000617 -0.096315995  
H -0.032963434 3.398712125 -0.847203398  
H -0.509880822 3.083425498 0.842751794  
N -1.213746428 1.689609884 -0.502725151  
H -1.277211164 1.346195145 -1.463710726  
C -2.255499233 1.339994634 0.309909916  
O -2.347345600 1.666937921 1.498383930  
C -3.315595190 0.462820928 -0.371734257  
N -3.184219141 0.513184943 -1.840799905  
H -3.705567073 -0.254179597 -2.269328843  
H -3.589553989 1.378698170 -2.203681170  
H -4.284877114 0.855037471 -0.016978644  
C -3.201896054 -0.986480637 0.154396153  
H -3.553562254 -0.977886537 1.194689120



```

H -3.916750539 -1.604280503 -0.415427273
C -1.825131836 -1.602534399 0.108029054
C -1.184286791 -1.917789952 -1.101340550
H -1.681503707 -1.705182070 -2.048112584
C 0.088524402 -2.491050571 -1.108963365
H 0.576389935 -2.716144792 -2.057809094
C 0.740113093 -2.783126327 0.091997646
H 1.738532938 -3.219064368 0.081431792
C 0.110497972 -2.482041687 1.301858117
H 0.602878662 -2.713578047 2.247740108
C -1.153468083 -1.884765099 1.307683761
H -1.636022304 -1.642503403 2.256432835

```

———— 264\_FGG114: PBE+MBD@rsSCS ————

```

O 3.877400936 1.425711244 -0.173475270
C 3.432897532 0.307869285 0.027214439
O 3.796428571 -0.761632149 -0.709245565
H 3.331178138 -1.584335724 -0.346879415
C 2.444866609 0.002459940 1.168028481
H 2.186905617 0.944562817 1.658620146
H 2.959325566 -0.651865505 1.890391741
N 1.208919416 -0.655198656 0.753688832
H 0.361938902 -0.093518759 0.664309538
C 1.178370933 -1.953578797 0.383340820
O 2.218077605 -2.646996962 0.289845512
C -0.175917453 -2.574363001 0.085771754
H -0.198491273 -3.543357255 0.608542777
H -0.229649563 -2.787450237 -0.993738849
N -1.315147508 -1.752149322 0.414549117
H -1.535525128 -1.460919019 1.371680638
C -2.224471851 -1.349165869 -0.521955822
O -2.160215710 -1.626405500 -1.724361943
C -3.340080677 -0.454257787 0.041058518
N -3.328328417 -0.447474993 1.518112974
H -3.935884018 -1.182171371 1.884221682
H -3.686033338 0.437792978 1.879249643
H -4.282962439 -0.857340511 -0.365569739
C -3.169920703 0.967021988 -0.545736101
H -3.386318903 0.893704696 -1.619659430
H -3.947794066 1.609846094 -0.101898318
C -1.803672390 1.577873505 -0.354644130
C -0.844158555 1.483260854 -1.375805455
H -1.101109082 0.957425688 -2.296567810
C 0.425768547 2.042658007 -1.222361916
H 1.160012667 1.958125735 -2.024067569
C 0.762775639 2.708634139 -0.041021190
H 1.760177151 3.131130705 0.076784734
C -0.179413736 2.801768494 0.986995081
H 0.071125861 3.322714354 1.912099257
C -1.450198660 2.242267039 0.829281616
H -2.180866219 2.341333853 1.634205223

```

———— 265\_FGG357: PBE+MBD@rsSCS ————

```

O -3.625378888 1.734630163 0.226159967
C -3.330217690 0.573742463 -0.001317366
O -3.816561410 -0.454298902 0.723847748

```

H -3.460699303 -1.322745274 0.347795850  
C -2.398742168 0.165797968 -1.157006035  
H -2.029984450 1.075840393 -1.637695672  
H -2.991850585 -0.411339506 -1.884491205  
N -1.251409329 -0.642071252 -0.757133538  
H -0.347463927 -0.185386426 -0.641500451  
C -1.369287542 -1.937433993 -0.392722288  
O -2.479001103 -2.511743374 -0.305766530  
C -0.084756914 -2.690584575 -0.077245506  
H -0.152935935 -3.667391235 -0.577616178  
H -0.058947556 -2.877043964 1.007986688  
N 1.126542568 -1.987620486 -0.423910840  
H 1.440754014 -1.867932028 -1.390995536  
C 2.009974830 -1.531504038 0.513553369  
O 1.876505848 -1.695937636 1.731287008  
C 3.183937519 -0.730415807 -0.080471985  
N 3.090174655 -0.652896322 -1.549433433  
H 2.622495494 0.214088292 -1.830193712  
H 4.015939016 -0.651618918 -1.977009202  
H 4.094096007 -1.293027006 0.177833400  
C 3.250121825 0.647972627 0.634570564  
H 3.400427464 0.462421070 1.706372760  
H 4.133389863 1.183556967 0.256108343  
C 1.999187830 1.459715813 0.415650391  
C 0.915767954 1.353028439 1.305424304  
H 1.012545423 0.710042907 2.180878776  
C -0.273900952 2.043975150 1.071929783  
H -1.106339076 1.949163702 1.769785578  
C -0.410718770 2.851786451 -0.061609363  
H -1.351829901 3.370719122 -0.242932354  
C 0.661365708 2.978459934 -0.947409243  
H 0.574835520 3.622595627 -1.823262157  
C 1.857085253 2.293231032 -0.705762321  
H 2.702872707 2.433255623 -1.383697612

———— 266\_FGG691: PBE+MBD@rsSCS ————

O 2.853821209 -1.535364095 0.222084586  
C 3.866934329 -1.043795938 -0.242994171  
O 5.060760074 -1.709553486 -0.305769310  
H 4.900787036 -2.593718980 0.085508772  
C 3.999935508 0.354688455 -0.832686462  
H 4.354461903 0.265435316 -1.869221385  
H 4.772440188 0.892542751 -0.264974243  
N 2.767477739 1.096736648 -0.762926863  
H 1.957904737 0.766100189 -1.309623148  
C 2.464686384 1.792327061 0.380709289  
O 3.289071658 2.088793751 1.250363297  
C 0.969749943 2.121899931 0.503350646  
H 0.598990922 2.588089708 -0.421403889  
H 0.836719140 2.811667973 1.341937393  
N 0.205689085 0.906959476 0.748535012  
H 0.052324924 0.547824563 1.696130608  
C -0.085311512 0.020697416 -0.227882643  
O 0.162166839 0.214712602 -1.438817097  
C -0.703706963 -1.293980411 0.265679657  
N -1.011498985 -1.227552029 1.702444657

```

H -0.876559622 -2.133345316 2.150127289
H -1.986772920 -0.949275745 1.846868511
H 0.107069905 -2.028034141 0.128470305
C -1.890084870 -1.702380950 -0.643231990
H -1.542099208 -1.661902658 -1.684804763
H -2.156185866 -2.744820067 -0.413715100
C -3.081604503 -0.804780477 -0.442016442
C -4.105839348 -1.161316959 0.447516015
H -4.073370590 -2.138917060 0.934084365
C -5.171630841 -0.294585093 0.704323881
H -5.958975132 -0.591569941 1.397979660
C -5.228172916 0.947468857 0.070347952
H -6.057563648 1.626446207 0.268350997
C -4.217919120 1.311511699 -0.824705977
H -4.258768912 2.277987228 -1.328444520
C -3.155132248 0.444739885 -1.078796873
H -2.364709321 0.733218633 -1.772800014

```

### 11.2.2 GFA: PBE+MBD@rsSCS

———— 236\_GFA15: PBE+MBD@rsSCS ————

```

O -0.823195254 -0.279386606 5.266774702
C 0.025277434 -0.273348718 4.391666520
O 0.912108638 -1.279290042 4.242088476
H 1.516216222 -1.080078510 3.453102045
C 0.201359463 0.897635036 3.390579434
C -0.806801718 2.008840702 3.633442890
H -1.830061567 1.645913930 3.472358454
H -0.739599256 2.359344942 4.668636423
H -0.616183285 2.851384457 2.956123666
H 1.231027937 1.271053004 3.540518763
N 0.103596970 0.446732756 1.997494488
H -0.703066055 0.753168251 1.413491232
C 1.072647723 -0.249252220 1.379597119
O 2.098216149 -0.683318451 1.962472146
C 0.905850858 -0.462855711 -0.127638015
H 1.610799696 -1.265549551 -0.378071503
N -0.413418205 -0.953101696 -0.535302788
H -0.441951406 -1.745052554 -1.190012604
C -1.549360878 -0.219111170 -0.605498564
O -1.759898479 0.841098979 0.021728295
C -2.605395602 -0.808670600 -1.539175503
H -3.108824151 0.051232129 -2.011943516
H -3.358229329 -1.309307616 -0.912379830
N -2.025205260 -1.781063379 -2.473530367
H -2.724700202 -2.441097751 -2.810710060
H -1.621329317 -1.308459872 -3.286625283
C 1.319510678 0.817834267 -0.909211633
H 0.766870974 1.680685720 -0.513448617
H 2.389097848 0.987173081 -0.715291951
C 1.038213833 0.655966332 -2.379122738
C 1.779063094 -0.244385134 -3.158182654
H 2.633256696 -0.763293630 -2.716730986
C 1.432825253 -0.492216244 -4.486999478
H 2.016923699 -1.197455706 -5.078513022
C 0.338821509 0.162006849 -5.062681800
H 0.067220586 -0.033345862 -6.100391086

```

C -0.391544129 1.079178987 -4.302418819  
H -1.234676023 1.608020882 -4.748404003  
C -0.043555060 1.321978680 -2.970660010  
H -0.625995086 2.026810036 -2.373917821

———— 237\_GFA07: PBE+MBD@rsSCS ————

O -0.501479183 0.805726632 5.472455895  
C -0.713923599 0.175568554 4.450833550  
O -1.959098232 -0.162165946 4.059478896  
H -1.910860546 -0.681082080 3.190619141  
C 0.422003796 -0.339368650 3.529989561  
C 1.787800932 0.095980866 4.034149096  
H 2.583275355 -0.330053811 3.409516594  
H 1.870930214 1.190196912 4.021465350  
H 1.926660049 -0.231356942 5.069529904  
H 0.340583043 -1.442256194 3.538692293  
N 0.251615079 0.098946918 2.139332531  
H 0.973360463 0.708681020 1.712420210  
C -0.655219043 -0.432510447 1.298191859  
O -1.574467552 -1.202304744 1.666246607  
C -0.483181927 0.003811772 -0.166553027  
H -0.497635709 1.109293300 -0.170277007  
N 0.817741541 -0.401924900 -0.695592892  
H 0.876254338 -1.099410282 -1.445600739  
C 1.952303112 0.309110799 -0.508698766  
O 2.069811187 1.231499621 0.324843972  
C 3.115123786 -0.108781498 -1.405327752  
H 3.843556702 -0.632367122 -0.768666384  
H 3.603283397 0.824446129 -1.734193974  
N 2.689236699 -1.006325233 -2.487091645  
H 3.459183200 -1.589482092 -2.812272978  
H 2.338600026 -0.482084416 -3.291098324  
C -1.605090000 -0.528023724 -1.065201375  
H -1.657426345 -1.622050374 -0.968087038  
H -2.558240438 -0.139371616 -0.681306707  
C -1.382529510 -0.127163962 -2.501175579  
C -0.944842058 -1.064175663 -3.446301382  
H -0.835454180 -2.111000963 -3.152613141  
C -0.646155508 -0.677429157 -4.755735263  
H -0.310894876 -1.421335202 -5.479232385  
C -0.785053203 0.657402898 -5.140587929  
H -0.558667305 0.960724304 -6.163093705  
C -1.233206230 1.598921150 -4.208426683  
H -1.354568062 2.641231329 -4.504364942  
C -1.529730296 1.208654209 -2.902449513  
H -1.877141115 1.953158607 -2.182036329

———— 238\_GFA10: PBE+MBD@rsSCS ————

O -0.371642510 1.747499946 -3.783272159  
C -0.248200799 1.938425004 -2.587175422  
O -1.277241788 2.352211222 -1.814795838  
H -0.969183901 2.426374185 -0.856782239  
C 1.096290488 1.753239075 -1.833635682  
C 2.211060204 1.340854883 -2.779239995  
H 2.301760265 2.069401354 -3.591583708  
H 3.166965266 1.279047002 -2.243578009

```

H  1.984295882  0.368221495 -3.237638398
H  1.329208953  2.719635835 -1.354858681
N  0.979880723  0.762866019 -0.754145161
H  1.282224037 -0.188806942 -0.965675879
C  0.280810577  0.964074560  0.383579556
O -0.301771726  2.047180896  0.634582692
C  0.176446963 -0.230954921  1.320312416
H  1.112534757 -0.813508922  1.309564261
N -0.037691784  0.245950332  2.663495931
H -0.455381940  1.166017128  2.826194234
C  0.255699618 -0.525305512  3.743522858
O  0.735194681 -1.666034369  3.664698179
C -0.068781134  0.123454128  5.089606483
H  0.765727970 -0.122490203  5.767176676
H -0.950168770 -0.404631812  5.481670609
N -0.379718561  1.555020314  4.980265564
H -1.005287453  1.857518351  5.725986887
H  0.466109701  2.121965863  5.048257962
C -0.971710046 -1.182036980  0.851892518
H -1.015858269 -1.984548234  1.602263246
H -1.919923254 -0.626406572  0.884961425
C -0.712684790 -1.729007460 -0.523149688
C  0.330590157 -2.646914316 -0.727470827
H  0.869702620 -3.046226742  0.134897249
C  0.683245408 -3.046715418 -2.018286540
H  1.495423418 -3.760201361 -2.161194159
C -0.003391589 -2.535051217 -3.123673272
H  0.279430952 -2.837616365 -4.131961158
C -1.056685787 -1.638295567 -2.929411360
H -1.591107479 -1.225402102 -3.784584842
C -1.407892962 -1.241565928 -1.637852885
H -2.211093099 -0.515880650 -1.495013846

```

———— 239\_GFA02: PBE+MBD@rsSCS ————

```

O  2.667635000  0.544931000  1.489993000
C  2.767247000  1.434063000  0.653691000
O  3.749097000  2.372549000  0.687744000
H  4.292752000  2.178028000  1.479815000
C  1.816278000  1.649430000 -0.509969000
C  1.034297000  2.964460000 -0.344212000
H  0.362458000  3.075020000 -1.202637000
H  0.433010000  2.941792000  0.574225000
H  1.717978000  3.820810000 -0.311083000
H  2.406458000  1.708170000 -1.439792000
N  0.956766000  0.488540000 -0.564416000
H  0.969510000 -0.119933000  0.251340000
C  0.259936000  0.110240000 -1.666107000
O  0.228371000  0.760010000 -2.719433000
C -0.544750000 -1.198270000 -1.496877000
H -0.238850000 -1.850730000 -2.327850000
N -0.233630000 -1.893010000 -0.261798000
H -0.617260000 -1.561803000  0.629660000
C  0.822530000 -2.756420000 -0.147634000
O  1.461010000 -3.206160000 -1.104158000
C  1.156570000 -3.123607000  1.303812000
H  2.242150000 -3.311165000  1.330483000

```

```
H 0.661420000 -4.081592000 1.523288000
N 0.679730000 -2.107046000 2.255522000
H 0.550490000 -2.501687000 3.186426000
H 1.357760000 -1.344672000 2.339604000
C -2.055710000 -0.890740000 -1.606203000
H -2.216600000 -0.399620000 -2.575576000
H -2.599810000 -1.846130000 -1.610104000
C -2.532310000 -0.010820000 -0.478749000
C -2.439935000 1.385910000 -0.578188000
H -2.085840000 1.829300000 -1.510626000
C -2.777508000 2.202499000 0.501199000
H -2.696087000 3.285993000 0.406030000
C -3.215489000 1.637043000 1.701762000
H -3.469339000 2.274807000 2.548959000
C -3.329935000 0.249466000 1.807618000
H -3.680720000 -0.200985000 2.736635000
C -2.994020000 -0.565387000 0.724095000
H -3.090300000 -1.650058000 0.811661000
```

———— 240\_GFA11: PBE+MBD@rsSCS ————

```
O -5.192797711 0.571597263 -0.234886121
C -4.025412851 0.917175054 -0.196782198
O -3.616086767 2.004940810 0.490583277
H -2.613150322 2.099903055 0.400073004
C -2.896700317 0.172153807 -0.954263021
C -3.431652008 -1.019466080 -1.731686754
H -4.228028060 -0.696480164 -2.410513464
H -2.629489764 -1.488765357 -2.315912433
H -3.862258204 -1.764654115 -1.050564982
H -2.449739886 0.911989737 -1.642246556
N -1.829802095 -0.266011678 -0.047448337
H -1.758223839 -1.268919829 0.208289713
C -0.912177261 0.567085392 0.475366490
O -0.981038763 1.816310238 0.365536784
C 0.202921354 -0.130998116 1.283679097
H -0.308978514 -0.555209531 2.166659699
N 0.811736167 -1.243808868 0.560735990
H 1.761313348 -1.140973472 0.181664557
C 0.253984007 -2.461708151 0.398590173
O -0.907007214 -2.757949841 0.755236004
C 1.159314503 -3.489575059 -0.277488072
H 0.529398991 -4.053903665 -0.984742682
H 1.455109970 -4.201873017 0.506755054
N 2.359627267 -2.884403891 -0.865103458
H 3.155814290 -3.518990859 -0.840248803
H 2.208033481 -2.618035703 -1.838160947
C 1.291754473 0.849925840 1.759984727
H 0.784967301 1.768453773 2.083795240
H 1.780965414 0.408185473 2.639715433
C 2.336358202 1.157809650 0.712589427
C 3.554933717 0.462388543 0.713913765
H 3.757449369 -0.263481084 1.505038021
C 4.515988391 0.691298943 -0.273654281
H 5.459643098 0.145833625 -0.251827339
C 4.270182936 1.626862723 -1.279247718
H 5.019946958 1.812875349 -2.048314700
```

C 3.064450138 2.334090569 -1.284625302  
H 2.872631609 3.075937111 -2.060832760  
C 2.104530402 2.102846343 -0.299084494  
H 1.160940190 2.648162180 -0.307270032

———— 241\_GFA09: PBE+MBD@rsSCS ————

O 1.696714000 3.786573000 0.410781000  
C 1.916783000 2.600077000 0.249295000  
O 2.365930000 1.810989000 1.250289000  
H 2.451729000 0.861963000 0.918879000  
C 1.727191000 1.875310000 -1.110091000  
C 1.285252000 2.836310000 -2.200476000  
H 1.216318000 2.317060000 -3.164851000  
H 0.308611000 3.274960000 -1.952842000  
H 1.999834000 3.661540000 -2.288164000  
H 2.697320000 1.415120000 -1.363066000  
N 0.754637000 0.778490000 -1.003244000  
H -0.203682000 0.982110000 -1.288329000  
C 0.978300000 -0.369400000 -0.327718000  
O 2.072010000 -0.621067000 0.233990000  
C -0.206550000 -1.317440000 -0.219585000  
H -0.802830000 -1.298020000 -1.146425000  
N 0.283670000 -2.659080000 -0.028929000  
H 1.222600000 -2.818905000 0.345517000  
C -0.474100000 -3.739500000 -0.353201000  
O -1.616700000 -3.661690000 -0.828634000  
C 0.205970000 -5.086590000 -0.105139000  
H 0.444460000 -5.497280000 -1.097254000  
H -0.559830000 -5.751319000 0.327345000  
N 1.442260000 -4.974631000 0.681196000  
H 2.109540000 -5.702303000 0.429538000  
H 1.256890000 -5.068339000 1.680265000  
C -1.144020000 -0.877073000 0.950397000  
H -1.937810000 -1.636796000 0.995325000  
H -0.572510000 -0.917961000 1.888971000  
C -1.710640000 0.495139000 0.722755000  
C -1.221403000 1.603998000 1.425654000  
H -0.475326000 1.457353000 2.209168000  
C -1.641702000 2.895892000 1.105539000  
H -1.226986000 3.747622000 1.644231000  
C -2.565033000 3.095505000 0.076728000  
H -2.887263000 4.104170000 -0.181608000  
C -3.076126000 1.995900000 -0.619388000  
H -3.808181000 2.143930000 -1.414048000  
C -2.652566000 0.704680000 -0.297696000  
H -3.052070000 -0.153190000 -0.843725000

———— 242\_GFA08: PBE+MBD@rsSCS ————

O -0.192205970 5.224507981 -0.570489405  
C -0.176334690 4.056231656 -0.914941996  
O 0.489918672 3.635280828 -2.011212174  
H 0.386254590 2.632817804 -2.102020182  
C -0.940576044 2.940327534 -0.157825982  
C -1.690719165 3.487023760 1.046137543  
H -2.278172655 2.692434131 1.524129996  
H -0.991275951 3.905962065 1.781154170

```

H -2.363295392  4.293561993  0.735593128
H -1.646428085  2.503652685 -0.887349061
N -0.043818190  1.860630085  0.269712635
H  0.203671299  1.772062361  1.273898648
C  0.455294454  0.933306278 -0.567036836
O  0.340543130  1.004373466 -1.815797710
C  1.244181511 -0.196460862  0.130923594
H  2.120930709  0.305939158  0.578480000
N  0.499544938 -0.809544651  1.226700582
H  0.082608615 -1.740254033  1.099878586
C  0.326838867 -0.259194402  2.445987223
O  0.699902056  0.892785316  2.758950027
C -0.414006857 -1.143518164  3.446104905
H -1.384066432 -0.656552566  3.624477037
H  0.139173377 -1.078203665  4.397625360
N -0.631382068 -2.507170139  2.950601202
H  0.098156002 -3.145562837  3.267040138
H -1.525147881 -2.885225849  3.259137233
C  1.734692256 -1.278842642 -0.850375420
H  2.056858130 -0.767988687 -1.767486546
H  2.617224607 -1.760567546 -0.405948199
C  0.700549322 -2.334640246 -1.164359639
C -0.328495529 -2.100929687 -2.089666608
H -0.359590695 -1.147426984 -2.616529665
C -1.301146841 -3.072605977 -2.326278611
H -2.091287980 -2.879209540 -3.052671472
C -1.265066006 -4.292152235 -1.644717235
H -2.024679507 -5.050553630 -1.833979283
C -0.241977644 -4.540051296 -0.729126672
H -0.196270276 -5.494861634 -0.204930212
C  0.731923822 -3.566746904 -0.494319648
H  1.538142500 -3.769940925  0.214379550

```

———— 243\_GFA13: PBE+MBD@rsSCS ————

```

O  1.086753485 -0.522164179 -3.010010354
C  0.072198127 -0.238929140 -3.628632262
O -0.137600467 -0.622223060 -4.921768285
H  0.655036463 -1.132981103 -5.188962774
C -1.093114899  0.610292706 -3.107183915
C -0.944557834  2.051314420 -3.604654385
H -0.909093615  2.083790715 -4.699742179
H -1.799553428  2.646926117 -3.262180548
H -0.024946254  2.503000785 -3.206798731
H -2.017944848  0.164156026 -3.498237076
N -1.124458721  0.581397973 -1.658542107
H -0.493933790  1.235216899 -1.167533295
C -1.358975333 -0.609419607 -1.020689458
O -1.880985772 -1.586922212 -1.567163376
C -0.835168689 -0.663954759  0.427514172
H -1.093136739 -1.666483548  0.793277263
N  0.630373451 -0.614134085  0.379824811
H  1.149593172 -1.496482597  0.314939677
C  1.388901921  0.454130129  0.042006979
O  0.966825510  1.623252799 -0.093029572
C  2.860581068  0.114578645 -0.180783803
H  3.398383497  0.326745090  0.756351364

```



```
H 3.226421893 0.828162518 -0.937115531
N 3.036067655 -1.301647884 -0.526822296
H 2.783190422 -1.449846126 -1.507071569
H 4.002333259 -1.599411410 -0.398761186
C -1.468544045 0.379175476 1.372011704
H -1.299611325 1.389984490 0.981041715
H -2.553609584 0.193246737 1.370221100
C -0.912498996 0.260639683 2.765676887
C -1.394196743 -0.716344055 3.646892600
H -2.222584270 -1.357397500 3.336307661
C -0.829862114 -0.878820351 4.912911570
H -1.218316306 -1.642687153 5.587191997
C 0.229230834 -0.061555837 5.316063168
H 0.674294547 -0.188502855 6.303533517
C 0.711031468 0.921111845 4.448337085
H 1.533376865 1.566891879 4.758246094
C 0.144355278 1.080584215 3.182613873
H 0.525264855 1.842392313 2.499920466
```

———— 244\_GFA12: PBE+MBD@rsSCS ————

```
O 5.214677171 -0.630689153 0.033193009
C 4.314356807 0.157972390 -0.196604540
O 4.141046559 0.715668794 -1.413287019
H 3.333936088 1.326506326 -1.392072152
C 3.306271573 0.629830971 0.883002233
C 3.582623782 -0.021793953 2.228028481
H 2.913302598 0.383364154 2.997767358
H 3.438899914 -1.108227589 2.165251998
H 4.621412334 0.155933858 2.524795131
H 3.424385306 1.726848384 0.950814560
N 1.917849150 0.364318066 0.488981145
H 1.373955984 -0.360948324 0.998482178
C 1.267601574 1.058512813 -0.461655393
O 1.812167726 1.939388626 -1.172621928
C -0.226428640 0.743846296 -0.623701684
H -0.521044732 1.223252762 -1.566443339
N -0.502371875 -0.683518068 -0.797452984
H -0.982552897 -1.005805994 -1.645931262
C -0.439022190 -1.645020760 0.147012702
O 0.071081530 -1.513323644 1.281729643
C -1.067641382 -2.973479893 -0.275551627
H -1.943263548 -3.108558530 0.376613923
H -0.355788031 -3.769456756 -0.007106288
N -1.475023063 -2.992912405 -1.687201436
H -0.829299909 -3.534204077 -2.260565895
H -2.407069325 -3.383485046 -1.811166359
C -1.046646891 1.380001373 0.529560978
H -0.668404206 1.007420370 1.491030677
H -0.858620388 2.464012919 0.494086571
C -2.516435747 1.081077912 0.400551238
C -3.304800183 1.739060456 -0.553632335
H -2.860225518 2.521259789 -1.173498542
C -4.652038841 1.412273486 -0.714865958
H -5.253192431 1.934680330 -1.459704387
C -5.233438853 0.420182445 0.079692174
H -6.285850438 0.165414082 -0.045141454
```

C -4.459083069 -0.235729629 1.039176986  
H -4.908944525 -1.002916450 1.670685136  
C -3.110584823 0.092389602 1.196331182  
H -2.505465592 -0.419983934 1.947248281

———— 245\_GFA06: PBE+MBD@rsSCS ————

O 0.731633662 5.400088543 0.812797903  
C 0.837713248 4.386751822 0.144193695  
O 2.023931594 3.961458092 -0.337539477  
H 1.887163310 3.104160528 -0.859586013  
C -0.374589071 3.507709356 -0.256819687  
C -1.678940166 4.051045411 0.302349794  
H -2.526892728 3.447219242 -0.046214537  
H -1.663991803 4.044844491 1.399681007  
H -1.820692605 5.088264347 -0.018677789  
H -0.398277801 3.513585204 -1.362421783  
N -0.199063806 2.111985569 0.164064712  
H -0.863066412 1.702358458 0.845634514  
C 0.613639137 1.248086649 -0.474146006  
O 1.440990923 1.596684309 -1.350068374  
C 0.449804900 -0.215070739 -0.031000972  
H 0.551176081 -0.230992547 1.069543343  
N -0.892492321 -0.703470120 -0.340184910  
H -1.038567557 -1.428253763 -1.051280230  
C -1.962146370 -0.476643353 0.453058450  
O -1.963693305 0.321328640 1.413709219  
C -3.199261581 -1.299191726 0.096748222  
H -4.070789110 -0.628718960 0.165768435  
H -3.312424747 -2.036897894 0.904746613  
N -3.065302314 -1.997550451 -1.189559226  
H -3.510930785 -2.913275121 -1.169592314  
H -3.490446303 -1.465607440 -1.948773478  
C 1.507089395 -1.126087824 -0.659633478  
H 1.443066920 -1.050608101 -1.755104945  
H 2.495101432 -0.732867762 -0.382303807  
C 1.339378508 -2.553196445 -0.207179197  
C 1.679476758 -2.932088187 1.099193742  
H 2.120280976 -2.196351854 1.776004867  
C 1.461950254 -4.235995649 1.543943795  
H 1.735202663 -4.515134368 2.561791874  
C 0.899095349 -5.186615944 0.687144322  
H 0.735766003 -6.208001040 1.030912179  
C 0.560255337 -4.821677158 -0.616634275  
H 0.127485000 -5.558330400 -1.293826739  
C 0.780213072 -3.514701455 -1.057883429  
H 0.518677264 -3.237063361 -2.081810021

———— 246\_GFA16: PBE+MBD@rsSCS ————

O -5.179338353 0.218789455 -1.487772271  
C -4.323720445 0.409326784 -0.638005371  
O -4.137817683 1.609412156 -0.059138252  
H -3.397224131 1.544795427 0.638262236  
C -3.447789767 -0.757644753 -0.124809296  
C -4.013523674 -1.294852727 1.198093774  
H -3.464408335 -2.196315892 1.499751397  
H -3.928730492 -0.547976045 1.996758842

H -5.071852073 -1.554807215 1.068497203  
 H -3.538069670 -1.532328438 -0.895644193  
 N -2.010132847 -0.466124983 -0.028612751  
 H -1.349116219 -1.030630736 -0.602909564  
 C -1.444962034 0.424896895 0.802102305  
 O -2.082030263 1.262529592 1.492177398  
 C 0.084255576 0.458637150 0.833998530  
 H 0.330878947 0.949025500 1.784493151  
 N 0.748660882 -0.846606854 0.877337749  
 H 1.523363267 -0.955147111 1.544527659  
 C 0.879431224 -1.710795083 -0.157712066  
 O 0.130733825 -1.753561095 -1.157379911  
 C 2.050609793 -2.680514220 -0.008642661  
 H 2.456194768 -2.824869061 -1.024245788  
 H 1.640931525 -3.650887248 0.308615044  
 N 3.020206407 -2.212959685 0.988772416  
 H 3.672441571 -1.541519796 0.574790104  
 H 3.566080534 -2.982950580 1.372782316  
 C 0.617985678 1.347350231 -0.328654096  
 H 0.188971305 0.999006708 -1.277915949  
 H 0.251506041 2.369356435 -0.152207915  
 C 2.120962508 1.294235596 -0.393474191  
 C 2.759996551 0.578490874 -1.415067939  
 H 2.158370897 0.130712495 -2.208527274  
 C 4.149075451 0.422573332 -1.419366820  
 H 4.631449993 -0.130784820 -2.226039037  
 C 4.920407396 0.979299986 -0.395804856  
 H 6.003952754 0.858927620 -0.396904671  
 C 4.293383321 1.709465416 0.619336701  
 H 4.889955457 2.160597909 1.412606203  
 C 2.906868980 1.866602708 0.617275520  
 H 2.427166336 2.437858073 1.415627325

———— 247\_GFA03: PBE+MBD@rsSCS ————

O -3.028799694 0.612401108 -1.594181211  
 C -3.018693131 1.365558541 -0.634006383  
 O -4.153600555 1.835781156 -0.041160712  
 H -4.900583697 1.456711663 -0.549954878  
 C -1.769601861 1.918413331 0.024592720  
 C -1.610585777 3.418797036 -0.268770305  
 H -2.463814539 3.980164726 0.131155201  
 H -0.693223600 3.773040664 0.214999038  
 H -1.537016213 3.596488208 -1.349649336  
 H -1.853847034 1.783575286 1.115679790  
 N -0.649770423 1.124578641 -0.454496848  
 H -0.870144317 0.458336033 -1.195904944  
 C 0.463612294 0.955108412 0.306204273  
 O 0.707383235 1.633743796 1.315309782  
 C 1.374943297 -0.187326837 -0.129868325  
 H 1.233797773 -0.425307435 -1.196627028  
 N 2.746822841 0.224930684 0.060238947  
 H 2.968334841 0.914520710 0.783070636  
 C 3.773501603 -0.366493717 -0.600793647  
 O 3.630771416 -1.265843311 -1.442581254  
 C 5.159756434 0.160254643 -0.221468981  
 H 5.723221469 0.264451403 -1.164155726

```
H 5.649536795 -0.645949587 0.344352369
N 5.114100332 1.368283614 0.613129509
H 5.940911552 1.448818133 1.203014040
H 5.060445068 2.213593808 0.043978426
C 1.045428436 -1.460357055 0.705740936
H 1.714707594 -2.252444128 0.340612692
H 1.304282692 -1.245091289 1.752503109
C -0.396884880 -1.866795994 0.591274849
C -0.861438613 -2.547119690 -0.543739430
H -0.149756936 -2.848633318 -1.315477934
C -2.217537210 -2.841099898 -0.694364812
H -2.563206353 -3.365327836 -1.585636920
C -3.131056463 -2.463205170 0.292436766
H -4.190215990 -2.691733986 0.173296031
C -2.679012577 -1.795558010 1.433140031
H -3.383979669 -1.506098631 2.213674899
C -1.322535582 -1.499210808 1.578405429
H -0.971685549 -0.969583897 2.466641203
```

———— 248\_GFA01: PBE+MBD@rsSCS ————

```
O -1.580870000 -0.547590000 -3.076591000
C -0.609820000 -1.286200000 -3.059676000
O 0.027630000 -1.706830000 -4.190516000
H -0.462120000 -1.306570000 -4.939167000
C 0.019710000 -1.873570000 -1.811226000
C -0.270890000 -3.378550000 -1.700022000
H 0.194900000 -3.753170000 -0.781434000
H -1.352330000 -3.561920000 -1.654962000
H 0.150030000 -3.916610000 -2.558245000
H 1.111620000 -1.732680000 -1.869952000
N -0.483870000 -1.115410000 -0.676666000
H -1.222450000 -0.443890000 -0.889452000
C 0.257560000 -0.981603000 0.455710000
O 1.258140000 -1.673332000 0.698406000
C -0.177490000 0.147317000 1.385175000
H -1.238050000 0.405838000 1.232702000
N -0.006840000 -0.285801000 2.753233000
H 0.677220000 -1.015456000 2.969100000
C -0.669873000 0.297642000 3.783521000
O -1.494629000 1.214114000 3.650410000
C -0.344420000 -0.288749000 5.159710000
H -1.207640000 -0.909167000 5.442239000
H -0.326529000 0.559931000 5.863556000
N 0.863050000 -1.124696000 5.161334000
H 1.702640000 -0.566841000 5.318661000
H 0.827260000 -1.837537000 5.888072000
C 0.685432000 1.409374000 1.080871000
H 0.328983000 2.202760000 1.753435000
H 1.725368000 1.169761000 1.346553000
C 0.591794000 1.827370000 -0.359380000
C 1.575753000 1.440610000 -1.280783000
H 2.447989000 0.885990000 -0.927288000
C 1.442532000 1.741780000 -2.637497000
H 2.217602000 1.432430000 -3.340121000
C 0.317767000 2.433080000 -3.094347000
H 0.207011000 2.663660000 -4.154334000
```

C -0.666461000 2.827480000 -2.184965000  
H -1.548162000 3.364900000 -2.534748000  
C -0.528638000 2.528310000 -0.828597000  
H -1.301743000 2.837110000 -0.121162000

———— 249\_GFA14: PBE+MBD@rsSCS ————

O 0.398686850 -3.095691159 -0.701172878  
C 0.084097190 -2.627496158 -1.785688258  
O 0.613680724 -3.076372852 -2.958732018  
H 1.252724513 -3.777140242 -2.711426796  
C -0.999214166 -1.559469757 -1.999293214  
C -0.882854078 -0.782067376 -3.311543180  
H -0.920491266 -1.461265725 -4.170816660  
H -1.715262305 -0.071133896 -3.382844929  
H 0.060612385 -0.226504807 -3.338536516  
H -1.944765689 -2.128096618 -2.006358112  
N -1.057843066 -0.689926461 -0.829634128  
H -1.737581582 -0.921461540 -0.095352851  
C 0.090185002 -0.092036210 -0.384252719  
O 1.136670464 -0.046565285 -1.043097843  
C -0.004585925 0.389463429 1.077538302  
H -1.033467826 0.714276020 1.295230221  
N 0.255253877 -0.796623904 1.891686958  
H 1.215933893 -1.145670502 1.986634053  
C -0.689719662 -1.760360069 2.064021622  
O -1.894970257 -1.608850768 1.789839527  
C -0.142991293 -3.074312174 2.616283874  
H -0.780843111 -3.868520324 2.194231961  
H -0.298238915 -3.075966352 3.705880222  
N 1.291820854 -3.212053905 2.333360629  
H 1.420868156 -3.489867383 1.357016609  
H 1.722325732 -3.920253187 2.926532367  
C 0.981924527 1.514867250 1.381600615  
H 1.013535487 1.655683809 2.472180822  
H 1.983369045 1.206432579 1.046511896  
C 0.567639580 2.792839696 0.697560514  
C -0.392519802 3.626774927 1.287273099  
H -0.798199657 3.368674138 2.268513211  
C -0.837190271 4.777459551 0.635329975  
H -1.585259102 5.414864443 1.107654042  
C -0.325131249 5.110546065 -0.621179227  
H -0.675667883 6.005723474 -1.135530526  
C 0.636455240 4.289643265 -1.214299572  
H 1.040535928 4.543103034 -2.195049627  
C 1.078923115 3.138487103 -0.560292017  
H 1.808874543 2.480907869 -1.033609446

———— 250\_GFA05: PBE+MBD@rsSCS ————

O -2.039099480 1.478774201 -1.737168617  
C -2.276412369 0.431356070 -2.311531746  
O -2.843160391 0.372361025 -3.553688622  
H -2.972144513 1.301232919 -3.838722222  
C -2.052794881 -0.979155208 -1.754858960  
C -3.355835132 -1.517067527 -1.157699407  
H -3.205013741 -2.542616737 -0.798290553  
H -3.681883985 -0.893988730 -0.312557511

H -4.149057622 -1.525094640 -1.913831303  
H -1.735971734 -1.608262187 -2.598869384  
N -1.007526373 -0.977388692 -0.749628855  
H -1.295213772 -0.888553551 0.225411405  
C 0.248818585 -0.548478182 -1.077371954  
O 0.607281913 -0.371283770 -2.248500040  
C 1.168729918 -0.278692524 0.112796751  
H 1.169671589 -1.146845535 0.793953016  
N 2.504963097 -0.089705681 -0.395478643  
H 2.635869225 0.036590310 -1.403104520  
C 3.590697650 -0.204866657 0.408193020  
O 3.526450899 -0.443316163 1.625532384  
C 4.933835004 -0.032509703 -0.301207872  
H 5.378592016 -1.036841704 -0.363951422  
H 5.576124814 0.551443807 0.379882983  
N 4.803318121 0.512192628 -1.658579624  
H 4.731191765 1.530387734 -1.639859727  
H 5.613124334 0.277327165 -2.231310967  
C 0.680931171 0.958743621 0.929928345  
H 1.544974296 1.277543855 1.530370153  
H 0.421945218 1.771800150 0.236558211  
C -0.472230720 0.634853339 1.840530758  
C -1.757073000 1.150190522 1.616037576  
H -1.921373863 1.819438275 0.770413422  
C -2.822822287 0.785388895 2.443481099  
H -3.816394194 1.195551916 2.258363642  
C -2.618844310 -0.101216446 3.502919346  
H -3.450977046 -0.389959898 4.145004027  
C -1.339028883 -0.611934248 3.740635256  
H -1.169135483 -1.295651598 4.572648509  
C -0.274882909 -0.245077696 2.917554431  
H 0.727723071 -0.636143356 3.106119611

———— 251\_GFA04: PBE+MBD@rsSCS ————

O 1.749194138 1.460431302 -2.100152673  
C 2.333487020 0.406747712 -2.276675059  
O 3.589244373 0.326580782 -2.811164994  
H 3.873954856 1.249027266 -2.979955769  
C 1.771364851 -0.993079437 -2.007418333  
C 1.193219533 -1.572926696 -3.300551783  
H 0.349788162 -0.962998746 -3.654607889  
H 1.959773906 -1.598641943 -4.083501749  
H 0.837494429 -2.595728184 -3.124311470  
H 2.607389997 -1.613997144 -1.655537561  
N 0.749619769 -0.952198099 -0.978936104  
H -0.219871679 -0.857630877 -1.284050472  
C 1.065663406 -0.498342502 0.271713709  
O 2.234900277 -0.321036339 0.636845983  
C -0.132317005 -0.210367365 1.177000629  
H -0.800656441 -1.087920232 1.205599494  
N 0.364613825 0.023266550 2.510415536  
H 1.361416689 0.212159323 2.645463826  
C -0.440741764 -0.093068331 3.594166935  
O -1.649924152 -0.369900691 3.528639021  
C 0.246375638 0.164773870 4.935727091  
H -0.170020779 -0.569996941 5.645427176

```

H -0.097915186  1.153011287  5.274829156
N  1.711110267  0.180387353  4.841259781
H  2.099255384 -0.759736480  4.922729072
H  2.128035870  0.747906232  5.577460564
C -0.969784999  0.997570568  0.653070114
H -1.587913870  1.317887798  1.504203916
H -0.291045784  1.821521865  0.390415270
C -1.857427299  0.636805210 -0.507696749
C -1.619941700  1.135505734 -1.797190427
H -0.779858169  1.812489145 -1.959148079
C -2.424572297  0.743503324 -2.870817892
H -2.227565377  1.141124386 -3.867365501
C -3.474998464 -0.154821086 -2.670546319
H -4.100220135 -0.464184875 -3.508418950
C -3.723519083 -0.652823327 -1.387523283
H -4.545891128 -1.349340394 -1.221621327
C -2.922438521 -0.259288762 -0.315550747
H -3.119728559 -0.644181255  0.687735858

```

### 11.2.3 GGF: PBE+MBD@rsSCS

———— 221\_GGF14: PBE+MBD@rsSCS ————

```

O -4.266090000 -0.642020000 -1.307375000
C -3.487880000 -0.182320000 -0.488191000
O -3.899702000  0.481540000  0.608606000
H -3.096939000  0.751429000  1.172379000
C -1.964850000 -0.396670000 -0.627194000
H -1.807820000 -0.687840000 -1.673061000
N -1.157356000  0.810810000 -0.428289000
H -0.505512000  1.092910000 -1.184240000
C -0.988185000  1.452351000  0.743909000
O -1.682634000  1.245948000  1.769545000
C  0.120438000  2.508128000  0.736907000
H  0.154646000  2.959595000  1.732983000
H -0.144852000  3.287527000  0.003742000
N  1.433551000  1.975170000  0.408889000
H  2.160706000  1.849097000  1.119357000
C  1.813091000  1.632990000 -0.842355000
O  1.060809000  1.685820000 -1.838682000
C  3.258803000  1.162450000 -0.958323000
H  3.795851000  1.934850000 -1.527883000
H  3.243677000  0.258590000 -1.589347000
N  3.895093000  0.974050000  0.351570000
H  4.890705000  1.188008000  0.318377000
H  3.791007000  0.005614000  0.660956000
C -1.535220000 -1.568945000  0.292395000
H -1.858780000 -1.365973000  1.322343000
H -2.086670000 -2.457790000 -0.051849000
C -0.050880000 -1.826016000  0.271895000
C  0.600520000 -2.224920000 -0.904868000
H  0.025040000 -2.355160000 -1.823950000
C  1.973440000 -2.469820000 -0.914904000
H  2.460500000 -2.788530000 -1.837172000
C  2.721520000 -2.326877000  0.258891000
H  3.790480000 -2.546300000  0.256581000
C  2.085080000 -1.922786000  1.435509000
H  2.655380000 -1.816699000  2.359736000

```

C 0.711380000 -1.665886000 1.436042000  
H 0.216860000 -1.346906000 2.355630000

———— 222\_GGF13: PBE+MBD@rsSCS ————

O -4.260388034 -1.251765500 0.710514143  
C -3.482395133 -0.452558925 0.216619150  
O -3.894705118 0.619353107 -0.487007080  
H -3.092463399 1.170971838 -0.782178411  
C -1.958790336 -0.583591908 0.431311386  
H -1.796280092 -1.616328562 0.763524004  
N -1.155179229 -0.429904350 -0.785237916  
H -0.519610818 -1.204249617 -1.053181121  
C -0.987145779 0.715112515 -1.474208030  
O -1.678497839 1.749720483 -1.304157563  
C 0.118302589 0.668310752 -2.533800515  
H 0.165866071 1.653862978 -3.007148641  
H -0.159549242 -0.076767838 -3.296793157  
N 1.427071077 0.329947351 -1.998238700  
H 2.150538804 1.037459429 -1.836648122  
C 1.777509366 -0.913316565 -1.604105404  
O 1.018095354 -1.904866178 -1.655437737  
C 3.185157434 -1.023564693 -1.030730076  
H 3.666424711 -1.887440462 -1.513579091  
H 3.051413278 -1.292617275 0.027677680  
N 3.954708650 0.223251215 -1.150012183  
H 4.703735463 0.141610261 -1.835953423  
H 4.375552055 0.484988166 -0.259984144  
C -1.531342588 0.382584294 1.567973885  
H -1.842691950 1.404211762 1.311939996  
H -2.097550978 0.083562460 2.463104429  
C -0.051397999 0.355547988 1.842315208  
C 0.762469296 1.427302027 1.452456554  
H 0.308044934 2.285377616 0.953081733  
C 2.135695662 1.415105003 1.707735937  
H 2.748035392 2.268194554 1.412841839  
C 2.718271432 0.320893861 2.351270905  
H 3.787423610 0.314273112 2.569256703  
C 1.918488161 -0.762000922 2.731505938  
H 2.363739109 -1.617397939 3.240701467  
C 0.546502151 -0.742344667 2.478206374  
H -0.071703063 -1.586729372 2.790563983

———— 223\_GGF07: PBE+MBD@rsSCS ————

O 4.119445000 1.429488000 0.622291000  
C 3.441091000 0.439315000 0.400804000  
O 3.911640000 -0.831704000 0.566363000  
H 4.839270000 -0.725283000 0.865032000  
C 2.005861000 0.488170000 -0.110101000  
H 2.097865000 0.734330000 -1.183684000  
N 1.312790000 -0.778170000 -0.057742000  
H 0.903410000 -1.107553000 0.830665000  
C 0.896310000 -1.409680000 -1.192594000  
O 1.203310000 -1.063830000 -2.340878000  
C -0.042730000 -2.591670000 -0.906133000  
H 0.436890000 -3.286520000 -0.199728000  
H -0.233020000 -3.110520000 -1.850676000



```

N -1.310160000 -2.148550000 -0.341276000
H -2.136470000 -1.996220000 -0.927075000
C -1.463160000 -1.762855000 0.945696000
O -0.551980000 -1.783080000 1.799550000
C -2.871310000 -1.286591000 1.293730000
H -2.748920000 -0.403289000 1.942338000
H -3.328880000 -2.074107000 1.910687000
N -3.693520000 -1.050141000 0.099558000
H -3.595180000 -0.080220000 -0.212892000
H -4.680560000 -1.218992000 0.287700000
C 1.232427000 1.598283000 0.625172000
H 1.217914000 1.369804000 1.702812000
H 1.807594000 2.530858000 0.519402000
C -0.184715000 1.787644000 0.142406000
C -1.187068000 2.117376000 1.065575000
H -0.930994000 2.196069000 2.123969000
C -2.501199000 2.345500000 0.653417000
H -3.261751000 2.611796000 1.388428000
C -2.840105000 2.231750000 -0.698387000
H -3.862742000 2.420410000 -1.027933000
C -1.853491000 1.883520000 -1.625300000
H -2.106724000 1.779480000 -2.680708000
C -0.539138000 1.665560000 -1.209539000
H 0.206936000 1.376720000 -1.951241000

```

———— 224\_GGF12: PBE+MBD@rsSCS ————

```

O 1.495276591 -3.083932750 -0.083956003
C 0.974638660 -1.873541591 0.280039447
O 1.668081858 -0.894524611 0.498185153
H 2.468305861 -2.968633206 -0.103044431
C -0.556184981 -1.937187706 0.335370091
H -0.811360768 -2.859825323 0.877260840
N -1.084895525 -0.808776237 1.071386842
H -1.289906038 0.058163105 0.562586693
C -0.787930802 -0.691208670 2.408079767
O -0.357176401 -1.628043038 3.087001260
C -0.960653918 0.730182788 2.961081052
H -0.806418584 0.699623365 4.044196972
H -1.963611740 1.119761421 2.737600200
N 0.016717106 1.614206262 2.340917306
H 1.005194320 1.559605032 2.604651479
C -0.198842166 2.151652075 1.111775033
O -1.305673117 2.137234601 0.540031741
C 1.043110478 2.747323549 0.454697296
H 1.009678610 3.838122277 0.597303812
H 0.930570568 2.559386646 -0.627358015
N 2.274078568 2.218031179 1.055416098
H 3.078118751 2.802740193 0.831844308
H 2.456583149 1.272096305 0.709534774
C -1.145543276 -2.019612061 -1.093978392
H -0.815100061 -2.970616109 -1.533683111
H -2.238974557 -2.065828904 -0.988826454
C -0.744892543 -0.867137171 -1.980447726
C 0.441344845 -0.925879398 -2.728392983
H 1.042527767 -1.837484898 -2.711403873
C 0.857208067 0.162756221 -3.494113524

```

```
H 1.780330063 0.099502583 -4.070928011
C 0.090271805 1.331059133 -3.524889993
H 0.414655220 2.183457217 -4.122483941
C -1.096526017 1.397165429 -2.793754095
H -1.698316006 2.305268111 -2.801885207
C -1.512166946 0.303063224 -2.033081823
H -2.440738845 0.369360961 -1.463152583
```

———— 225\_GGF10: PBE+MBD@rsSCS ————

```
O -1.253288124 4.228500254 0.164840202
C -0.172276707 3.432106651 0.454675056
O 0.778177101 3.817032791 1.107537565
H -1.073194665 5.090621538 0.593682020
C -0.371841846 2.037109098 -0.119590308
H -0.672999191 2.154690853 -1.172497158
N 0.860623331 1.288129285 -0.122531676
H 1.233890725 0.903839723 0.758281932
C 1.406382677 0.818471814 -1.281384608
O 1.007513597 1.110439342 -2.416231015
C 2.559990060 -0.166646856 -1.038203409
H 3.305139233 0.287520079 -0.367270919
H 3.026526902 -0.387210398 -2.003282965
N 2.087306063 -1.407582349 -0.440288570
H 1.866294235 -2.230074607 -1.008582923
C 1.772750186 -1.531064959 0.869697706
O 1.886636774 -0.614379787 1.708481693
C 1.256118105 -2.913147006 1.262521391
H 0.420003554 -2.744982668 1.961555228
H 2.057955304 -3.400043983 1.836900083
N 0.913176034 -3.735606824 0.094901746
H 1.042672518 -4.727914109 0.286221828
H -0.065492337 -3.590389206 -0.167403944
C -1.483197784 1.314730243 0.676809084
H -1.203626708 1.297309956 1.742370222
H -2.401276278 1.918783684 0.603195422
C -1.753619613 -0.097095958 0.214818877
C -2.055989302 -1.085544265 1.161371434
H -2.051005460 -0.827524967 2.222217646
C -2.363241959 -2.389447838 0.767896511
H -2.607268242 -3.139969161 1.520946847
C -2.356843175 -2.730165777 -0.588120519
H -2.607145566 -3.744290454 -0.902621234
C -2.035538108 -1.757153125 -1.539052718
H -2.014404742 -2.013386075 -2.598605746
C -1.739748946 -0.452570168 -1.141747047
H -1.474145645 0.284158228 -1.901097732
```

———— 226\_GGF15: PBE+MBD@rsSCS ————

```
O 3.878670000 -1.552350000 -0.935275000
C 3.363850000 -0.712470000 -0.218844000
O 4.071206000 0.277566000 0.365900000
H 3.447694000 0.851414000 0.920826000
C 1.858150000 -0.702606000 0.133900000
H 1.810480000 -0.776252000 1.235886000
N 1.218124000 0.565180000 -0.224227000
H 0.559847000 0.612880000 -1.017639000
```

C	1.330234000	1.663536000	0.550029000
O	2.163293000	1.756357000	1.482819000
C	0.368851000	2.803373000	0.217545000
H	0.645464000	3.216730000	-0.765630000
H	0.501335000	3.579808000	0.977459000
N	-1.026410000	2.398095000	0.176006000
H	-1.646320000	2.503696000	0.983727000
C	-1.574347000	1.746720000	-0.877792000
O	-0.930124000	1.418650000	-1.894453000
C	-3.061541000	1.445530000	-0.724654000
H	-3.246759000	0.494050000	-1.247488000
H	-3.604721000	2.228330000	-1.275687000
N	-3.478939000	1.461621000	0.683976000
H	-4.468163000	1.690889000	0.773905000
H	-3.340454000	0.536565000	1.100441000
C	1.109430000	-1.873140000	-0.499370000
H	1.190180000	-1.805300000	-1.594165000
H	1.640780000	-2.794210000	-0.217758000
C	-0.339340000	-1.945260000	-0.081256000
C	-0.702340000	-1.976868000	1.274157000
H	0.071160000	-1.954108000	2.044501000
C	-2.041420000	-2.047939000	1.657763000
H	-2.300810000	-2.078760000	2.716748000
C	-3.048300000	-2.099733000	0.687420000
H	-4.094980000	-2.176579000	0.984082000
C	-2.699600000	-2.074640000	-0.665188000
H	-3.475080000	-2.124950000	-1.430588000
C	-1.356950000	-1.989930000	-1.041871000
H	-1.093320000	-1.954000000	-2.099948000

———— 227\_GGF04: PBE+MBD@rsSCS ————

O	-0.315411344	1.086395807	3.917055349
C	0.485390231	0.314474855	3.426244228
O	1.567905662	-0.175374102	4.115752498
H	1.519517554	0.230665579	5.006256007
C	0.472073083	-0.223215659	2.000368224
H	0.556684377	-1.319769652	2.069115660
N	-0.781301675	0.056832630	1.345024661
H	-0.961097816	0.995381085	0.959108535
C	-1.621053911	-0.943104266	0.949889874
O	-1.476145168	-2.137743655	1.239897924
C	-2.755527419	-0.441160997	0.044521891
H	-3.265639682	0.411059400	0.518470548
H	-3.467943857	-1.259595827	-0.096460855
N	-2.246064495	-0.017875002	-1.252219138
H	-2.223411698	-0.651603254	-2.055769570
C	-1.621232204	1.165926377	-1.451903413
O	-1.465312512	2.033280316	-0.568513100
C	-1.107086148	1.374343609	-2.874136466
H	-0.115809043	1.848241421	-2.778945070
H	-1.770398801	2.112988877	-3.347483399
N	-1.109556849	0.132883831	-3.659278537
H	-0.213945149	-0.351243432	-3.555945438
H	-1.249356122	0.319642319	-4.651139908
C	1.669860841	0.360301402	1.219683783
H	1.609965014	1.460318662	1.246397604

```
H 2.591137915 0.086627122 1.757386923
C 1.767413446 -0.090681182 -0.218448395
C 2.295369818 0.789695379 -1.173339348
H 2.575741025 1.799944371 -0.868906334
C 2.468162762 0.395169614 -2.500482123
H 2.891264764 1.093969462 -3.223054488
C 2.101017501 -0.893655676 -2.899790590
H 2.248460496 -1.212325272 -3.932710423
C 1.553462979 -1.772710341 -1.960763775
H 1.253101451 -2.776655634 -2.262379316
C 1.387088013 -1.374918961 -0.632536189
H 0.942178963 -2.074348206 0.076880167
```

———— 227\_GGF04r: PBE+MBD@rsSCS ————

```
O -0.255719000 1.079813000 3.924390000
C 0.518765000 0.285604000 3.427215000
O 1.577864000 -0.255241000 4.114856000
H 1.545965000 0.140706000 5.010338000
C 0.495479000 -0.233746000 1.994767000
H 0.565534000 -1.331911000 2.051740000
N -0.754600000 0.067082000 1.342209000
H -0.925730000 1.009329000 0.961854000
C -1.609198000 -0.922868000 0.953056000
O -1.482859000 -2.116824000 1.253058000
C -2.738354000 -0.410505000 0.047187000
H -3.249162000 0.435872000 0.530544000
H -3.450328000 -1.227391000 -0.105063000
N -2.231031000 0.029742000 -1.244409000
H -2.214997000 -0.591698000 -2.057754000
C -1.619187000 1.221021000 -1.437149000
O -1.453844000 2.077232000 -0.544862000
C -1.138409000 1.453171000 -2.867527000
H -0.161483000 1.958474000 -2.789947000
H -1.833999000 2.172643000 -3.323667000
N -1.122998000 0.215857000 -3.658643000
H -0.219418000 -0.254911000 -3.561657000
H -1.271539000 0.404739000 -4.648670000
C 1.697652000 0.338727000 1.211542000
H 1.644306000 1.438961000 1.233111000
H 2.619201000 0.059435000 1.745985000
C 1.777753000 -0.125088000 -0.224027000
C 2.213294000 0.767295000 -1.213103000
H 2.439636000 1.798373000 -0.935911000
C 2.362391000 0.358072000 -2.539594000
H 2.714816000 1.066756000 -3.290264000
C 2.061830000 -0.958274000 -2.902088000
H 2.191262000 -1.288363000 -3.934006000
C 1.601271000 -1.849951000 -1.928356000
H 1.348838000 -2.874610000 -2.202033000
C 1.461138000 -1.437779000 -0.602065000
H 1.085380000 -2.147585000 0.136795000
```

———— 228\_GGF08: PBE+MBD@rsSCS ————

```
O -4.009734820 -0.713968510 -0.627645416
C -2.838965355 -0.927445471 0.055191505
O -2.401086148 -2.040879170 0.279304689
```

```

H -4.347776092 -1.605840276 -0.851789221
C -2.200454649 0.383108046 0.472488471
H -2.949378135 0.931088653 1.070347701
N -1.052871637 0.084097240 1.301572714
H -0.657451606 -0.868961856 1.292850025
C -0.397568745 1.063487136 1.978429063
O -0.772883009 2.244530849 2.018968829
C 0.872249761 0.579215519 2.696793733
H 0.609407635 -0.234098955 3.391068933
H 1.271143987 1.425519651 3.264647941
N 1.891729271 0.090394144 1.781471590
H 2.672000366 0.675511480 1.475941916
C 1.846059182 -1.144900333 1.228398118
O 0.940347504 -1.969809531 1.450010287
C 3.006922478 -1.471086542 0.292554744
H 2.563499887 -1.950436970 -0.596001208
H 3.609167921 -2.240131913 0.797727507
N 3.845083872 -0.301601195 -0.009555933
H 3.513477917 0.160121134 -0.858810006
H 4.816962770 -0.568903721 -0.158469213
C -1.867258178 1.296656473 -0.746157142
H -2.737478485 1.291572506 -1.417997772
H -1.755872481 2.313799071 -0.351460254
C -0.613348180 0.909836485 -1.485342638
C 0.510093607 1.745627884 -1.432931246
H 0.462155444 2.659868362 -0.838410716
C 1.674437482 1.429409715 -2.136753650
H 2.525394185 2.112273702 -2.107659055
C 1.741661734 0.252079315 -2.886501666
H 2.643314494 0.006671237 -3.449664447
C 0.635429801 -0.602326110 -2.926500774
H 0.677600703 -1.522894350 -3.509144561
C -0.531892408 -0.271300270 -2.238313224
H -1.391310074 -0.941470425 -2.296252626

```

———— 229\_GGF11: PBE+MBD@rsSCS ————

```

O -0.555980000 3.600750000 -0.944154000
C 0.486038000 3.038200000 -0.306028000
O 1.641795000 3.342790000 -0.550659000
H -1.427920000 3.230130000 -0.575906000
C 0.087203000 2.022719000 0.797753000
H -0.500800000 2.606430000 1.528301000
N -0.787855000 0.967807000 0.288553000
H -0.394004000 0.029404000 0.209987000
C -2.085614000 1.142090000 -0.023915000
O -2.636417000 2.268100000 -0.039819000
C -2.875670000 -0.120270000 -0.346778000
H -3.569835000 0.118650000 -1.162778000
H -3.471290000 -0.365453000 0.547276000
N -2.068070000 -1.273260000 -0.672051000
H -1.698080000 -1.437650000 -1.612870000
C -1.797320000 -2.269350000 0.226751000
O -2.161790000 -2.256606000 1.407033000
C -1.002870000 -3.429700000 -0.375744000
H -1.721880000 -4.248690000 -0.525939000
H -0.295610000 -3.768223000 0.398413000

```

```
N -0.383600000 -3.082050000 -1.662250000
H  0.556000000 -2.702600000 -1.517123000
H -0.295380000 -3.899870000 -2.264089000
C  1.300690000  1.399945000  1.513008000
H  2.062981000  2.186818000  1.590366000
H  0.994153000  1.123848000  2.531419000
C  1.870662000  0.180796000  0.825456000
C  2.646107000  0.291890000 -0.341039000
H  2.850873000  1.282980000 -0.747499000
C  3.146270000 -0.848960000 -0.968675000
H  3.748970000 -0.746620000 -1.871537000
C  2.891470000 -2.119080000 -0.439561000
H  3.308660000 -3.006580000 -0.917101000
C  2.122530000 -2.240124000  0.719968000
H  1.929960000 -3.223144000  1.151027000
C  1.607450000 -1.098203000  1.340431000
H  1.002850000 -1.201291000  2.244482000
```

———— 230\_GGF09: PBE+MBD@rsSCS ————

```
O -0.299760909 -2.092187966 -2.221573500
C -0.203502842 -0.996501436 -2.742534222
O  0.366803779 -0.807251645 -3.976538892
H  0.635482404 -1.698646391 -4.281548492
C -0.670291846  0.317850840 -2.147812460
H -1.346476746  0.789497466 -2.881432592
N -1.400453362  0.031226777 -0.930875668
H -1.330391411 -0.909451693 -0.515032491
C -2.076695031  1.004466390 -0.264101946
O -2.215876713  2.161576788 -0.687491987
C -2.650067878  0.550663971  1.088674668
H -3.348587355 -0.284605588  0.926411235
H -3.193263929  1.398988679  1.516677789
N -1.626075037  0.108100723  2.022126969
H -1.176721309  0.750970147  2.677636378
C -1.067318951 -1.125146086  1.953740524
O -1.415629940 -1.997234231  1.136961415
C  0.075561860 -1.366855169  2.933968231
H  0.987555132 -1.407729984  2.319232359
H -0.065349933 -2.375631363  3.354322397
N  0.216128902 -0.299769604  3.937132395
H  1.196699901 -0.129447459  4.156869702
H -0.257943264 -0.541152349  4.807541162
C  0.512476238  1.314439492 -1.942012186
H  1.075517730  1.362719252 -2.884537227
H  0.057402320  2.297741282 -1.769772677
C  1.414132338  0.962906038 -0.789229392
C  2.376860915 -0.052222799 -0.891274285
H  2.496253101 -0.593361932 -1.832073391
C  3.195943830 -0.373135465  0.192076330
H  3.940858686 -1.163271736  0.093197264
C  3.072441474  0.325679518  1.396712616
H  3.728104038  0.087727070  2.235769543
C  2.119492034  1.340926423  1.510043215
H  2.017401964  1.897155648  2.442595586
C  1.294381412  1.649284770  0.427112769
H  0.548877399  2.442179621  0.515570861
```

## ——— 231\_GGF01: PBE+MBD@rsSCS ———

O 2.077544427 -2.993368703 0.952113806  
C 1.097587713 -2.298565573 0.732117035  
O 0.298050894 -1.885851713 1.730376709  
H -0.434217541 -1.258558757 1.468189050  
C 0.782974878 -1.879292502 -0.728190003  
H 0.695575242 -2.828483027 -1.276236886  
N -0.449530054 -1.139767165 -0.897323227  
H -0.396135048 -0.125737876 -0.821756439  
C -1.685005850 -1.718168689 -0.889083618  
O -1.884876752 -2.931646898 -0.962018923  
C -2.858790818 -0.734513602 -0.756440959  
H -3.532030341 -1.179746316 -0.009427416  
H -3.397830162 -0.694986438 -1.711493346  
N -2.489572691 0.617234406 -0.367427638  
H -2.697164651 1.440186111 -0.940974552  
C -1.936000487 0.903154338 0.836704400  
O -1.619424196 0.037978264 1.675837692  
C -1.701050910 2.388476942 1.094121252  
H -0.702575526 2.476064659 1.553258737  
H -2.427057774 2.691719695 1.862617477  
N -1.881416015 3.202845467 -0.115400635  
H -0.983203082 3.344540768 -0.583103263  
H -2.262887555 4.121482609 0.105694740  
C 1.963008202 -1.060733967 -1.301553746  
H 2.885098622 -1.591896048 -1.030105828  
H 1.883058536 -1.056372506 -2.397799173  
C 1.979212257 0.358476559 -0.786342735  
C 2.380133448 0.649314201 0.528240826  
H 2.731488857 -0.155688216 1.175647241  
C 2.332495875 1.955644379 1.015220955  
H 2.646225057 2.160692168 2.038813185  
C 1.895567797 3.001622291 0.196118648  
H 1.879243504 4.024779273 0.573439514  
C 1.504020672 2.727937446 -1.116515856  
H 1.191878804 3.538955794 -1.776836336  
C 1.538477981 1.415178330 -1.597683144  
H 1.236612686 1.206333299 -2.626237542

## ——— 232\_GGF06: PBE+MBD@rsSCS ———

O -0.548696473 1.560623797 4.086602001  
C -0.392565476 0.528628453 3.464037441  
O -0.630051937 -0.692081383 4.016698670  
H -0.454524647 -1.347260259 3.298424214  
C 0.111486110 0.492366652 2.012592402  
H 1.191189118 0.708613001 2.080029088  
N -0.001034320 -0.836118110 1.414765156  
H -0.872613216 -1.067244611 0.896620415  
C 1.123361520 -1.491368562 0.948044664  
O 2.277667387 -1.189181521 1.254984466  
C 0.789146228 -2.637787344 -0.017904778  
H 0.036208419 -3.301666777 0.434781487  
H 1.707009869 -3.204255175 -0.201861389  
N 0.274626979 -2.138874078 -1.284997001  
H 0.870076876 -2.042323422 -2.113796827  
C -0.983309230 -1.672098176 -1.450036375

O -1.834796766 -1.620699801 -0.536185066  
C -1.298869827 -1.206509745 -2.867586180  
H -1.897461097 -0.285934830 -2.769645194  
H -1.956965874 -1.968326267 -3.310910333  
N -0.088548611 -1.059523591 -3.684127911  
H 0.276163122 -0.105953480 -3.610387387  
H -0.274015885 -1.249395880 -4.667750898  
C -0.606161414 1.563550162 1.182401454  
H -1.682441273 1.329506670 1.152419886  
H -0.520410141 2.510451326 1.737550000  
C -0.098162162 1.734464361 -0.228313200  
C -0.992895646 2.137678438 -1.230779233  
H -2.045050555 2.283030747 -0.977745670  
C -0.560387337 2.357908658 -2.539047281  
H -1.272654478 2.680876423 -3.299562703  
C 0.784090133 2.164239094 -2.873263348  
H 1.128675921 2.341975785 -3.892800438  
C 1.682889632 1.750433910 -1.886311109  
H 2.732742822 1.591331240 -2.134835898  
C 1.246418317 1.539783791 -0.576623054  
H 1.968423910 1.209180506 0.171149929

———— 233\_GGF03: PBE+MBD@rsSCS ————

O -1.494518597 -2.232743948 0.699152150  
C -2.110681221 -1.293272560 1.173515517  
O -3.462779341 -1.313281101 1.372571481  
H -3.767587327 -2.189237587 1.055628415  
C -1.506501214 0.036708507 1.580456999  
H -1.791367591 0.263461420 2.619981788  
N -0.068339307 -0.090202644 1.517864737  
H 0.317954471 -0.730370654 0.827081480  
C 0.761763905 0.719191452 2.228822682  
O 0.366373985 1.546667437 3.058197773  
C 2.258732817 0.540623560 1.941237370  
H 2.741509818 0.215850668 2.873217931  
H 2.649299375 1.536259512 1.689048029  
N 2.582856254 -0.361725040 0.857365038  
H 2.645408174 -1.376518597 0.976379231  
C 2.794026648 0.075548999 -0.419266284  
O 2.792732953 1.264478781 -0.760243735  
C 2.985616657 -1.053175270 -1.434715729  
H 3.790247494 -0.741009105 -2.118740129  
H 2.060929644 -1.073022576 -2.032524894  
N 3.193911579 -2.367593936 -0.806713638  
H 4.185383649 -2.597101946 -0.741159875  
H 2.740379075 -3.113336120 -1.332057106  
C -2.041490752 1.190793274 0.676754055  
H -3.129931893 1.254099872 0.811724179  
H -1.598936209 2.116228675 1.070094117  
C -1.679577167 0.986949158 -0.769293001  
C -0.430057127 1.400265210 -1.252427924  
H 0.259384796 1.937483880 -0.600376728  
C -0.043213160 1.122733020 -2.564715125  
H 0.939860605 1.446770634 -2.906751253  
C -0.907958494 0.434483567 -3.418700393  
H -0.610768097 0.220914824 -4.445842954



C -2.162810274 0.031926150 -2.954142796  
H -2.846719582 -0.496978940 -3.618649581  
C -2.543312987 0.305394521 -1.639513480  
H -3.524680560 -0.013594094 -1.281838347

———— 234\_GGF02: PBE+MBD@rsSCS ————

O 1.871230579 -2.675512262 0.811434727  
C 0.845089917 -2.920923880 -0.055173330  
O 0.956597131 -3.662653036 -1.017453919  
H 2.638103090 -3.184655025 0.475136441  
C -0.441753903 -2.209275963 0.341654665  
H -1.023374485 -2.964100290 0.904482491  
N -0.173222715 -1.094062540 1.229794925  
H 0.768475449 -0.672653748 1.274624750  
C -1.171080294 -0.461469508 1.900277961  
O -2.354256767 -0.829525132 1.903247819  
C -0.685879342 0.777418738 2.675385276  
H 0.081904708 0.466982480 3.401605728  
H -1.544664597 1.187439094 3.215499709  
N -0.124915297 1.812413969 1.817906497  
H -0.662455008 2.641564321 1.552950114  
C 1.110785158 1.745916171 1.273253167  
O 1.897135740 0.790763968 1.437752228  
C 1.496710142 2.948747632 0.416879785  
H 1.965069772 2.543039744 -0.495344234  
H 2.284937173 3.484482246 0.965774904  
N 0.366360105 3.852422706 0.162291802  
H -0.098691430 3.597640553 -0.711312268  
H 0.672365180 4.820985596 0.083217178  
C -1.295910477 -1.835318240 -0.897580721  
H -1.237928513 -2.681547797 -1.597082866  
H -2.334004815 -1.743944928 -0.555820079  
C -0.875781982 -0.552616208 -1.567074141  
C -1.684428774 0.587090798 -1.464507110  
H -2.613971491 0.526611983 -0.895584921  
C -1.323123253 1.783612418 -2.088382464  
H -1.985728703 2.648698756 -2.022249514  
C -0.127724302 1.865697928 -2.807441976  
H 0.154847518 2.794242889 -3.305723925  
C 0.695467298 0.739397540 -2.903285553  
H 1.626319643 0.790689462 -3.469089813  
C 0.319417714 -0.459672750 -2.296993098  
H 0.953283832 -1.341012685 -2.405360236

———— 235\_GGF05: PBE+MBD@rsSCS ————

O -1.951825995 0.817192574 1.994967809  
C -2.342454925 1.139304420 0.886404004  
O -3.670264316 1.238341626 0.564659623  
H -4.163546180 1.019484530 1.382630099  
C -1.467420577 1.464075957 -0.309033955  
H -1.728654520 2.472915762 -0.667038936  
N -0.082467608 1.482921114 0.106799229  
H 0.208379249 0.803283748 0.820005209  
C 0.824505112 2.253207580 -0.561517933  
O 0.509310945 3.040228922 -1.462990304  
C 2.288337973 2.098209616 -0.126939104

```

H 2.644905735 3.079369636 0.215827441
H 2.870892786 1.826317019 -1.016990419
N 2.508009635 1.076779870 0.879636226
H 1.979370667 1.168773065 1.747101490
C 2.783593811 -0.225023385 0.525578272
O 3.291903255 -0.552486155 -0.550250248
C 2.359093187 -1.235932620 1.598448415
H 3.028311605 -1.132894260 2.466468973
H 2.511453783 -2.239278611 1.174527490
N 0.974507479 -0.953697380 2.019294538
H 0.309934447 -1.472431479 1.438099071
H 0.805009328 -1.227270937 2.986505261
C -1.711990671 0.476598464 -1.491443728
H -2.784243703 0.480035476 -1.729990509
H -1.173900359 0.892157882 -2.354264017
C -1.221654039 -0.911046828 -1.181093698
C 0.081392541 -1.294932651 -1.528289674
H 0.721573811 -0.599848806 -2.073973649
C 0.578438232 -2.551010355 -1.174439570
H 1.600322967 -2.816557761 -1.445162463
C -0.224639639 -3.444258933 -0.460695802
H 0.157813028 -4.427736613 -0.185663692
C -1.527883140 -3.075204778 -0.110861305
H -2.163163588 -3.770087081 0.439228451
C -2.021359960 -1.819801753 -0.471090513
H -3.042109356 -1.542022876 -0.200184084

```

#### 11.2.4 WGG: PBE+MBD@rsSCS

———— 206\_WGG06: PBE+MBD@rsSCS ————

```

O -1.744711986 -3.470522003 -0.034940062
C -0.597472839 -3.191999996 0.295570404
O 0.417325032 -3.209320784 -0.581256454
H 1.256280820 -2.839485220 -0.130022937
C -0.221624697 -2.797808669 1.731852055
H 0.505213462 -3.535488760 2.111884098
H -1.127677755 -2.842532019 2.342565344
N 0.344308068 -1.457270726 1.849028676
H -0.165658961 -0.707355825 2.354862391
C 1.563190070 -1.136468983 1.376700068
O 2.277547212 -1.925543438 0.710507201
C 2.065539179 0.261422186 1.751509997
H 3.041198369 0.389727027 1.272819088
H 2.200510657 0.290554485 2.845282848
N 1.206191689 1.366153481 1.352773571
H 1.461878909 1.956297458 0.557477244
C 0.022821403 1.665467155 1.934644768
O -0.499714656 0.979736357 2.840667338
C -0.675968519 2.905686741 1.376508730
H -1.158904606 3.384829543 2.247249402
N 0.289246674 3.786847779 0.698039144
H 0.849385937 4.303905005 1.378860631
H -0.206139796 4.478289177 0.131756537
C -1.806479894 2.468700291 0.399974009
H -2.094427945 3.364164288 -0.180103632
H -2.680273396 2.206403471 1.012279994
C -1.497113387 1.308080396 -0.492780499

```

```

C -2.135643611  0.086370413 -0.410389766
H -2.936032277 -0.226923799  0.253678678
N -1.613779167 -0.791952429 -1.335768034
H -1.835232996 -1.785731145 -1.369993310
C -0.588816774 -0.167023558 -2.015870307
C  0.281610058 -0.675692720 -2.984147622
H  0.219387050 -1.715529729 -3.305025711
C  1.246101335  0.185824789 -3.495710897
H  1.948534319 -0.179238754 -4.245130032
C  1.335383395  1.522714932 -3.054107646
H  2.098505332  2.173905407 -3.481728501
C  0.477416362  2.021498938 -2.079587002
H  0.580135952  3.048339257 -1.730771909
C -0.501673020  1.172977981 -1.527308897

```

———— 207\_WGG08: PBE+MBD@rsSCS ————

```

O  0.481563865  3.235111591  2.023820954
C  0.709754844  3.076115554  0.831239947
O -0.217862686  3.328765057 -0.107449024
H  0.133139009  3.013857237 -1.013788216
C  2.062303834  2.570037451  0.303625741
H  2.734682740  2.449116278  1.157236782
H  2.480821313  3.329856017 -0.377250801
N  1.972961108  1.291915878 -0.398019395
H  2.408905904  0.440678202 -0.006577818
C  1.371720157  1.165217872 -1.597700461
O  0.775276300  2.108489627 -2.171529177
C  1.473843949 -0.218989143 -2.239582950
H  2.534734721 -0.452562059 -2.415280374
H  0.955030513 -0.172437915 -3.201919600
N  0.900075801 -1.298628426 -1.446467709
H -0.073758742 -1.554369354 -1.608405948
C  1.536351385 -1.836200161 -0.374683458
O  2.637312501 -1.407509652  0.032389620
C  0.831898062 -2.999939809  0.317786252
H  0.042557086 -3.377468027 -0.351724127
N  1.824714286 -4.061980867  0.488039904
H  2.660337824 -3.663620529  0.926435561
H  1.462924593 -4.791793224  1.105008554
C  0.166193770 -2.502565649  1.634947003
H  0.967705083 -2.308244059  2.364692463
H -0.432188926 -3.343315484  2.027735448
C -0.659652682 -1.269764632  1.455479200
C -0.462771013 -0.061250271  2.092452728
H  0.249433850  0.204836416  2.867520190
N -1.335666830  0.888214985  1.599503849
H -1.283829454  1.878271617  1.831005158
C -2.086774613  0.324432119  0.590718455
C -3.023958359  0.904165022 -0.268012783
H -3.272707315  1.962844232 -0.196224067
C -3.607368805  0.087716094 -1.232403675
H -4.333442896  0.512184555 -1.925317210
C -3.276191832 -1.280023356 -1.328738961
H -3.769079053 -1.895460857 -2.081612835
C -2.339086696 -1.855282579 -0.474770445
H -2.116235564 -2.921414854 -0.549794721

```

C -1.708410031 -1.050371896 0.494842948

———— 208\_WGG04: PBE+MBD@rsSCS ————

O -1.420766765 2.288539583 -1.976504032  
C -0.801357324 2.569354541 -0.961443249  
O -1.367999549 3.254843436 0.049914830  
H -0.676850032 3.398878756 0.778318701  
C 0.683303147 2.206598332 -0.758958810  
H 1.256616346 3.148472989 -0.737282589  
H 1.009544059 1.607210023 -1.613600140  
N 0.965584914 1.449367486 0.461100066  
H 1.252094264 0.470600347 0.370917864  
C 0.877624763 1.993690136 1.694093530  
O 0.501820068 3.175277210 1.885455263  
C 1.199631238 1.065650041 2.865321936  
H 1.105414869 1.650691621 3.785978691  
H 2.224933389 0.678779229 2.773836136  
N 0.296450523 -0.069805003 2.894864231  
H -0.664731658 0.011708354 3.236398104  
C 0.564140992 -1.210823976 2.205608044  
O 1.648304416 -1.418477917 1.635049577  
C -0.593389706 -2.222739016 2.184520662  
H -0.361685078 -2.968761862 2.963323124  
N -1.845752074 -1.554084870 2.577581486  
H -2.250539086 -1.085192312 1.759949424  
H -2.530622159 -2.233898668 2.910111646  
C -0.639874512 -2.953426548 0.819144856  
H -1.439885041 -3.707713438 0.880163113  
H 0.303932751 -3.501405297 0.689383963  
C -0.852093385 -2.043429833 -0.352278642  
C -2.040035548 -1.469690078 -0.770505190  
H -3.046425101 -1.582437489 -0.376395947  
N -1.828933735 -0.716159094 -1.912840508  
H -2.473055341 -0.026132693 -2.284866539  
C -0.491279271 -0.769501188 -2.245686212  
C 0.195950492 -0.165452142 -3.303937504  
H -0.318406077 0.484214799 -4.010689964  
C 1.563901926 -0.401277513 -3.393112589  
H 2.134726763 0.055946369 -4.201822407  
C 2.228175674 -1.217339976 -2.450301987  
H 3.302157330 -1.376685970 -2.549395617  
C 1.540266381 -1.818993729 -1.402705245  
H 2.065086559 -2.426350271 -0.666700049  
C 0.154657576 -1.599023370 -1.284630027

———— 209\_WGG03: PBE+MBD@rsSCS ————

O -2.010452746 3.223895815 0.493219741  
C -0.816843107 3.069599965 0.718433988  
O 0.117798621 3.327712125 -0.212023614  
H 1.026682971 3.017046774 0.133572941  
C -0.282157573 2.561554202 2.067502453  
H -1.132507321 2.433578150 2.743154312  
H 0.396910741 3.323150309 2.485483813  
N 0.425570345 1.287405368 1.968382982  
H 0.036718750 0.430384147 2.397752436  
C 1.622029251 1.166199288 1.359769832

```

O  2.196392720  2.113888580  0.770116989
C  2.260803215 -0.221521657  1.443519805
H  2.462877210 -0.456455115  2.499618011
H  3.210518998 -0.175844390  0.901076954
N  1.452715769 -1.300501702  0.885874693
H  1.575535324 -1.526335841 -0.102332891
C  0.374504546 -1.828154967  1.526732383
O -0.018469716 -1.400407640  2.634324645
C -0.321849007 -3.005305706  0.828390025
H  0.353051542 -3.398485547  0.052440923
N -0.623586024 -4.100573090  1.750218944
H  0.239814247 -4.536294185  2.082032226
H -1.091002321 -3.714786134  2.576847766
C -1.628939453 -2.523327034  0.156107666
H -2.370662693 -2.345429589  0.950395549
H -2.005613420 -3.365012682 -0.446366917
C -1.452919621 -1.277797442 -0.649984840
C -2.100379103 -0.077112193 -0.445659093
H -2.878809273  0.175884719  0.267787320
N -1.616884928  0.882132931 -1.313265776
H -1.855034481  1.870212018 -1.253675415
C -0.604361642  0.331641253 -2.069189935
C  0.246708519  0.922884309 -3.006212071
H  0.165171605  1.982102309 -3.250279147
C  1.216458402  0.116142691 -3.595059320
H  1.903656212  0.548537459 -4.321862077
C  1.325255069 -1.252199953 -3.269759914
H  2.081446602 -1.859540151 -3.767615697
C  0.478018335 -1.839505579 -2.333845493
H  0.557856254 -2.907109242 -2.118444406
C -0.496242823 -1.044300572 -1.698130788

```

———— 210\_WGG05: PBE+MBD@rsSCS ————

```

O -0.861557709 -1.770542274  0.286380062
C -1.797949349 -1.252533704 -0.298177799
O -2.561690085 -1.923714868 -1.215330363
H -2.199612803 -2.833204024 -1.249872650
C -2.288206923  0.179621280 -0.138957017
H -3.375640501  0.148522003  0.015674672
H -2.095793480  0.716114828 -1.079577333
N -1.640037241  0.859502150  0.954158591
H -0.768804097  1.359619643  0.764918997
C -1.887383468  0.450245086  2.239250754
O -2.847652917 -0.262244200  2.547532589
C -0.819278632  0.888569787  3.249278284
H -1.161226644  0.609871921  4.251117164
H -0.649383138  1.973212758  3.198838450
N  0.438195609  0.222409965  2.944395941
H  0.539963785 -0.785263338  3.097449904
C  1.311206885  0.736219606  2.039975112
O  1.224992908  1.893645160  1.588128069
C  2.435717085 -0.231323539  1.632126024
H  3.268177552 -0.022726549  2.326595559
N  2.004149273 -1.614031494  1.872235642
H  2.798217239 -2.254937353  1.855275253
H  1.340674221 -1.903078382  1.143615931

```

C 2.953572702 0.082484532 0.202912122  
H 3.907348770 -0.454606963 0.082481558  
H 3.180444188 1.157398579 0.155452465  
C 2.024860190 -0.298666770 -0.907011519  
C 1.949866162 -1.541701325 -1.501621577  
H 2.530732756 -2.438271802 -1.306281578  
N 0.979893023 -1.541407361 -2.490327837  
H 0.767427953 -2.319504397 -3.101726752  
C 0.411107339 -0.285669320 -2.564247924  
C -0.587415041 0.203250067 -3.411857016  
H -1.062594969 -0.433563600 -4.158875282  
C -0.957782614 1.536852886 -3.262476671  
H -1.734661958 1.952173201 -3.904515447  
C -0.342851279 2.358429605 -2.292178401  
H -0.658213514 3.397966290 -2.201511520  
C 0.651825002 1.869076019 -1.451626324  
H 1.109773184 2.503447524 -0.693343438  
C 1.045319533 0.522950375 -1.572817693

———— 211\_WGG02: PBE+MBD@rsSCS ————

O 1.991742618 -1.150099747 -2.871177253  
C 2.502805048 -0.348375741 -2.095716412  
O 3.749992648 -0.500917834 -1.630355980  
H 3.921913706 0.206284354 -0.921339945  
C 1.769462473 0.900809162 -1.578042280  
H 0.809054112 0.999689994 -2.092309690  
H 2.387817586 1.785337079 -1.796450083  
N 1.523713756 0.843904155 -0.141607882  
H 0.597426888 0.575406766 0.192304100  
C 2.517939809 0.991634333 0.760171564  
O 3.713150914 1.157825710 0.421133613  
C 2.130303188 0.931541094 2.232139336  
H 2.565428320 1.811608792 2.725665553  
H 2.613323107 0.037041920 2.655644493  
N 0.712523412 0.834277401 2.475573851  
H 0.086516235 1.645579857 2.494497081  
C 0.095843678 -0.359454089 2.732983396  
O 0.693938709 -1.436864213 2.831558022  
C -1.435793735 -0.250215455 2.841334607  
H -1.685148943 -0.495528748 3.885863709  
N -1.883544632 1.130819730 2.576602935  
H -2.713693442 1.357850794 3.123185030  
H -2.130937510 1.244365222 1.589141657  
C -2.066226750 -1.328579812 1.922369532  
H -3.160118182 -1.283592162 2.042720506  
H -1.736783265 -2.311467648 2.284946896  
C -1.681153665 -1.163413007 0.484040010  
C -0.637458589 -1.807278892 -0.157022235  
H 0.061128892 -2.536599058 0.241890533  
N -0.555162480 -1.392422730 -1.472791256  
H 0.219849388 -1.592979170 -2.112477320  
C -1.526499144 -0.440528426 -1.703233844  
C -1.805193903 0.299496116 -2.857339400  
H -1.219978918 0.165411779 -3.768079657  
C -2.866518576 1.198837802 -2.803287407  
H -3.110587003 1.793331940 -3.683612116

C -3.643702299 1.341740266 -1.634331396  
H -4.484996787 2.034776873 -1.637088327  
C -3.361525388 0.608081581 -0.486737279  
H -3.989649225 0.715811381 0.400193558  
C -2.272172055 -0.284977368 -0.493740221

———— 212\_WGG14: PBE+MBD@rsSCS ————

O -1.300204956 -3.591255090 -0.148617730  
C -0.703829394 -2.909544842 -0.970494992  
O -1.351090468 -2.187235825 -1.901405752  
H -0.665399845 -1.697086476 -2.470269345  
C 0.834213380 -2.821322370 -1.026672741  
H 1.168499099 -3.235792612 -1.991101961  
H 1.241609762 -3.426954625 -0.212884335  
N 1.359819527 -1.461958484 -0.897910011  
H 1.692738213 -1.168960213 0.024739996  
C 1.223058195 -0.551961645 -1.883464193  
O 0.612939309 -0.813785060 -2.951498805  
C 1.772295190 0.841698153 -1.644582572  
H 2.387569375 1.116422500 -2.516664299  
H 2.395557232 0.913573922 -0.742102166  
N 0.632845974 1.727721832 -1.482417092  
H -0.275776315 1.485116377 -1.889104561  
C 0.607689503 2.740471042 -0.577120033  
O 1.598391520 3.160919889 0.036589795  
C -0.803410407 3.282853144 -0.305083181  
H -0.701768512 4.378330152 -0.210010498  
N -1.743452174 2.876965133 -1.363516672  
H -2.707205981 2.911851251 -1.027225829  
H -1.680167117 3.504927193 -2.166515203  
C -1.268381249 2.746973612 1.074097950  
H -2.282081034 3.140777845 1.255394403  
H -0.616984621 3.206854901 1.831158903  
C -1.252272152 1.258007482 1.237423554  
C -2.285110794 0.375941401 0.992597681  
H -3.288439355 0.569035445 0.624341806  
N -1.895674199 -0.915676397 1.299058448  
H -2.401104462 -1.762263915 1.052613434  
C -0.584904592 -0.898285335 1.728801046  
C 0.245359612 -1.949896143 2.130754710  
H -0.119513232 -2.976257098 2.146938359  
C 1.559657429 -1.634513873 2.470159186  
H 2.237892161 -2.428744134 2.784135568  
C 2.025365299 -0.300053559 2.425529462  
H 3.059509572 -0.088164610 2.699431550  
C 1.184501360 0.747725280 2.058114772  
H 1.559787022 1.770021103 2.014212860  
C -0.145089873 0.459185649 1.697618489

———— 213\_WGG15: PBE+MBD@rsSCS ————

O -1.520656439 -3.334780857 0.739677387  
C -2.237503166 -2.433368194 0.316261095  
O -3.263220855 -1.950545654 1.027719647  
H -3.716193529 -1.202298302 0.498857485  
C -2.041101590 -1.814031372 -1.079067849  
H -2.914094105 -2.100810845 -1.689986073

H -1.143374589 -2.255737486 -1.521513059  
N -1.894038883 -0.362182341 -1.103680633  
H -0.995190898 0.069197632 -1.389791657  
C -2.891654223 0.484980674 -0.789199617  
O -4.013728657 0.107689332 -0.367360366  
C -2.576668499 1.971165478 -0.983417558  
H -3.471644252 2.533329053 -0.699855428  
H -2.359745948 2.149742957 -2.049528347  
N -1.448815566 2.436042410 -0.187888680  
H -1.574876638 3.118565445 0.562171495  
C -0.160532594 2.181710534 -0.529200542  
O 0.158330402 1.454588057 -1.490674186  
C 0.878066519 2.799095299 0.404353260  
H 1.794464853 2.901575284 -0.202277907  
N 0.377092387 4.065952490 0.963672394  
H 0.494838166 4.837125357 0.304046889  
H 0.895447361 4.309315793 1.810136069  
C 1.161892179 1.833371516 1.587900865  
H 0.315510885 1.920274814 2.288637666  
H 2.052667862 2.223125898 2.111723947  
C 1.346505006 0.407605616 1.199506275  
C 0.454357620 -0.616214172 1.439918976  
H -0.482289199 -0.603978877 1.990558231  
N 0.906842194 -1.785882969 0.861706960  
H 0.357967761 -2.646598219 0.834868647  
C 2.101557960 -1.533565527 0.217499163  
C 2.924639463 -2.381284225 -0.530321509  
H 2.670045039 -3.431017988 -0.680886795  
C 4.082864184 -1.834664273 -1.075394632  
H 4.746041333 -2.466471200 -1.666149757  
C 4.417302378 -0.478605356 -0.875714795  
H 5.336656114 -0.088539411 -1.312553423  
C 3.595204470 0.362530229 -0.135070706  
H 3.866551203 1.410379769 0.007358094  
C 2.414617290 -0.156185370 0.422099974

———— 214\_WGG01: PBE+MBD@rsSCS ————

O -3.063120000 -1.219220000 -1.344281000  
C -2.446730000 -0.379300000 -1.990869000  
O -2.552505000 0.933170000 -1.735640000  
H -1.914308000 1.443920000 -2.342922000  
C -1.500760000 -0.749910000 -3.143945000  
H -1.885190000 -0.290530000 -4.068884000  
H -1.508090000 -1.837280000 -3.261283000  
N -0.123830000 -0.312710000 -2.934743000  
H 0.605130000 -0.976410000 -2.612585000  
C 0.236196000 0.986820000 -2.969214000  
O -0.578536000 1.923890000 -3.147872000  
C 1.729314000 1.240370000 -2.747657000  
H 1.922454000 2.299200000 -2.944802000  
H 2.313914000 0.628100000 -3.451783000  
N 2.140453000 0.925960000 -1.389033000  
H 2.350331000 1.649480000 -0.691649000  
C 2.315580000 -0.334900000 -0.934868000  
O 2.091520000 -1.355490000 -1.623245000  
C 2.836220000 -0.414217000 0.510258000



H	3.888640000	-0.731616000	0.417626000
N	2.815382000	0.923066000	1.129467000
H	3.583760000	1.035785000	1.789579000
H	1.940813000	1.054787000	1.648514000
C	2.064800000	-1.504828000	1.293602000
H	2.571480000	-1.649235000	2.260754000
H	2.151180000	-2.447541000	0.736139000
C	0.627320000	-1.145831000	1.497094000
C	-0.419530000	-1.461363000	0.652889000
H	-0.418770000	-2.069980000	-0.245597000
N	-1.591040000	-0.897106000	1.111757000
H	-2.467170000	-0.929071000	0.588700000
C	-1.328330000	-0.184539000	2.260964000
C	-2.177341000	0.575300000	3.071107000
H	-3.233763000	0.693483000	2.827828000
C	-1.624501000	1.178250000	4.197198000
H	-2.258574000	1.780322000	4.848004000
C	-0.258632000	1.020698000	4.515489000
H	0.135550000	1.493178000	5.415575000
C	0.587372000	0.272859000	3.703662000
H	1.639336000	0.150908000	3.970324000
C	0.065340000	-0.334549000	2.545204000

———— 215\_WGG07: PBE+MBD@rsSCS ————

O	1.301003865	0.157398739	3.595469192
C	0.703445287	0.976181666	2.910766045
O	1.348867140	1.908847371	2.189557980
H	0.662741341	2.472404359	1.692689216
C	-0.834886377	1.026388479	2.821046035
H	-1.173031048	1.988528282	3.237518273
H	-1.239261543	0.210788955	3.426125790
N	-1.361690216	0.896283100	1.462245389
H	-1.699084967	-0.025716111	1.172303846
C	-1.224416281	1.879122931	0.549457895
O	-0.610243325	2.946093604	0.806169588
C	-1.775911394	1.637324930	-0.842705971
H	-2.394581085	2.506389930	-1.119598273
H	-2.395738290	0.732283306	-0.913119784
N	-0.636057933	1.478964393	-1.728889221
H	0.272875100	1.883369575	-1.483471115
C	-0.609224422	0.575355275	-2.742692837
O	-1.598902409	-0.039245011	-3.164353242
C	0.802655655	0.307075349	-3.284229890
H	0.703136851	0.209928146	-4.379628241
N	1.738490686	1.369764695	-2.878986612
H	1.668755242	2.174599884	-3.504290213
H	2.703462338	1.038093360	-2.920777544
C	1.272010203	-1.069737171	-2.745358083
H	2.287130772	-1.247719385	-3.137247655
H	0.625205931	-1.830975481	-3.205196779
C	1.253556493	-1.231957746	-1.256147610
C	2.284768374	-0.985364705	-0.372914519
H	3.286166567	-0.612300632	-0.564846628
N	1.896183669	-1.295745781	0.917773319
H	2.402335088	-1.052389569	1.764654024
C	0.586732228	-1.728608108	0.899592267

```

C -0.242156310 -2.133380367 1.951110049
H 0.122344727 -2.150620181 2.977920496
C -1.555775684 -2.473533274 1.634064040
H -2.234555286 -2.788571235 2.427191986
C -2.019911872 -2.430219460 0.298913657
H -3.052721309 -2.706732410 0.085676604
C -1.179797026 -2.061962090 -0.748907388
H -1.554004564 -2.022026120 -1.771944801
C 0.147647785 -1.696572492 -0.458440286

```

———— 216\_WGG11: PBE+MBD@rsSCS ————

```

O -4.595489699 -0.119300438 0.033739161
C -3.293556980 0.248221997 0.183299781
O -2.939614114 1.418386812 0.212869079
H -5.112009924 0.711628346 -0.029033878
C -2.391417231 -0.977196762 0.235146786
H -2.157888709 -1.252231225 -0.804773908
H -2.960643636 -1.797574255 0.691442955
N -1.160380028 -0.769486457 0.954855328
H -0.300267067 -0.562062352 0.451012455
C -1.186336038 -0.691556220 2.321472511
O -2.237105456 -0.781061240 2.964560927
C 0.162764048 -0.515253653 3.017913063
H 0.140336922 -1.152270077 3.914332603
H 0.251036633 0.527527019 3.360882191
N 1.304232423 -0.787923499 2.177121870
H 1.451436145 -1.697446086 1.729541575
C 2.267833213 0.132824414 1.893498460
O 2.339969746 1.254297699 2.412327272
C 3.238996215 -0.313835224 0.783093950
H 4.243871915 -0.334291176 1.232079194
N 2.915269384 -1.672016993 0.304664083
H 2.326157426 -1.630770313 -0.531682558
H 3.759261070 -2.187630425 0.059188551
C 3.208106684 0.778552358 -0.320824684
H 3.899897253 0.479762845 -1.123736233
H 3.591337877 1.709738507 0.117160401
C 1.823080407 0.994269362 -0.849586178
C 0.892360898 1.873512736 -0.329085643
H 1.001836440 2.566960952 0.498484080
N -0.309064369 1.757508012 -1.001764296
H -1.206109245 2.065299571 -0.622471120
C -0.194062352 0.758312160 -1.947281488
C -1.144670766 0.242701558 -2.834349935
H -2.160057991 0.640557194 -2.867990660
C -0.743888240 -0.784016925 -3.685364179
H -1.459930083 -1.208709186 -4.388777524
C 0.580759471 -1.269756979 -3.667333467
H 0.865668205 -2.059568522 -4.362299432
C 1.527641683 -0.750431199 -2.790532234
H 2.554114804 -1.122891714 -2.809154409
C 1.147705067 0.266712380 -1.893304450

```

———— 217\_WGG09: PBE+MBD@rsSCS ————

```

O -1.439086927 -0.762944375 -3.693394912
C -0.172686395 -0.649069168 -3.264258029

```

O 0.645714682 -1.552326111 -3.396984707  
 H -1.954970695 0.058370579 -3.402790615  
 C 0.159550873 0.692823300 -2.593841956  
 H -0.101124404 1.506165119 -3.288365739  
 H 1.229309049 0.736998129 -2.373142792  
 N -0.577240736 0.890284240 -1.350588900  
 H -0.112753593 0.681103313 -0.464510484  
 C -1.890869138 1.203082209 -1.359760229  
 O -2.547292754 1.299639309 -2.422170928  
 C -2.563972007 1.457400084 -0.018191563  
 H -3.442442832 0.798694056 0.032505980  
 H -2.925285637 2.496177142 -0.021996065  
 N -1.748800150 1.190207745 1.149209793  
 H -1.077989181 1.883835031 1.466648802  
 C -1.889290657 0.024685052 1.871696309  
 O -2.724400652 -0.836505278 1.577976328  
 C -0.935548021 -0.141262089 3.060495400  
 H -0.345234309 0.781226132 3.196115184  
 N -1.639111886 -0.412101628 4.317127579  
 H -2.219374705 0.386124911 4.584885152  
 H -2.279374847 -1.198559988 4.169198596  
 C 0.018519924 -1.315040387 2.758175080  
 H -0.590727281 -2.231521758 2.728324739  
 H 0.698321423 -1.406513989 3.619681519  
 C 0.774406636 -1.174267268 1.477781400  
 C 0.657734014 -1.973117043 0.358456242  
 H -0.002254096 -2.817724657 0.184943738  
 N 1.547035658 -1.564996682 -0.620252827  
 H 1.505786624 -1.853641454 -1.601643655  
 C 2.230404067 -0.455901620 -0.163082789  
 C 3.202969796 0.330534329 -0.791909780  
 H 3.557521066 0.096595705 -1.796846478  
 C 3.716806545 1.410161705 -0.078671220  
 H 4.475540162 2.042976659 -0.538711273  
 C 3.287775326 1.689242436 1.236699892  
 H 3.728318068 2.530910239 1.771297225  
 C 2.328996579 0.901328963 1.864548688  
 H 2.027403367 1.114740355 2.891766294  
 C 1.770190046 -0.183686250 1.162508001

———— 218\_WGG13: PBE+MBD@rsSCS ————

O -1.592059083 2.396041608 1.677125114  
 C -0.756279356 3.065199130 0.862708152  
 O 0.192840008 3.705728790 1.290465234  
 H -2.288722081 1.921233616 1.109082450  
 C -1.093685564 2.971224512 -0.639144798  
 H -0.346832374 3.545555362 -1.192867232  
 H -2.087035741 3.418715774 -0.800500074  
 N -1.105657023 1.604661813 -1.163793313  
 H -0.267498879 1.279481596 -1.654106107  
 C -2.070826668 0.725610423 -0.832155144  
 O -3.000989371 1.020288592 -0.037693018  
 C -1.972883494 -0.684019935 -1.381454448  
 H -1.181674030 -0.805509038 -2.133065006  
 H -2.939346398 -0.943724404 -1.842451767  
 N -1.658346407 -1.546037291 -0.250585336

```

H -1.981585482 -1.250843901 0.666788115
C -0.837489910 -2.627571498 -0.352979986
O -0.465686447 -3.095950422 -1.437813450
C -0.327729646 -3.176484112 0.977008017
H -0.936179459 -2.766176570 1.802082909
N -0.481457158 -4.628913688 0.952487694
H 0.092888877 -5.065763238 1.675950898
H -0.155814041 -4.973283951 0.043950785
C 1.144981724 -2.691362900 1.174155152
H 1.751878487 -3.198497896 0.407056563
H 1.479059813 -3.075721789 2.151021223
C 1.364795772 -1.213086192 1.097502251
C 1.348334693 -0.306828947 2.139389768
H 1.176275070 -0.473418062 3.198871782
N 1.624931589 0.966514008 1.671804733
H 1.520346794 1.828825333 2.199060499
C 1.803515736 0.913816003 0.305365912
C 2.088268041 1.935902126 -0.606754137
H 2.214645949 2.965800144 -0.274390261
C 2.169927998 1.586701161 -1.953552621
H 2.389165240 2.356181981 -2.694681832
C 1.990998326 0.248247019 -2.373749166
H 2.067843847 0.009164328 -3.434763289
C 1.742318444 -0.770767985 -1.457748019
H 1.598901197 -1.796793145 -1.796895491
C 1.639638009 -0.447468353 -0.092034753

```

———— 219\_WGG10: PBE+MBD@rsSCS ————

```

O 1.511198025 -0.761317867 3.337614962
C 2.230800566 -0.338788287 2.438005289
O 3.254542879 -1.051997795 1.954704605
H 3.709495364 -0.522275097 1.208077064
C 2.038836338 1.058716825 1.822140259
H 2.908656962 1.668562987 2.120931661
H 1.137766386 1.499074894 2.258706104
N 1.900892850 1.091363223 0.369640219
H 1.004961615 1.381248725 -0.064728281
C 2.899320889 0.775773004 -0.475889231
O 4.016913074 0.343248209 -0.098321581
C 2.589275982 0.984423852 -1.960726566
H 3.485139881 0.707014316 -2.524058473
H 2.372889390 2.052251964 -2.128835547
N 1.462884090 0.192419359 -2.434732676
H 1.592698321 -0.563247169 -3.109914886
C 0.173349288 0.531256841 -2.182022286
O -0.147220207 1.492407225 -1.455079104
C -0.864105937 -0.403506176 -2.800048361
H -1.779859908 0.202923281 -2.907773764
N -0.360830980 -0.964539016 -4.065765063
H -0.880973188 -1.809164844 -4.311519590
H -0.475642953 -0.304679444 -4.837476281
C -1.152117174 -1.584076479 -1.831204781
H -0.304692362 -2.283962133 -1.911296709
H -2.040008915 -2.110148893 -2.224077741
C -1.344740370 -1.191680721 -0.407301201
C -0.457341867 -1.426511257 0.621913914

```

H 0.479268240 -1.977639623 0.617741488  
N -0.915948929 -0.842645455 1.786825381  
H -0.371930318 -0.815318947 2.650843643  
C -2.111252190 -0.202567612 1.526261138  
C -2.939667446 0.549136876 2.365452786  
H -2.689304028 0.709345610 3.415057687  
C -4.097774267 1.087078036 1.810923230  
H -4.765427670 1.679833469 2.436521591  
C -4.425659691 0.878697326 0.454590229  
H -5.343816977 1.311940388 0.057692628  
C -3.597083444 0.136153042 -0.378413078  
H -3.861532930 -0.011606679 -1.426961966  
C -2.417582390 -0.415198955 0.148506288

———— 220\_WGG12: PBE+MBD@rsSCS ————

O -1.391814769 -3.492669981 -0.075931768  
C -0.825921622 -2.832044276 -0.933909436  
O -1.504891010 -2.078781175 -1.818958477  
H -0.840196705 -1.626622469 -2.441241853  
C 0.707258590 -2.806646703 -1.098681934  
H 0.956211268 -3.238766054 -2.080681336  
H 1.147465487 -3.424481799 -0.311644757  
N 1.293991447 -1.468076521 -1.016167355  
H 1.706968529 -1.188712349 -0.121360743  
C 1.119653117 -0.552980488 -1.988864410  
O 0.422866284 -0.786244552 -3.011331112  
C 1.710978896 0.830107798 -1.789281912  
H 2.302001085 1.087711288 -2.682464041  
H 2.358373248 0.909634490 -0.905141049  
N 0.578294660 1.725324210 -1.602168342  
H -0.303243129 1.458212228 -2.034842295  
C 0.557755148 2.706804294 -0.654403805  
O 1.577778000 3.118658927 -0.086052714  
C -0.843917383 3.220131504 -0.268684595  
H -0.776910090 4.319197573 -0.262428519  
N -1.973675082 2.834592138 -1.110549799  
H -1.868907119 3.110345962 -2.086504107  
H -2.179922769 1.834645495 -1.048099146  
C -1.116080282 2.766039184 1.191214133  
H -2.087125876 3.192557480 1.480029770  
H -0.347221588 3.218343668 1.832553609  
C -1.121144121 1.279138794 1.376182394  
C -2.202622824 0.426202666 1.263656868  
H -3.240312753 0.655603286 1.039422205  
N -1.815638308 -0.876303504 1.529606112  
H -2.370853158 -1.708054596 1.350889293  
C -0.463492036 -0.896047589 1.798979414  
C 0.376618526 -1.969691190 2.112934824  
H -0.010398911 -2.986346611 2.173506069  
C 1.726814940 -1.688180321 2.310240744  
H 2.412858903 -2.498616829 2.557914647  
C 2.220636997 -0.366655700 2.210867723  
H 3.281784920 -0.181246360 2.379230168  
C 1.374887642 0.702245249 1.926118297  
H 1.767877895 1.715327286 1.842761852  
C 0.008493950 0.447865546 1.707915383

## 11.2.5 WG: PBE+MBD@rsSCS

———— 191\_WG03: PBE+MBD@rsSCS ————

O 0.896666305 -3.083986924 -0.703273997  
C 1.623896256 -2.112315143 -0.581675687  
O 2.362382242 -1.897830597 0.526249043  
H 2.792590440 -0.976959484 0.463496002  
C 1.796125947 -1.054139564 -1.690748153  
H 1.198933055 -1.366903680 -2.551952895  
H 2.858627142 -1.030714375 -1.983030769  
N 1.378662239 0.287751350 -1.302007131  
H 0.513443564 0.696446017 -1.666734028  
C 1.991741001 1.021316588 -0.353747180  
O 2.999485109 0.627335813 0.284661960  
C 1.320609538 2.354310113 -0.033187099  
H 2.133584872 3.062112472 0.208316667  
N 0.480992690 2.785836924 -1.161120204  
H -0.182204196 3.500987105 -0.859168262  
H 1.050215712 3.195576885 -1.904264242  
C 0.460049293 2.160628477 1.253734461  
H -0.165068270 3.062260058 1.372786820  
H 1.152656008 2.145534931 2.106485421  
C -0.355914288 0.906982067 1.259731709  
C 0.031934841 -0.264913733 1.875769944  
H 0.903607769 -0.463148336 2.490827973  
N -0.852899726 -1.278976110 1.569105984  
H -0.691232935 -2.260623608 1.763873944  
C -1.827799594 -0.786537837 0.723261407  
C -2.907497409 -1.437117485 0.121009988  
H -3.083851385 -2.501919920 0.275430151  
C -3.743875260 -0.676831430 -0.690068475  
H -4.594577595 -1.152046169 -1.178465967  
C -3.510190333 0.699979458 -0.889143568  
H -4.190146408 1.267401321 -1.524935275  
C -2.428827325 1.340829990 -0.295096542  
H -2.263378740 2.404225115 -0.468374779  
C -1.555010559 0.600517710 0.521720781

———— 192\_WG10: PBE+MBD@rsSCS ————

O 2.158038994 -2.678065791 0.684582920  
C 1.023324258 -2.005554961 1.034231527  
O 0.965256514 -1.228703943 1.972761695  
H 2.853819840 -2.374155726 1.303840751  
C -0.129188727 -2.382214291 0.133233884  
H -0.343354895 -3.454297743 0.287820435  
H 0.164191270 -2.272390402 -0.921841179  
N -1.269525480 -1.540983973 0.402130452  
H -1.292591467 -1.018264221 1.282883633  
C -2.016132342 -1.030307825 -0.616155798  
O -1.957509863 -1.427793041 -1.788079852  
C -2.904481614 0.151903754 -0.216654019  
H -3.830121603 0.050329695 -0.810662140  
N -3.133548458 0.183493806 1.235679448  
H -3.541366617 1.078058936 1.514068687  
H -3.789135225 -0.548196609 1.516136799  
C -2.206414552 1.460396711 -0.675310150

```

H -2.874424869  2.299069126 -0.417504712
H -2.150712819  1.430080015 -1.773147518
C -0.844436874  1.678188687 -0.096012488
C -0.542014722  2.293744804  1.099259537
H -1.199695726  2.759907004  1.825924115
N  0.824270345  2.260087069  1.317610894
H  1.288967557  2.587439358  2.154779326
C  1.435324794  1.601912709  0.269635846
C  2.782283123  1.299214442  0.053648745
H  3.552608751  1.591569128  0.768508690
C  3.104339969  0.605578881 -1.109614873
H  4.145387203  0.352690050 -1.312519812
C  2.106214495  0.226313956 -2.032126528
H  2.395134063 -0.318293692 -2.931251566
C  0.766442244  0.529315161 -1.813827543
H  0.003017821  0.208812143 -2.523589199
C  0.408272611  1.226837782 -0.645767008

```

———— 193\_WG06: PBE+MBD@rsSCS ————

```

O -1.979670000  2.275920000 -0.547478000
C -1.013093000  2.460536000  0.377536000
O -0.118835000  3.276589000  0.229183000
H -2.551372000  1.488900000 -0.267054000
C -1.137117000  1.568364000  1.627928000
H -2.120405000  1.738371000  2.092536000
H -0.353783000  1.858688000  2.333950000
N -0.995897000  0.141876000  1.339757000
H -0.071230000 -0.274669000  1.448821000
C -1.913310000 -0.553212000  0.628199000
O -2.985440000 -0.033608000  0.233948000
C -1.548470000 -1.985132000  0.261138000
H -0.796340000 -2.349874000  0.979502000
N -2.746800000 -2.808878000  0.380669000
H -2.612890000 -3.705610000 -0.089714000
H -3.527580000 -2.325530000 -0.072722000
C -0.891390000 -1.969870000 -1.161940000
H -1.681200000 -1.741210000 -1.893296000
H -0.544910000 -2.996970000 -1.365863000
C  0.215380000 -0.972760000 -1.264537000
C  0.173026000  0.222680000 -1.949471000
H -0.591197000  0.610030000 -2.615527000
N  1.282834000  0.988910000 -1.640191000
H  1.378816000  1.972120000 -1.870013000
C  2.047001000  0.318140000 -0.706157000
C  3.210426000  0.708140000 -0.038473000
H  3.673754000  1.677060000 -0.225583000
C  3.748060000 -0.180159000  0.888985000
H  4.651840000  0.095791000  1.431976000
C  3.146010000 -1.431152000  1.138549000
H  3.600360000 -2.104478000  1.865119000
C  1.988420000 -1.818947000  0.470482000
H  1.543160000 -2.796460000  0.665109000
C  1.412890000 -0.938650000 -0.465730000

```

———— 194\_WG02: PBE+MBD@rsSCS ————

```

O -1.887609324  2.339893126 -0.518256390

```

```
C -0.927734493  2.481219493  0.421110767
O -0.006616278  3.271029421  0.296897103
H -2.483973396  1.563895404 -0.259249229
C -1.095909896  1.575744138  1.656016824
H -2.080653891  1.768886632  2.108001058
H -0.314465276  1.833634121  2.376508250
N -0.992866805  0.148640837  1.350057122
H -0.073996853 -0.285113109  1.446295857
C -1.915375588 -0.511177083  0.607798583
O -2.968878352  0.042994106  0.208695013
C -1.592834968 -1.963834234  0.237818896
H -0.877038666 -2.364927436  0.973278398
N -2.764989137 -2.833075590  0.222247787
H -3.125661002 -2.963673917  1.169668722
H -3.510075886 -2.370921546 -0.308221418
C -0.920624403 -1.975203009 -1.165596641
H -1.698596549 -1.749852012 -1.911636673
H -0.587416393 -3.007772409 -1.349968725
C  0.189837694 -0.982085874 -1.265717668
C  0.161266984  0.210997526 -1.954054563
H -0.597378969  0.602954888 -2.624086504
N  1.279060019  0.966490985 -1.645446183
H  1.384826726  1.948288103 -1.876161857
C  2.033035247  0.291405605 -0.705876242
C  3.196088607  0.671628758 -0.031998620
H  3.670657079  1.635166131 -0.218819305
C  3.719193282 -0.220104648  0.900950854
H  4.621278554  0.049071905  1.449783333
C  3.104522414 -1.464927039  1.150385728
H  3.548483489 -2.140988426  1.881345508
C  1.947055359 -1.842736722  0.476064453
H  1.492311676 -2.816858879  0.665157591
C  1.385463992 -0.957971245 -0.464341830
```

———— 195\_WG01: PBE+MBD@rsSCS ————

```
O -3.005360348 -0.925704205  1.247190551
C -3.103691213  0.405077211  1.455493000
O -3.133408718  0.895003178  2.570238588
H -2.949053983 -1.099389831  0.245342292
C -3.208254552  1.253342277  0.172676941
H -3.283625934  2.303439155  0.468438324
H -4.131405037  0.963260869 -0.356336061
N -2.071097545  1.101428965 -0.725057663
H -1.426731120  1.873642063 -0.927109898
C -1.805146426 -0.020511400 -1.414011860
O -2.483689901 -1.074118735 -1.307094690
C -0.574423155  0.051975121 -2.325467073
H -0.954081131 -0.067940264 -3.353005149
N  0.073745646  1.369925365 -2.210223565
H  0.430443423  1.689089278 -3.109720381
H  0.864854411  1.321670295 -1.560852993
C  0.350561167 -1.149175431 -1.993321828
H  1.158934768 -1.179359557 -2.739748112
H -0.236561345 -2.070617337 -2.106409332
C  0.910625667 -1.042692181 -0.609266772
C  0.307481109 -1.477712087  0.554082575
```



H	-0.621293806	-2.020528020	0.695357070
N	1.065730175	-1.097957551	1.645518050
H	0.814599712	-1.271171407	2.611225278
C	2.177423823	-0.402234685	1.214124575
C	3.221676522	0.181731869	1.935906397
H	3.254252568	0.138066033	3.025251539
C	4.222245249	0.824691829	1.212477376
H	5.050706486	1.291812356	1.744571847
C	4.186113716	0.877814529	-0.196769150
H	4.992372102	1.381925526	-0.729998045
C	3.146083160	0.294615215	-0.912583789
H	3.140089349	0.332468597	-2.003775627
C	2.111694165	-0.354666041	-0.211521416

———— 196\_WG14: PBE+MBD@rsSCS ————

O	0.518198809	2.314126577	2.755855643
C	0.996612240	1.292959753	1.993584399
O	1.881785184	1.426835378	1.163297505
H	1.000363922	3.118425045	2.471608581
C	0.312477803	-0.010153970	2.328979690
H	-0.779508025	0.110784734	2.266360613
H	0.539715428	-0.261874410	3.379099909
N	0.755076682	-1.032078372	1.407428848
H	1.528842046	-0.763515082	0.798599137
C	-0.077301609	-2.037210231	1.018518043
O	-1.152143880	-2.280760379	1.586746415
C	0.375285486	-2.823752518	-0.211972901
H	1.467899630	-2.714058882	-0.332881318
N	0.048398852	-4.228676025	0.014668206
H	-0.851182695	-4.267672336	0.504933311
H	-0.051924052	-4.725630223	-0.872179293
C	-0.305425835	-2.207451919	-1.475726347
H	-1.394563312	-2.319001452	-1.351847783
H	-0.013155211	-2.835608890	-2.332568955
C	0.049041149	-0.779086772	-1.734666795
C	1.139874205	-0.311945380	-2.438902026
H	1.903128336	-0.862907888	-2.980217212
N	1.165458328	1.073140233	-2.406681536
H	1.886220617	1.653961362	-2.815930517
C	0.093742885	1.530219650	-1.666242810
C	-0.286668028	2.832414569	-1.331268931
H	0.285226363	3.697182616	-1.670177160
C	-1.421241315	2.984146590	-0.539227784
H	-1.747034964	3.985577215	-0.257232397
C	-2.158240270	1.865102914	-0.095577769
H	-3.040888990	2.023980329	0.524460250
C	-1.777844652	0.570505571	-0.433187278
H	-2.346508971	-0.286971634	-0.069817299
C	-0.633361154	0.384337826	-1.229666440

———— 197\_WG07: PBE+MBD@rsSCS ————

O	2.275890293	0.620595998	2.719522470
C	1.132712485	0.987867983	2.066576681
O	1.107775095	1.816853854	1.174044879
H	3.001458068	1.120933275	2.290868356
C	-0.073782299	0.264097477	2.634012833

```

H -0.205449560  0.593207993  3.679514730
H  0.112557879 -0.819690984  2.662308750
N -1.237215811  0.501768285  1.822876905
H -1.410445458  1.430040868  1.430610168
C -1.914510742 -0.514747141  1.224587603
O -1.799043008 -1.708827593  1.538335132
C -2.814689685 -0.075948777  0.058069689
H -3.823328750 -0.446287434  0.294676021
N -2.859497696  1.386891587 -0.078495470
H -2.193660512  1.688369415 -0.798542071
H -3.786854042  1.708287979 -0.351728853
C -2.323724942 -0.804617674 -1.231079161
H -3.090433241 -0.662233009 -2.007877794
H -2.267577337 -1.880284130 -1.011418050
C -1.004136286 -0.287498095 -1.709425079
C -0.815961706  0.737364025 -2.617083019
H -1.547022485  1.279207039 -3.210548893
N  0.535688222  1.011409006 -2.748873690
H  0.933481467  1.724410696 -3.346756798
C  1.251466003  0.168013446 -1.921890356
C  2.628788249  0.077356600 -1.702286271
H  3.331182423  0.734503652 -2.216734127
C  3.070037110 -0.884060195 -0.798283827
H  4.138414549 -0.986703041 -0.604345790
C  2.159311845 -1.733963831 -0.135231603
H  2.541369302 -2.479082640  0.563306037
C  0.789421461 -1.638584859 -0.353557015
H  0.093595524 -2.287358544  0.178744067
C  0.310454585 -0.669635233 -1.254967453

```

———— 198\_WG09: PBE+MBD@rsSCS ————

```

O  0.500885858  2.322301461  2.690818594
C  1.002109949  1.279956645  1.973198192
O  1.896964590  1.394882443  1.150222624
H  0.971327660  3.123138807  2.378386458
C  0.330574405 -0.019294125  2.349893574
H -0.763207127  0.089691779  2.301310417
H  0.577496161 -0.242224721  3.402355399
N  0.759121282 -1.065642898  1.446268670
H  1.541758955 -0.813414790  0.840838564
C -0.119692062 -2.020021109  1.017476098
O -1.220395573 -2.210189981  1.555562044
C  0.327067723 -2.832668661 -0.205474362
H  1.424581369 -2.786979588 -0.301116274
N -0.070587090 -4.240354779 -0.117366514
H -1.047801139 -4.264484312  0.195059887
H  0.463479232 -4.701383687  0.623612862
C -0.296417114 -2.207699708 -1.479819778
H -1.390944538 -2.309628615 -1.397979531
H  0.017039435 -2.839108858 -2.322998795
C  0.072392112 -0.776957864 -1.708834478
C  1.174905603 -0.313818531 -2.395824561
H  1.941682975 -0.868478262 -2.927884682
N  1.208602383  1.070572914 -2.359372468
H  1.934773358  1.647428315 -2.764267191
C  0.126940295  1.532153667 -1.636808826

```

```

C -0.256103445  2.835916444 -1.311180097
H  0.322414370  3.699094084 -1.643018155
C -1.407285512  2.992213167 -0.544136018
H -1.738920820  3.995329865 -0.275073822
C -2.156864433  1.875787157 -0.114906910
H -3.053920020  2.037323027  0.483261293
C -1.772765275  0.579748282 -0.441703839
H -2.351018915 -0.276078901 -0.090851599
C -0.612597654  0.388759336 -1.213906776

```

———— 199\_WG15: PBE+MBD@rsSCS ————

```

O -2.831966321  0.836978358  0.367782770
C -2.269030334  0.277698220 -0.557851152
O -1.553100798  0.930033010 -1.518216707
H -1.410269694  1.858156188 -1.217926028
C -2.245297431 -1.225335457 -0.803021832
H -2.884925722 -1.449646596 -1.672493023
H -2.650819828 -1.738406146  0.076014897
N -0.887368122 -1.692279284 -1.018226194
H -0.273530179 -1.167613510 -1.647076552
C -0.235783221 -2.470439839 -0.104838746
O -0.779892644 -3.067949946  0.831620464
C  1.288147911 -2.503260447 -0.291826210
H  1.598505716 -3.549191022 -0.118298642
N  1.681019796 -1.997307922 -1.618848456
H  2.682727686 -1.796628185 -1.636794380
H  1.506787326 -2.702024061 -2.338425717
C  1.920076812 -1.637874932  0.837004754
H  2.980446039 -1.469802936  0.580732095
H  1.913045486 -2.248328793  1.750005064
C  1.215377172 -0.347997213  1.120985772
C  0.330227301 -0.165551861  2.163578741
H  0.022233903 -0.870451477  2.929369374
N -0.204854540  1.107573189  2.118303640
H -0.997306495  1.420375782  2.666435905
C  0.293231998  1.765000391  1.012529925
C -0.021341168  3.028139453  0.501015585
H -0.741574057  3.678036585  0.999120209
C  0.616932248  3.421838466 -0.675154668
H  0.399952612  4.401834074 -1.100785935
C  1.548623403  2.575680036 -1.314874011
H  2.031512068  2.915541656 -2.231130375
C  1.848743119  1.317199674 -0.805751327
H  2.545141436  0.665771388 -1.332749286
C  1.211594521  0.879861158  0.368789047

```

———— 200\_WG13: PBE+MBD@rsSCS ————

```

O -2.574152877 -0.640351081 -2.399110180
C -1.947414889 -1.026021322 -1.252881836
O -1.086663224 -1.890842855 -1.213537469
H -2.165182673 -1.161544156 -3.121403599
C -2.484267893 -0.280508460 -0.052462082
H -3.537534365 -0.579056382  0.089792962
H -2.486802848  0.802925660 -0.240657095
N -1.665848490 -0.560433014  1.105231007
H -1.082319672 -1.394392992  1.038537145

```

```
C -1.250413161  0.450163541  1.928692485
O -1.750868297  1.583076608  1.905472249
C -0.082460769  0.114220440  2.873252415
H -0.342713592  0.589071077  3.832182029
N  0.220549600 -1.294681807  3.118054276
H -0.607856534 -1.834254430  3.370050304
H  0.666993383 -1.723656707  2.302355789
C  1.192091913  0.821911402  2.337787057
H  1.974149459  0.696174126  3.100184385
H  0.972950413  1.895505022  2.255211248
C  1.652502692  0.279903734  1.021256213
C  2.532599129 -0.765545415  0.821490014
H  3.101410416 -1.338651195  1.547897095
N  2.660675538 -1.021953455 -0.534381226
H  3.236495557 -1.748355266 -0.940442324
C  1.859761417 -0.145970804 -1.240213422
C  1.639977088 -0.028340108 -2.615381339
H  2.132709030 -0.689761345 -3.328980024
C  0.760172239  0.962831395 -3.040386988
H  0.566296702  1.085680408 -4.106429183
C  0.118332750  1.815116603 -2.116371245
H -0.562586997  2.582067358 -2.486439322
C  0.335002779  1.691349484 -0.748428234
H -0.181273633  2.343157437 -0.042428159
C  1.213905813  0.694075501 -0.287184947
```

———— 201\_WG12: PBE+MBD@rsSCS ————

```
O  1.677426158 -2.884807393 -0.511806660
C  2.204280162 -1.785715669 -0.451021386
O  2.891498515 -1.372624194  0.633470932
H  3.103746987 -0.383625795  0.525153010
C  2.145351581 -0.761722114 -1.602726294
H  1.671817826 -1.242033753 -2.464040623
H  3.171159543 -0.466804049 -1.872763682
N  1.385167457  0.439345444 -1.264879971
H  0.423930669  0.509876936 -1.591534530
C  1.791075680  1.335214249 -0.334630558
O  2.886679847  1.218145936  0.267603645
C  0.821592523  2.472768579  0.004655777
H  1.460947412  3.343407511  0.220646516
N -0.144109206  2.851483632 -1.023039893
H -0.892258460  2.164763600 -1.139986021
H  0.292505761  3.036491948 -1.926023855
C  0.081336526  2.084158586  1.320972624
H -0.656017683  2.877292954  1.516425182
H  0.814552704  2.102960342  2.138220714
C -0.548680739  0.728299438  1.241915976
C  0.033206371 -0.437108761  1.696586269
H  0.949914842 -0.576604686  2.259890939
N -0.704252315 -1.531112600  1.286572273
H -0.383689398 -2.491623006  1.350584439
C -1.776073990 -1.095537598  0.533647940
C -2.777245687 -1.820663065 -0.117683564
H -2.791453123 -2.910759031 -0.095795733
C -3.757216853 -1.100642415 -0.794594113
H -4.551417274 -1.636092410 -1.314627555
```

C -3.748994001 0.309783376 -0.806521761  
H -4.547653371 0.842020256 -1.323240000  
C -2.749617335 1.030481946 -0.161181504  
H -2.776046964 2.122027777 -0.156820656  
C -1.724357166 0.332722029 0.508482122

———— 202\_WG08: PBE+MBD@rsSCS ————

O 0.782167832 -0.640804271 3.573462807  
C 1.232547877 0.522613735 3.065048316  
O 1.931706302 1.292405938 3.701747675  
H 0.246319849 -1.135577325 2.865758537  
C 0.851654625 0.796376700 1.601436297  
H 1.423978287 0.101704190 0.960514577  
H 1.162160598 1.817859461 1.365072629  
N -0.569651702 0.666747820 1.290438090  
H -1.073813441 1.443272842 0.854543102  
C -1.222815412 -0.508602150 1.225663583  
O -0.766588506 -1.587451295 1.675932795  
C -2.557124508 -0.465130418 0.486004960  
H -3.217710285 -1.198019940 0.980984229  
N -3.094138809 0.904979346 0.481014670  
H -3.817532268 1.003248139 -0.233641896  
H -3.526030214 1.125970782 1.380318374  
C -2.319055044 -0.953972850 -0.971099871  
H -3.285216888 -0.895620809 -1.498597662  
H -2.053641978 -2.019815673 -0.921358490  
C -1.261400697 -0.191991823 -1.703288999  
C -1.416428585 0.983743548 -2.405942283  
H -2.317444529 1.545742520 -2.631617553  
N -0.181852613 1.443958717 -2.832839754  
H -0.031098061 2.260838831 -3.411578038  
C 0.800450321 0.563000628 -2.419687757  
C 2.186384622 0.604496535 -2.595891173  
H 2.666730624 1.416429390 -3.142800708  
C 2.932192836 -0.433603914 -2.045061109  
H 4.015972360 -0.433235334 -2.160392874  
C 2.310417600 -1.485527290 -1.340051121  
H 2.926345979 -2.281578350 -0.921486107  
C 0.931319372 -1.521329061 -1.164232217  
H 0.468044675 -2.328631977 -0.596675576  
C 0.149617778 -0.484679642 -1.705895455

———— 203\_WG11: PBE+MBD@rsSCS ————

O 1.485273370 -0.434138139 -1.401027222  
C 2.548530605 0.138057666 -0.769198718  
O 3.521853918 -0.481826319 -0.378739873  
H 1.585341799 -1.408331239 -1.308540679  
C 2.392485221 1.651842057 -0.632866673  
H 2.954460739 2.120887653 -1.454253742  
H 2.874952987 1.935077396 0.310833253  
N 1.029974256 2.125440091 -0.628666490  
H 0.489509395 2.238648882 -1.488571577  
C 0.293344753 2.177297699 0.514150466  
O 0.761100235 2.020192741 1.651319662  
C -1.205511802 2.454737560 0.291310620  
H -1.394363886 3.432249374 0.762017651

N -1.528426858 2.555459275 -1.141097667  
H -2.248775772 3.256410668 -1.310805878  
H -1.884296652 1.653002202 -1.475664270  
C -2.048661814 1.391204314 1.057134746  
H -3.089325814 1.747446485 1.088698154  
H -1.680222286 1.351743676 2.091760228  
C -1.982325168 0.041623016 0.417011629  
C -2.813130478 -0.425668109 -0.583662261  
H -3.713354618 0.016834056 -1.000950170  
N -2.371768261 -1.663491309 -1.025467598  
H -2.823828745 -2.226941783 -1.734190084  
C -1.243566543 -2.021928191 -0.313399349  
C -0.421271355 -3.147805462 -0.429411671  
H -0.626588483 -3.932122465 -1.159515754  
C 0.672087836 -3.232070544 0.431815759  
H 1.335438871 -4.095383354 0.372170446  
C 0.928964941 -2.224326652 1.386939899  
H 1.795236784 -2.322858871 2.040471218  
C 0.118348762 -1.100017029 1.486749700  
H 0.351344576 -0.305981482 2.195954310  
C -0.980375510 -0.974839864 0.617510933

———— 204\_WG04: PBE+MBD@rsSCS ————

O 0.774329057 -0.376930957 -3.946688621  
C -0.411164541 -0.944263439 -3.651499465  
O -1.105843242 -1.493206554 -4.489767414  
H 1.191402882 -0.002767865 -3.098128024  
C -0.814419367 -0.898669881 -2.166558091  
H -0.146532519 -1.578322782 -1.609086263  
H -1.836312893 -1.279998480 -2.087800235  
N -0.764259960 0.419532495 -1.547911749  
H -1.609559002 0.890630298 -1.211126826  
C 0.369436931 1.084541361 -1.276155924  
O 1.504043579 0.719676066 -1.679091239  
C 0.205132280 2.337867762 -0.414302879  
H 0.652532772 3.157138568 -0.997852015  
N -1.215145277 2.626325682 -0.166153387  
H -1.456432372 2.389430137 0.801807599  
H -1.434074950 3.608465368 -0.324274778  
C 1.043652808 2.173530870 0.889812452  
H 1.141428123 3.167446089 1.351441757  
H 2.052193864 1.842722799 0.601735817  
C 0.417527084 1.220800173 1.855850312  
C -0.402293379 1.562679459 2.914576195  
H -0.661489016 2.544825818 3.298986446  
N -0.880288166 0.418670423 3.530965248  
H -1.462512456 0.399707905 4.358920208  
C -0.371041752 -0.691302909 2.882890339  
C -0.568107191 -2.052118484 3.134608110  
H -1.209478444 -2.393362196 3.947484124  
C 0.090487373 -2.956724842 2.308254445  
H -0.039253178 -4.025726124 2.476444728  
C 0.929957166 -2.515207926 1.264169535  
H 1.441963400 -3.254028995 0.646748887  
C 1.121060254 -1.161282326 1.013715035  
H 1.773552117 -0.833193973 0.204385695

C 0.455960015 -0.220296541 1.821840978

———— 205\_WG05: PBE+MBD@rsSCS ————

O -4.548392840 -0.640700241 0.102231826  
 C -4.328054795 0.499354192 0.785077265  
 O -5.229661565 1.219285979 1.177679006  
 H -3.659064586 -1.085137835 -0.107256737  
 C -2.847851895 0.809287548 1.080709532  
 H -2.486532177 0.051570072 1.797403899  
 H -2.801469854 1.792040170 1.558304492  
 N -1.973326820 0.813550393 -0.084342134  
 H -1.508401678 1.665889791 -0.414868707  
 C -1.624210036 -0.291952087 -0.763468903  
 O -2.125048233 -1.424152125 -0.543684530  
 C -0.566819308 -0.081132692 -1.852780390  
 H -1.094974254 -0.226980921 -2.809495270  
 N -0.058508763 1.300562240 -1.811667439  
 H 0.162395854 1.640283030 -2.746760277  
 H 0.802626637 1.345493935 -1.257859777  
 C 0.514148148 -1.182403751 -1.713262353  
 H 1.185018350 -1.122259183 -2.583950125  
 H 0.010829598 -2.157738346 -1.754276085  
 C 1.290101963 -1.039850015 -0.442113039  
 C 0.953514362 -1.562757744 0.790065571  
 H 0.121828110 -2.206730833 1.059163914  
 N 1.863328122 -1.136274283 1.743187849  
 H 1.856794024 -1.408454780 2.718256990  
 C 2.812254168 -0.329198487 1.143897480  
 C 3.922607370 0.325148594 1.684500752  
 H 4.166529690 0.252459751 2.744954287  
 C 4.713818663 1.071925228 0.816520701  
 H 5.593430885 1.587064870 1.201808254  
 C 4.405653335 1.162373583 -0.557150092  
 H 5.055671799 1.747439769 -1.207279339  
 C 3.299912632 0.511404130 -1.092117076  
 H 3.084366438 0.578397044 -2.160397317  
 C 2.476020658 -0.248826998 -0.240115231

### 11.2.6 FGG: PBE+TS

———— 252\_FGG55: PBE+TS ————

O -3.274604970 0.107726241 -2.317321312  
 C -3.137980114 -0.043470805 -1.116643076  
 O -3.223034854 0.984709581 -0.243979613  
 H -3.004673654 0.648119485 0.685001582  
 C -2.891785254 -1.427368191 -0.479909935  
 H -2.861707351 -2.160646545 -1.289773808  
 H -3.745200429 -1.661880604 0.177755487  
 N -1.647659331 -1.544124159 0.280579847  
 H -0.886096826 -2.148667481 -0.062410881  
 C -1.427712180 -0.904657251 1.448716548  
 O -2.240492336 -0.099250845 1.957912393  
 C -0.100875846 -1.240527354 2.146124828  
 H -0.075667745 -2.316254474 2.374349608  
 H -0.082818614 -0.679962930 3.085277470  
 N 1.098701537 -0.900485006 1.380329162  
 H 1.520831865 0.011613154 1.542924626

C 1.516648633 -1.608271456 0.295210969  
O 0.912243540 -2.623570486 -0.108656350  
C 2.766680740 -1.077812402 -0.435267860  
N 3.483345014 -2.123712202 -1.160893534  
H 2.804185242 -2.693935647 -1.674257660  
H 3.936482616 -2.759544261 -0.501288523  
H 3.454740469 -0.648037641 0.309271750  
C 2.360462591 0.056461319 -1.421094255  
H 3.282432312 0.343890842 -1.946054298  
H 1.676699047 -0.362707655 -2.174333092  
C 1.721675788 1.244607546 -0.744034409  
C 2.476388972 2.070298090 0.106886615  
H 3.549226476 1.896493421 0.214160620  
C 1.873021232 3.114300399 0.812327540  
H 2.475751717 3.744540660 1.466867135  
C 0.502873532 3.355117821 0.672349835  
H 0.029593426 4.166872565 1.224905920  
C -0.255321860 2.553754302 -0.184111714  
H -1.323535437 2.727709986 -0.306739974  
C 0.351936238 1.507350475 -0.882627214  
H -0.249753189 0.880321512 -1.542557426

———— 253\_FGG99: PBE+TS ————

O 1.120200267 0.018178926 -1.284121060  
C 2.102785060 0.056088347 -0.566020969  
O 3.235565125 -0.664140429 -0.813130047  
H 3.044919942 -1.201376558 -1.609743454  
C 2.259832647 0.895060566 0.701007218  
H 3.125437462 1.557443185 0.559088537  
H 2.485710004 0.222987639 1.538520849  
N 1.085786234 1.683197899 0.987063657  
H 0.283956479 1.223127496 1.425759837  
C 0.821392233 2.796662684 0.223854303  
O 1.674019965 3.365728723 -0.461354735  
C -0.653685455 3.229322789 0.247414007  
H -0.741123340 4.160734964 -0.319841247  
H -0.997779614 3.389276892 1.278529091  
N -1.492010808 2.201293275 -0.357965097  
H -1.490414899 2.065327501 -1.372164164  
C -1.931255307 1.126734773 0.348183940  
O -1.815920013 1.030180240 1.584650250  
C -2.597513121 0.036836198 -0.515553954  
N -2.048079852 0.096857710 -1.876457141  
H -1.084404468 -0.252387709 -1.892049043  
H -2.603366154 -0.463572823 -2.522759125  
H -3.660449537 0.327250742 -0.584366856  
C -2.569657467 -1.346282502 0.195264313  
H -2.988907116 -1.209272240 1.200894745  
H -3.253602321 -2.006586983 -0.359044045  
C -1.213680551 -2.001846949 0.289659146  
C -0.732681901 -2.809071070 -0.752053337  
H -1.357956842 -2.979231002 -1.630556732  
C 0.523961945 -3.414955562 -0.674943047  
H 0.872584064 -4.046131976 -1.493186892  
C 1.321801488 -3.229549505 0.455282594  
H 2.297598341 -3.710342834 0.525913122



C 0.851325036 -2.434951897 1.505086596  
 H 1.459378176 -2.301657821 2.401026683  
 C -0.401706187 -1.826200264 1.421990118  
 H -0.769061514 -1.207735424 2.241120936

———— 254\_FGG300: PBE+TS ————

O -1.275215000 -1.644434000 0.293521000  
 C -2.263265000 -2.116562000 -0.243727000  
 O -2.496304000 -3.459815000 -0.323485000  
 H -1.742744000 -3.898884000 0.123222000  
 C -3.387228000 -1.329641000 -0.915101000  
 H -4.328695000 -1.585063000 -0.408568000  
 H -3.473162000 -1.664263000 -1.958137000  
 N -3.188396000 0.096558000 -0.844552000  
 H -2.440908000 0.521918000 -1.406419000  
 C -3.552834000 0.777393000 0.293516000  
 O -4.313711000 0.320134000 1.150427000  
 C -2.860405000 2.143685000 0.431683000  
 H -3.318249000 2.677892000 1.269644000  
 H -2.971759000 2.732899000 -0.489288000  
 N -1.436613000 1.955047000 0.691848000  
 H -1.105473000 1.721120000 1.631612000  
 C -0.553315000 1.653409000 -0.295790000  
 O -0.844176000 1.688370000 -1.507204000  
 C 0.846067000 1.253755000 0.210691000  
 N 0.736796000 0.722880000 1.579464000  
 H 1.656456000 0.680805000 2.020155000  
 H 0.370118000 -0.233277000 1.547816000  
 H 1.432882000 2.186702000 0.273730000  
 C 1.532758000 0.321705000 -0.819750000  
 H 0.928197000 -0.592297000 -0.912182000  
 H 1.511041000 0.820390000 -1.798178000  
 C 2.945051000 -0.025224000 -0.423940000  
 C 3.232224000 -1.230129000 0.235119000  
 H 2.422692000 -1.937797000 0.424745000  
 C 4.534554000 -1.538622000 0.638079000  
 H 4.736221000 -2.483369000 1.144121000  
 C 5.575963000 -0.641778000 0.389867000  
 H 6.593552000 -0.880342000 0.699990000  
 C 5.304575000 0.563331000 -0.265261000  
 H 6.113011000 1.266321000 -0.468363000  
 C 4.002231000 0.866411000 -0.666616000  
 H 3.801063000 1.806777000 -1.184687000

———— 255\_FGG252: PBE+TS ————

O -2.867279126 -1.329355740 -0.553910338  
 C -3.880075307 -0.737510189 -0.221277178  
 O -5.136695096 -1.213913900 -0.468104646  
 H -5.021365412 -2.064218205 -0.940948654  
 C -3.944571867 0.600644831 0.512716507  
 H -4.512019806 0.463326584 1.443484603  
 H -4.508787137 1.302795754 -0.117276174  
 N -2.637561585 1.148937581 0.778119380  
 H -2.037899008 0.678594373 1.468873220  
 C -1.982551893 1.838711890 -0.215298950  
 O -2.543768503 2.310183960 -1.207506870

C	-0.460188465	1.899600892	-0.005763865
H	-0.216457592	2.267122730	1.001180947
H	-0.034058040	2.572721560	-0.755283453
N	0.112830202	0.569353485	-0.166694939
H	0.383440956	0.223578361	-1.089603564
C	0.085363438	-0.367139099	0.810284606
O	-0.329342695	-0.151122422	1.967306652
C	0.622811690	-1.740800329	0.394794414
N	0.451199563	-1.924907431	-1.054975013
H	-0.542415619	-2.037815744	-1.272612497
H	0.938250573	-2.764061027	-1.372509448
H	0.045600413	-2.462716711	0.998903643
C	2.112407956	-1.884880516	0.815768294
H	2.135699589	-1.896658448	1.914096751
H	2.459244688	-2.875253529	0.478876142
C	3.029687753	-0.801626897	0.299337964
C	3.606111224	-0.874153636	-0.976914164
H	3.422251988	-1.748650188	-1.602538442
C	4.409456028	0.160497272	-1.461434407
H	4.848074454	0.084949159	-2.456983316
C	4.653935354	1.287422965	-0.672617749
H	5.285046149	2.093232075	-1.047954090
C	4.090875306	1.369876786	0.603521809
H	4.280259922	2.242496385	1.229702316
C	3.286960484	0.334131019	1.082479214
H	2.840529418	0.408603350	2.075760295

## ———— 256\_FGG366: PBE+TS ————

O	-1.983841000	1.761040000	0.432181000
C	-3.120163000	1.959211000	0.038015000
O	-3.751575000	3.165039000	0.159798000
H	-3.120122000	3.764233000	0.609736000
C	-4.027688000	0.939421000	-0.648937000
H	-4.302313000	1.326627000	-1.639913000
H	-4.951371000	0.859553000	-0.058579000
N	-3.416699000	-0.362463000	-0.758945000
H	-2.651431000	-0.493487000	-1.432315000
C	-3.409792000	-1.199536000	0.332576000
O	-4.152519000	-1.059594000	1.307449000
C	-2.329113000	-2.290786000	0.254478000
H	-2.376936000	-2.820087000	-0.707294000
H	-2.494266000	-2.997841000	1.072923000
N	-1.005827000	-1.689873000	0.388160000
H	-0.645478000	-1.429900000	1.310918000
C	-0.389346000	-1.051092000	-0.640109000
O	-0.801552000	-1.072040000	-1.816452000
C	0.878316000	-0.287918000	-0.239719000
N	0.802371000	0.112362000	1.172889000
H	1.719815000	0.421227000	1.501362000
H	0.151652000	0.895074000	1.276125000
H	0.926884000	0.568957000	-0.935050000
C	2.120968000	-1.179129000	-0.485598000
H	2.052788000	-2.059980000	0.170285000
H	2.079217000	-1.532303000	-1.525449000
C	3.410122000	-0.437346000	-0.226936000
C	4.113653000	-0.613364000	0.973995000

H	3.748548000	-1.336336000	1.706181000
C	5.275296000	0.117264000	1.239744000
H	5.808894000	-0.035368000	2.178062000
C	5.752304000	1.036715000	0.303952000
H	6.657491000	1.607828000	0.509877000
C	5.065055000	1.215836000	-0.900713000
H	5.436631000	1.925788000	-1.640289000
C	3.905234000	0.485715000	-1.161996000
H	3.374792000	0.630551000	-2.105409000

———— 257\_FGG215: PBE+TS ————

O	3.203829558	-2.087176788	0.364940851
C	3.066400862	-0.916832306	0.051129787
O	3.280592523	-0.477196057	-1.203856195
H	3.167619221	0.528077288	-1.230195505
C	2.702978761	0.160920737	1.096640337
H	3.620378626	0.739480914	1.302603382
H	2.419944145	-0.364804411	2.012264908
N	1.616345563	1.079571746	0.752437553
H	0.763216795	1.093000108	1.328107248
C	1.693009276	1.995882153	-0.235200461
O	2.666641077	2.085712157	-1.019105258
C	0.493535958	2.946186775	-0.353202046
H	0.684279133	3.593664780	-1.214103329
H	0.437195756	3.565444845	0.556121922
N	-0.782260657	2.270852131	-0.545172550
H	-1.240313462	2.226781206	-1.459383899
C	-1.489950516	1.708298046	0.462509922
O	-1.079366197	1.652949263	1.639446643
C	-2.861280950	1.145284172	0.038124109
N	-2.971044046	1.127034991	-1.430944682
H	-3.941330008	1.224988681	-1.728145360
H	-2.624219037	0.236943807	-1.800266562
H	-3.596351024	1.875743296	0.414655889
C	-3.145761503	-0.209588274	0.749081801
H	-3.107463686	-0.035550623	1.832465875
H	-4.175334707	-0.504287886	0.496087347
C	-2.172250014	-1.298275420	0.366215735
C	-2.342025541	-2.055305398	-0.804799642
H	-3.242499540	-1.922747643	-1.409084640
C	-1.387715388	-3.000980306	-1.193690637
H	-1.535331313	-3.573920659	-2.109420979
C	-0.253520674	-3.215386140	-0.409242710
H	0.501654128	-3.940059535	-0.711446837
C	-0.090830099	-2.496023778	0.777551285
H	0.789729912	-2.671303243	1.394443886
C	-1.039151687	-1.547483412	1.158165608
H	-0.908351244	-0.981894218	2.081265201

———— 258\_FGG224: PBE+TS ————

O	3.528823977	-1.183005479	1.551760921
C	3.260160612	-0.418917297	0.639690036
O	3.314671289	-0.793872501	-0.653943722
H	3.001918425	-0.027077893	-1.237267108
C	2.881928359	1.054146027	0.893557792
H	3.685635030	1.685366064	0.477747347

H	2.850416257	1.199569776	1.976280279
N	1.596459858	1.484560968	0.345841614
H	0.831777511	1.773110744	0.980711766
C	1.354251480	1.603918379	-0.973946293
O	2.166756362	1.257957459	-1.863604868
C	0.014497699	2.256106350	-1.348157687
H	-0.041060328	2.255195715	-2.440445165
H	0.034575773	3.301691619	-0.999813688
N	-1.181172451	1.603529144	-0.826412867
H	-1.820381569	1.111024205	-1.453623007
C	-1.576890099	1.642024064	0.466321189
O	-0.902415412	2.149499855	1.387402723
C	-2.924771545	0.965210625	0.748650059
N	-3.730246910	0.876027411	-0.482437668
H	-4.176088717	1.771570426	-0.689340885
H	-4.477229411	0.188377503	-0.375397422
H	-3.396390254	1.580912773	1.534629724
C	-2.680113749	-0.440482863	1.365646043
H	-2.228117708	-0.282185331	2.353578622
H	-3.666713047	-0.899583576	1.540924165
C	-1.802450634	-1.365018734	0.553035104
C	-0.457202969	-1.546638924	0.907580960
H	-0.061654943	-1.031833166	1.784835185
C	0.378310185	-2.383995011	0.165762665
H	1.414300052	-2.525439782	0.470337767
C	-0.118474268	-3.041163300	-0.961452534
H	0.533932030	-3.690103077	-1.545257618
C	-1.456517210	-2.873119863	-1.326555096
H	-1.855446901	-3.392546942	-2.198317373
C	-2.292393504	-2.050123352	-0.569426855
H	-3.339683270	-1.946692016	-0.854894103

## ———— 259\_FGG380: PBE+TS ————

O	-2.654800491	-2.601991580	0.779378242
C	-2.847805370	-1.433845356	0.487162192
O	-3.414094935	-0.560987124	1.344185109
H	-3.507759372	0.339094600	0.888744200
C	-2.502662555	-0.877636591	-0.910814486
H	-3.453269244	-0.687755736	-1.437561442
H	-1.957957796	-1.658894537	-1.446704435
N	-1.684715681	0.335342112	-0.938126727
H	-0.730589771	0.293320638	-1.324923731
C	-2.119448601	1.537813587	-0.508471121
O	-3.239128325	1.714288967	0.027783712
C	-1.146652534	2.707577763	-0.709210572
H	-1.638772583	3.604246274	-0.321410130
H	-0.959499635	2.837303183	-1.786913132
N	0.130135942	2.532152199	-0.028232504
H	0.356307940	3.050260932	0.822374822
C	1.126879916	1.754218758	-0.523580843
O	1.012881870	1.083084635	-1.566163560
C	2.393755441	1.705313427	0.339394098
N	2.505366465	2.920229048	1.167346308
H	2.908906514	3.694196345	0.637051268
H	3.113666499	2.755192554	1.971065823
H	3.229163198	1.572727657	-0.369264338

C 2.343463262 0.471417609 1.281470405  
 H 3.296901463 0.454889192 1.835418301  
 H 1.546532993 0.642681833 2.020791346  
 C 2.125617274 -0.853747088 0.593117196  
 C 3.134896472 -1.434651714 -0.187519531  
 H 4.101015247 -0.935392888 -0.281254641  
 C 2.916919952 -2.641925370 -0.850470663  
 H 3.711644327 -3.076292372 -1.457469767  
 C 1.685496109 -3.293587365 -0.735437170  
 H 1.518068279 -4.240579899 -1.249024209  
 C 0.675694061 -2.734451173 0.050593759  
 H -0.287430464 -3.232731122 0.164514642  
 C 0.899716110 -1.521637275 0.707768943  
 H 0.109559023 -1.092246120 1.326389638

———— 260\_FGG412: PBE+TS ————

O 3.583076983 0.202222545 0.423946378  
 C 2.510287599 -0.365095105 0.312648041  
 O 1.441443768 -0.109167287 1.121725495  
 H 1.724447086 0.630882660 1.698819159  
 C 2.232919481 -1.428737718 -0.747229807  
 H 2.889571274 -2.279428833 -0.515049929  
 H 2.560058077 -1.010124183 -1.707518314  
 N 0.872723458 -1.903970243 -0.842985741  
 H 0.173431030 -1.351917414 -1.346969714  
 C 0.418826863 -2.909844759 -0.031427057  
 O 1.153693849 -3.604905494 0.675581006  
 C -1.111176233 -3.079257254 -0.052600022  
 H -1.360514598 -3.917510089 0.605231045  
 H -1.451890893 -3.302196514 -1.074100468  
 N -1.800632592 -1.879808310 0.405120593  
 H -1.934476072 -1.694106360 1.401246784  
 C -2.064229137 -0.828791499 -0.409863298  
 O -1.813691548 -0.829770664 -1.630714728  
 C -2.733360472 0.366871454 0.299957425  
 N -2.423702651 0.327489227 1.738351428  
 H -1.493440050 0.720786483 1.907476742  
 H -3.092640596 0.883634591 2.271452509  
 H -3.817707348 0.187726843 0.201897230  
 C -2.432421790 1.704120862 -0.431451732  
 H -2.716422941 1.578501496 -1.484342763  
 H -3.097541912 2.467016533 0.000608885  
 C -0.999346998 2.170936891 -0.339403457  
 C -0.550164680 2.915546053 0.762949593  
 H -1.257378216 3.196591077 1.546151320  
 C 0.780948154 3.336816429 0.855871522  
 H 1.105523579 3.924080331 1.715785616  
 C 1.685002375 3.028818424 -0.162496596  
 H 2.724650407 3.345899541 -0.091561518  
 C 1.246239881 2.302820927 -1.273628062  
 H 1.944957832 2.067879687 -2.077274353  
 C -0.078458960 1.874546927 -1.357906177  
 H -0.417604008 1.300443744 -2.220298035

———— 261\_FGG444: PBE+TS ————

O 2.386649782 -2.680752778 1.030715720

C 2.656578761 -1.702787785 0.353918390  
O 2.616882905 -1.729331736 -0.994044267  
H 2.860380345 -0.815890593 -1.351529353  
C 3.090783843 -0.361657758 0.979039570  
H 4.138360175 -0.172461350 0.691846662  
H 3.040493300 -0.470950109 2.065849074  
N 2.274268634 0.788188724 0.594380476  
H 1.588963178 1.189767027 1.256242386  
C 2.280283896 1.310786481 -0.650061934  
O 2.949184865 0.832853963 -1.595711420  
C 1.398786452 2.552481968 -0.840932862  
H 1.583577142 2.925851179 -1.852254692  
H 1.694665193 3.323731337 -0.112353470  
N -0.025211608 2.275231446 -0.696899598  
H -0.667746623 2.305197888 -1.494116416  
C -0.635168913 2.083006578 0.493643532  
O -0.028129932 2.034853681 1.584828723  
C -2.167224140 1.944915628 0.413886916  
N -2.625321016 1.962025430 -0.985270105  
H -3.501739897 2.472270038 -1.081202355  
H -2.786708399 1.006373492 -1.317427368  
H -2.545458247 2.853150450 0.909831530  
C -2.652677626 0.721333989 1.244216212  
H -2.147416258 0.757660864 2.218530134  
H -3.730470574 0.845313932 1.422938805  
C -2.397864446 -0.596910153 0.552617343  
C -3.387898880 -1.177983518 -0.257268174  
H -4.370268590 -0.704863104 -0.325792591  
C -3.142371990 -2.366082181 -0.952097777  
H -3.925353490 -2.802459945 -1.572935845  
C -1.901161533 -2.995577970 -0.841685948  
H -1.705686498 -3.922440857 -1.380886507  
C -0.910846479 -2.439674269 -0.026406315  
H 0.054839188 -2.932940340 0.081994359  
C -1.158987501 -1.250423906 0.661059770  
H -0.385983019 -0.830805745 1.306336395

———— 262\_FGG470: PBE+TS ————

O -2.539149871 0.845525359 1.813066078  
C -3.028200614 0.954579069 0.702765014  
O -3.886338650 1.964891749 0.359147060  
H -3.995121553 2.511460729 1.164943023  
C -2.772628364 0.040031269 -0.469728424  
H -2.359494866 0.643823807 -1.296861471  
H -3.731679034 -0.353282029 -0.842527499  
N -1.883229460 -1.032308656 -0.089537483  
H -1.389733217 -0.981358984 0.809639554  
C -1.584821015 -2.031769009 -0.966382703  
O -2.104691068 -2.137348883 -2.084033836  
C -0.530754448 -3.027732596 -0.449548481  
H -0.469727801 -3.840977935 -1.179032146  
H -0.849724248 -3.431877508 0.523248759  
N 0.787010134 -2.426920222 -0.293233041  
H 1.507870508 -2.509404996 -1.012522952  
C 1.146631034 -1.712156161 0.799658349  
O 0.385182771 -1.494926738 1.760543698

C 2.600623638 -1.196104836 0.775858589  
N 3.202800914 -1.390056906 -0.554047271  
H 3.032325092 -0.569190132 -1.142526746  
H 4.213109207 -1.508268493 -0.485055627  
H 3.141461963 -1.847704311 1.481337627  
C 2.673112589 0.252827216 1.338448269  
H 2.169737974 0.255475894 2.314002654  
H 3.733489834 0.493277486 1.505384287  
C 2.048252726 1.277874896 0.423519750  
C 0.692537258 1.623516323 0.550209403  
H 0.101175596 1.180663682 1.351579364  
C 0.105015781 2.532493751 -0.331029346  
H -0.943360579 2.806162390 -0.207288550  
C 0.854595416 3.108577497 -1.360714228  
H 0.390609084 3.814882706 -2.049421215  
C 2.206446479 2.785408564 -1.489346971  
H 2.805879717 3.243745262 -2.276292249  
C 2.797161949 1.883501440 -0.599601750  
H 3.863622124 1.663670307 -0.686620488

———— 263\_FGG80: PBE+TS ————

O 3.907577993 -1.374313421 -0.367269898  
C 3.475235245 -0.249398519 -0.187162608  
O 3.817913241 0.792423122 -0.975476480  
H 3.358136720 1.624334292 -0.635816279  
C 2.528088531 0.099241175 0.977763602  
H 3.058308995 0.788253560 1.655292532  
H 2.301046124 -0.823461035 1.515067718  
N 1.266082603 0.716497958 0.571259974  
H 0.411159824 0.165791367 0.640573447  
C 1.195616731 2.001981826 0.163053196  
O 2.217295601 2.703823371 -0.019522024  
C -0.193122253 2.600519841 -0.039396216  
H -0.084320912 3.412261458 -0.770458407  
H -0.510940378 3.039145328 0.920584729  
N -1.225354015 1.669189940 -0.443808677  
H -1.288520218 1.330520705 -1.406294935  
C -2.288911921 1.340416673 0.351895824  
O -2.404482249 1.682959618 1.533072583  
C -3.343331563 0.461140111 -0.344750619  
N -3.219659019 0.546197211 -1.814183139  
H -3.720686654 -0.225455307 -2.257745657  
H -3.647010865 1.408061069 -2.159304483  
H -4.314026598 0.834801452 0.024368603  
C -3.214796908 -1.003568177 0.148471302  
H -3.582320454 -1.027320167 1.182232505  
H -3.913552394 -1.617178978 -0.444583546  
C -1.829816520 -1.611111093 0.112963345  
C -1.164174556 -1.906464686 -1.088706202  
H -1.640498085 -1.678264912 -2.041822342  
C 0.108568453 -2.481091438 -1.080505029  
H 0.616193928 -2.688311912 -2.022312390  
C 0.736132157 -2.796281731 0.127534248  
H 1.730863707 -3.240083674 0.127570154  
C 0.085782714 -2.508188094 1.329676156  
H 0.560611927 -2.750504097 2.281103409

C -1.177579580 -1.908373894 1.320051993  
 H -1.675509349 -1.676188944 2.262583608

———— 264\_FGG114: PBE+TS ————

O 3.936321769 1.348304843 -0.258928062  
 C 3.481185234 0.238572565 -0.041958514  
 O 3.820946575 -0.841538764 -0.776204704  
 H 3.347021490 -1.653804795 -0.407061198  
 C 2.506726163 -0.041816334 1.120618240  
 H 2.270494318 0.910430966 1.600302997  
 H 3.024737968 -0.688585704 1.847155429  
 N 1.250878712 -0.685540354 0.737291669  
 H 0.410232140 -0.114509788 0.667671948  
 C 1.184109863 -1.982982955 0.366089010  
 O 2.203560712 -2.701486030 0.251272531  
 C -0.193387260 -2.568448479 0.086476125  
 H -0.236798518 -3.532012441 0.616949078  
 H -0.256854893 -2.787713874 -0.990346504  
 N -1.316399868 -1.717756495 0.413073656  
 H -1.540318421 -1.434563503 1.370874480  
 C -2.243118868 -1.337004464 -0.519484570  
 O -2.192306170 -1.636836202 -1.716365757  
 C -3.361463791 -0.437832637 0.039311188  
 N -3.377255808 -0.456062730 1.516934809  
 H -3.977017044 -1.207420852 1.861195895  
 H -3.753946913 0.416399783 1.888557581  
 H -4.296583953 -0.830682811 -0.394142501  
 C -3.179936070 0.998275612 -0.522618665  
 H -3.398172710 0.948331149 -1.597110879  
 H -3.955951369 1.635654518 -0.069809866  
 C -1.811747942 1.611470449 -0.322931500  
 C -0.841352035 1.506541140 -1.333978341  
 H -1.087898962 0.975351914 -2.254170043  
 C 0.429737386 2.061954990 -1.170680144  
 H 1.173904419 1.963097322 -1.960513928  
 C 0.756398064 2.739498793 0.006990340  
 H 1.753284816 3.162220225 0.129182841  
 C -0.197952321 2.848133756 1.022275275  
 H 0.044722715 3.378046495 1.943734784  
 C -1.469136038 2.289665038 0.857153766  
 H -2.206664392 2.398651654 1.654190533

———— 265\_FGG357: PBE+TS ————

O -3.737601019 1.669194189 0.239457922  
 C -3.412044824 0.514542409 0.024110655  
 O -3.885705124 -0.519318072 0.749851301  
 H -3.504155174 -1.381701206 0.388293617  
 C -2.456802714 0.132417116 -1.124803396  
 H -2.094922418 1.059697436 -1.575736360  
 H -3.034256688 -0.428374461 -1.877698579  
 N -1.296757956 -0.666624848 -0.732843069  
 H -0.390445513 -0.208013831 -0.665225086  
 C -1.381117305 -1.963267883 -0.360755658  
 O -2.474426211 -2.561164572 -0.241054620  
 C -0.069913011 -2.691631949 -0.077723410  
 H -0.127173705 -3.662548786 -0.591297462



```

H -0.023246374 -2.890476833 1.004168911
N 1.125823032 -1.959663240 -0.433098741
H 1.438695960 -1.845305737 -1.401401678
C 2.034459792 -1.536887334 0.500175702
O 1.924904557 -1.736820351 1.714000033
C 3.202616323 -0.721070144 -0.092466135
N 3.112298749 -0.643537165 -1.562529006
H 2.665633224 0.230793549 -1.851250635
H 4.037630584 -0.667121833 -1.988713364
H 4.115775894 -1.277257482 0.166387445
C 3.264289011 0.660684016 0.627537627
H 3.406154901 0.475753977 1.699973135
H 4.151045045 1.196909522 0.259031752
C 2.016894331 1.482207442 0.404894708
C 0.929303824 1.381696244 1.290755855
H 1.016809183 0.738823540 2.166855669
C -0.255353259 2.080840181 1.053696690
H -1.091352271 1.989031919 1.746599693
C -0.382061084 2.893196184 -0.077377721
H -1.314452909 3.428078921 -0.255981786
C 0.692874391 3.012060353 -0.960746472
H 0.610987684 3.656472882 -1.836398168
C 1.883153399 2.318633280 -0.716135064
H 2.730437675 2.452752569 -1.392554304

```

———— 266\_FGG691: PBE+TS ————

```

O 2.986227244 -1.629144906 0.188552833
C 3.994256059 -1.107362895 -0.252017111
O 5.203888396 -1.746386012 -0.309711905
H 5.055446830 -2.640796333 0.061634377
C 4.103343275 0.306092349 -0.815526380
H 4.471945721 0.241584788 -1.849274350
H 4.855014715 0.853877204 -0.229723910
N 2.853645084 1.022407454 -0.750137848
H 2.054543968 0.681410771 -1.302480022
C 2.538944891 1.750702764 0.370141040
O 3.357312849 2.085198662 1.231373093
C 1.040463264 2.086786449 0.474505866
H 0.687502044 2.550989534 -0.458015183
H 0.908365583 2.786950495 1.304599601
N 0.246557142 0.889549979 0.725111279
H 0.063329153 0.554415713 1.674948804
C -0.069943552 0.001216578 -0.243571083
O 0.202632269 0.165820741 -1.451639807
C -0.757096210 -1.280698968 0.258910315
N -1.059652559 -1.195892015 1.696619381
H -0.947186981 -2.101254897 2.150103908
H -2.026292483 -0.893241557 1.843940905
H 0.015050554 -2.054990134 0.124073984
C -1.964159837 -1.647421241 -0.649272116
H -1.624289135 -1.589755490 -1.692054998
H -2.240059285 -2.691322665 -0.442226036
C -3.156709407 -0.749350221 -0.426073811
C -4.187917899 -1.129720236 0.448048211
H -4.155225881 -2.115680598 0.916816385
C -5.262581638 -0.275130954 0.712099807

```

H	-6.055030548	-0.592274007	1.390695836
C	-5.323421870	0.978401886	0.101146452
H	-6.159574633	1.647694186	0.304528684
C	-4.309730152	1.365115053	-0.780590783
H	-4.357021334	2.337147005	-1.272580377
C	-3.237285366	0.511101153	-1.041692827
H	-2.450293271	0.818960364	-1.731261214

**11.2.7 GFA: PBE+TS**

———— 236\_GFA15: PBE+TS ————

O	-0.666451000	-0.233237000	5.394016000
C	0.121846000	-0.236372000	4.464480000
O	1.034201000	-1.217795000	4.303104000
H	1.587250000	-1.032349000	3.475855000
C	0.194151000	0.904605000	3.410366000
C	-0.849430000	1.983488000	3.665693000
H	-1.864032000	1.579281000	3.558854000
H	-0.753268000	2.367699000	4.686415000
H	-0.722795000	2.813979000	2.959115000
H	1.210498000	1.329241000	3.502096000
N	0.054551000	0.408901000	2.031242000
H	-0.764091000	0.710350000	1.465344000
C	1.027335000	-0.257614000	1.384711000
O	2.083562000	-0.651361000	1.940004000
C	0.843670000	-0.489838000	-0.123778000
H	1.523834000	-1.317880000	-0.355805000
N	-0.485560000	-0.950731000	-0.540203000
H	-0.519539000	-1.729100000	-1.208695000
C	-1.622584000	-0.215466000	-0.587289000
O	-1.829646000	0.830435000	0.062402000
C	-2.690761000	-0.784383000	-1.523567000
H	-3.186907000	0.087653000	-1.979920000
H	-3.443610000	-1.283816000	-0.896269000
N	-2.134932000	-1.752432000	-2.476664000
H	-2.837835000	-2.419765000	-2.789993000
H	-1.755134000	-1.283207000	-3.301512000
C	1.312471000	0.767709000	-0.923003000
H	0.779877000	1.652688000	-0.550867000
H	2.380642000	0.907859000	-0.703507000
C	1.068067000	0.610640000	-2.405130000
C	1.839313000	-0.267298000	-3.182283000
H	2.678571000	-0.796696000	-2.726125000
C	1.546414000	-0.475559000	-4.531578000
H	2.158929000	-1.158297000	-5.120921000
C	0.475053000	0.193949000	-5.131460000
H	0.248334000	0.033384000	-6.185729000
C	-0.291000000	1.082314000	-4.371895000
H	-1.118040000	1.622711000	-4.833992000
C	0.004192000	1.286612000	-3.020526000
H	-0.601187000	1.976117000	-2.429780000

———— 237\_GFA07: PBE+TS ————

O	-0.559979775	0.732555191	5.509125365
C	-0.749974377	0.116376901	4.475242119
O	-1.987202569	-0.241738818	4.070653443
H	-1.925242848	-0.742001396	3.194445737

```

C  0.403871728 -0.361120014  3.548765387
C  1.768586320  0.068911763  4.070441624
H  2.566300520 -0.340823554  3.437186047
H  1.855447821  1.163052873  4.088002401
H  1.909181631 -0.288569379  5.095965390
H  0.334763406 -1.464322143  3.529094336
N  0.237402870  0.106939716  2.162783471
H  0.957316521  0.730561463  1.758480432
C -0.644456452 -0.430885680  1.295036664
O -1.551262759 -1.225436129  1.636476799
C -0.457130952  0.030563813 -0.167149496
H -0.464183080  1.134423123 -0.150198894
N  0.849075217 -0.371866619 -0.689965904
H  0.918021109 -1.071674566 -1.435491242
C  1.983327435  0.337076711 -0.487195842
O  2.091927532  1.255989006  0.350115239
C  3.158677965 -0.084182630 -1.370230224
H  3.880949101 -0.599049375 -0.720094182
H  3.647426439  0.847510619 -1.700233849
N  2.750327566 -0.989354497 -2.453121621
H  3.511130893 -1.606179525 -2.732842400
H  2.447073160 -0.475187308 -3.281567645
C -1.579102276 -0.484267446 -1.082616501
H -1.648180273 -1.576809281 -0.984539735
H -2.530053441 -0.085187895 -0.703813940
C -1.362703924 -0.094343521 -2.528258970
C -0.960646704 -1.049352384 -3.472917029
H -0.849684484 -2.091872028 -3.166894593
C -0.709368412 -0.688805701 -4.800171569
H -0.406123879 -1.449128044 -5.520620601
C -0.858346096  0.639018717 -5.205773018
H -0.672850976  0.920542426 -6.242540365
C -1.264711073  1.600075223 -4.274310801
H -1.393414019  2.637527280 -4.583984964
C -1.514505488  1.235819849 -2.950238125
H -1.835243373  1.996533255 -2.235262945

```

———— 238\_GFA10: PBE+TS ————

```

O -0.441200603  1.790915481 -3.745707868
C -0.290524547  1.990780480 -2.554857792
O -1.300282321  2.428045844 -1.769525012
H -0.984379800  2.484255103 -0.814527126
C  1.069774757  1.792837824 -1.825348234
C  2.169850321  1.382787911 -2.793625972
H  2.266794170  2.125779389 -3.592150054
H  3.130159464  1.297575736 -2.269070017
H  1.929045363  0.422530958 -3.269562348
H  1.315251416  2.754841393 -1.345814162
N  0.971641184  0.793004784 -0.747869441
H  1.295528100 -0.147932295 -0.966316157
C  0.278363336  0.971665101  0.399113566
O -0.311021709  2.045162324  0.669467103
C  0.184069167 -0.238684165  1.324032861
H  1.129800054 -0.802050693  1.323188890
N -0.051226222  0.225373921  2.671632537
H -0.507947517  1.126489638  2.832518652

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```

C  0.327821519 -0.503818708  3.756628944
O  0.888657819 -1.606528792  3.683263716
C -0.011981508  0.140803649  5.105266872
H  0.853454191 -0.037953668  5.764751580
H -0.843500285 -0.445065255  5.523879435
N -0.426410804  1.546712729  4.991640528
H -1.077841972  1.803519784  5.731937830
H  0.372495690  2.177971009  5.059540790
C -0.948280810 -1.208560473  0.834837514
H -0.995268882 -2.014415424  1.580313554
H -1.902058173 -0.663730919  0.862325293
C -0.685792031 -1.758302649 -0.543535836
C  0.316114941 -2.722284073 -0.747683925
H  0.839023689 -3.145307003  0.112586794
C  0.649505131 -3.140484924 -2.038544142
H  1.427741056 -3.890799648 -2.180675157
C -0.013003214 -2.600953186 -3.145227588
H  0.253312805 -2.920521379 -4.152702234
C -1.020106433 -1.651925179 -2.953262849
H -1.533425704 -1.213640053 -3.808454719
C -1.354528264 -1.239535590 -1.662188451
H -2.122425371 -0.477208982 -1.522326376

```

———— 239\_GFA02: PBE+TS ————

```

O  2.747461526  0.691358312  1.406022667
C  2.831872907  1.554719569  0.543329041
O  3.806418493  2.503720302  0.541859799
H  4.358787508  2.333485128  1.333355733
C  1.868155160  1.719556495 -0.624227133
C  1.058747480  3.026924891 -0.492931751
H  0.397896208  3.117718757 -1.362153678
H  0.444216909  3.004021828  0.416366781
H  1.726121181  3.896304459 -0.460887540
H  2.455628309  1.760189456 -1.556299228
N  1.027965617  0.538722289 -0.633128407
H  1.076192255 -0.052347675  0.193295898
C  0.289754835  0.122469331 -1.694391034
O  0.219303203  0.731565189 -2.768842422
C -0.512461701 -1.178745587 -1.446505503
H -0.230932733 -1.861021200 -2.261080998
N -0.160474119 -1.836307305 -0.200721881
H -0.530275266 -1.510009172  0.696947799
C  0.798188853 -2.809291259 -0.115736878
O  1.358026019 -3.324545122 -1.088310353
C  1.136957858 -3.217744179  1.324549765
H  2.220428119 -3.417660639  1.338171303
H  0.637662288 -4.180021428  1.510288098
N  0.677062030 -2.235962997  2.319598752
H  0.505333746 -2.673227092  3.223571914
H  1.372693253 -1.501017147  2.463756818
C -2.033357758 -0.888253314 -1.529164800
H -2.219603702 -0.407811297 -2.498806718
H -2.560363750 -1.852337050 -1.523908295
C -2.529659740 -0.015479835 -0.399912094
C -2.442459142  1.383911070 -0.481465289
H -2.061828711  1.842085569 -1.395673247

```

C	-2.833394762	2.187871385	0.590321829
H	-2.757358164	3.272654468	0.508298377
C	-3.325162349	1.608575748	1.763951309
H	-3.632770447	2.236949813	2.600353771
C	-3.428790548	0.218878051	1.853731180
H	-3.818159259	-0.243439528	2.761155628
C	-3.035739039	-0.583779886	0.779453401
H	-3.126744570	-1.669437399	0.853918385

———— 240\_GFA11: PBE+TS ————

O	-5.277277767	0.560912828	-0.165229216
C	-4.109064545	0.903703373	-0.189386134
O	-3.676414459	2.024034309	0.430397275
H	-2.679377105	2.114930533	0.302074828
C	-3.0074444056	0.121434429	-0.959447294
C	-3.568225756	-1.103282409	-1.669620566
H	-4.386626298	-0.811021645	-2.336192944
H	-2.783742494	-1.593346452	-2.260815403
H	-3.972317352	-1.824448580	-0.947582211
H	-2.589992213	0.830871222	-1.695684648
N	-1.900858150	-0.282404541	-0.078794069
H	-1.806660245	-1.277990954	0.194768814
C	-0.961055753	0.567786396	0.376683934
O	-1.030521785	1.810780392	0.218631054
C	0.177166369	-0.100080208	1.188532170
H	-0.326098564	-0.516927531	2.079253514
N	0.806359929	-1.220001471	0.488568304
H	1.766363432	-1.122328022	0.138659149
C	0.274331303	-2.455763017	0.369637809
O	-0.888151022	-2.757768566	0.714684853
C	1.212257333	-3.503205489	-0.236070472
H	0.625276773	-4.062140762	-0.982436209
H	1.432547077	-4.214966948	0.572893691
N	2.461138580	-2.929593677	-0.751460612
H	3.264833755	-3.522361234	-0.555085416
H	2.425850645	-2.776983862	-1.758524367
C	1.248605188	0.907279685	1.660744230
H	0.725849758	1.834177538	1.929964653
H	1.703203812	0.504603592	2.576119696
C	2.346874095	1.193934436	0.656981071
C	3.609812338	0.602237427	0.815392643
H	3.794308033	-0.042126886	1.677443530
C	4.637088437	0.834897280	-0.103086479
H	5.613758070	0.373672845	0.044719181
C	4.413175602	1.667044492	-1.200874599
H	5.213581007	1.855851149	-1.916421625
C	3.160784911	2.265838674	-1.368114094
H	2.982053045	2.925288904	-2.218038758
C	2.136141831	2.033840498	-0.449301618
H	1.161942244	2.504232253	-0.580682664

———— 241\_GFA09: PBE+TS ————

O	1.746372660	3.771711423	0.439261100
C	1.958448809	2.584956570	0.272996416
O	2.415559383	1.793597101	1.268844914
H	2.483350970	0.842916256	0.940078126

C 1.757909821 1.869373517 -1.095377979  
C 1.310602513 2.843878283 -2.175610880  
H 1.228264411 2.331445952 -3.142878398  
H 0.341375518 3.291852822 -1.916219308  
H 2.032579921 3.661963218 -2.268212906  
H 2.727858934 1.416299936 -1.360787291  
N 0.783323756 0.768097161 -1.003394333  
H -0.165567691 0.972463008 -1.313699383  
C 0.987754273 -0.380529059 -0.320170472  
O 2.069918988 -0.637119908 0.259451981  
C -0.208384326 -1.322867155 -0.223687493  
H -0.787211623 -1.310817986 -1.160073438  
N 0.271586849 -2.669055085 -0.014823817  
H 1.192252157 -2.831292588 0.400684507  
C -0.467179060 -3.753019810 -0.376651458  
O -1.585889293 -3.679029541 -0.904998137  
C 0.205317393 -5.102042099 -0.098187194  
H 0.477830456 -5.515102444 -1.080138771  
H -0.575863872 -5.764450431 0.309174646  
N 1.411754325 -4.992921554 0.735135619  
H 2.107493167 -5.691789821 0.479830899  
H 1.196048332 -5.127005313 1.723026504  
C -1.165024791 -0.863010337 0.932443249  
H -1.962186978 -1.617598352 0.979231502  
H -0.604449566 -0.899291102 1.876728076  
C -1.731444553 0.512607593 0.696872550  
C -1.215258999 1.627578449 1.373135766  
H -0.447055529 1.485387998 2.134572436  
C -1.635515324 2.919296125 1.051482663  
H -1.197207638 3.772306625 1.568052144  
C -2.590593692 3.114723762 0.050843864  
H -2.914542101 4.122798362 -0.206858870  
C -3.131465182 2.010933432 -0.615142379  
H -3.888248222 2.155783189 -1.386521398  
C -2.704841189 0.719667350 -0.295151487  
H -3.126974006 -0.138566549 -0.821813571

———— 242\_GFA08: PBE+TS ————

O -0.111042758 5.263503970 -0.557430797  
C -0.140112417 4.097782931 -0.908463692  
O 0.497074502 3.666824020 -2.019680468  
H 0.370359453 2.669809398 -2.112911220  
C -0.934075634 2.996345607 -0.150273617  
C -1.687906170 3.555402611 1.048836301  
H -2.297271046 2.770538546 1.515547987  
H -0.994683342 3.959949037 1.797304511  
H -2.343464398 4.374006658 0.732959745  
H -1.645002081 2.575718148 -0.883057575  
N -0.064074366 1.891436314 0.281368529  
H 0.192317422 1.806502315 1.281351329  
C 0.413728733 0.950567239 -0.555977988  
O 0.290456470 1.022164094 -1.802543243  
C 1.199896279 -0.193684556 0.132269724  
H 2.089627991 0.300131691 0.561830896  
N 0.474773382 -0.805317970 1.244743158  
H 0.063716522 -1.738559259 1.130304880

C 0.343004385 -0.261871237 2.474657979  
O 0.721335057 0.889622838 2.778582786  
C -0.354659954 -1.156502899 3.501874818  
H -1.315640923 -0.671408853 3.726889376  
H 0.241154620 -1.094853066 4.427471940  
N -0.590525399 -2.520936064 3.013724647  
H 0.130159177 -3.169806016 3.327859559  
H -1.489232067 -2.886352653 3.322289529  
C 1.674641861 -1.278807969 -0.859347560  
H 1.988707399 -0.765980627 -1.777435806  
H 2.564502586 -1.756231561 -0.427001707  
C 0.652460084 -2.351553712 -1.176640310  
C -0.412137438 -2.118497497 -2.063373953  
H -0.497108366 -1.144980386 -2.545695022  
C -1.347755173 -3.120364852 -2.325950940  
H -2.164474752 -2.924109475 -3.021353081  
C -1.239061438 -4.371979236 -1.712366599  
H -1.968031045 -5.154202941 -1.925102402  
C -0.183829163 -4.617615837 -0.832604149  
H -0.081869828 -5.594431394 -0.359383941  
C 0.751663718 -3.613335083 -0.569168393  
H 1.582859118 -3.816252271 0.109742772

———— 243\_GFA13: PBE+TS ————

O 1.092174000 -0.515175000 -3.090143000  
C 0.062548000 -0.233092000 -3.682046000  
O -0.181113000 -0.620257000 -4.969128000  
H 0.606229000 -1.126257000 -5.258863000  
C -1.093662000 0.617717000 -3.131484000  
C -0.958915000 2.060594000 -3.637026000  
H -0.933093000 2.087392000 -4.732364000  
H -1.813956000 2.653640000 -3.290398000  
H -0.037657000 2.520712000 -3.253697000  
H -2.027201000 0.170008000 -3.498828000  
N -1.095314000 0.590983000 -1.680373000  
H -0.450054000 1.235463000 -1.198999000  
C -1.374605000 -0.579247000 -1.021377000  
O -1.959531000 -1.534679000 -1.541413000  
C -0.824588000 -0.651081000 0.422979000  
H -1.077310000 -1.660568000 0.770478000  
N 0.643371000 -0.604253000 0.368984000  
H 1.154932000 -1.489666000 0.302661000  
C 1.412413000 0.459221000 0.035404000  
O 1.002215000 1.632208000 -0.093706000  
C 2.883054000 0.109662000 -0.194289000  
H 3.424788000 0.326129000 0.739083000  
H 3.244312000 0.820745000 -0.954672000  
N 3.058641000 -1.308316000 -0.536098000  
H 2.837174000 -1.457990000 -1.523099000  
H 4.015882000 -1.617277000 -0.373061000  
C -1.462784000 0.368296000 1.399029000  
H -1.312145000 1.389119000 1.028892000  
H -2.545135000 0.171952000 1.394765000  
C -0.906868000 0.237997000 2.797230000  
C -1.389654000 -0.740337000 3.679005000  
H -2.211125000 -1.389182000 3.366289000

C	-0.835780000	-0.892687000	4.951955000
H	-1.225295000	-1.656705000	5.625818000
C	0.213409000	-0.065669000	5.362525000
H	0.647028000	-0.181929000	6.356169000
C	0.698632000	0.915684000	4.494645000
H	1.515132000	1.567571000	4.807328000
C	0.141600000	1.066358000	3.222988000
H	0.523755000	1.830016000	2.544038000

## ——— 244\_GFA12: PBE+TS ———

O	5.478071576	-0.314101449	-0.031365834
C	4.494858104	0.380826665	-0.220884466
O	4.283971600	1.020990884	-1.389904636
H	3.408336926	1.527131198	-1.343290107
C	3.417368876	0.642538759	0.869601056
C	3.741231884	-0.070259758	2.175484394
H	3.000489438	0.186900633	2.943903195
H	3.748172919	-1.159061743	2.037806816
H	4.735406875	0.223416748	2.528651803
H	3.410472449	1.736917237	1.024992065
N	2.066464193	0.260207568	0.424814420
H	1.563996278	-0.500252316	0.924705398
C	1.355085769	0.975239735	-0.464207546
O	1.825587149	1.948925313	-1.104654861
C	-0.125055283	0.610427028	-0.654464850
H	-0.378003343	1.023526155	-1.638352381
N	-0.432483517	-0.821991398	-0.742142344
H	-1.072890448	-1.116291654	-1.488647292
C	-0.400305274	-1.730695207	0.262417302
O	0.241976866	-1.607799645	1.326008574
C	-1.233086977	-2.986151275	-0.008947228
H	-1.675390319	-3.268904724	0.960634919
H	-0.532878549	-3.789583051	-0.280963796
N	-2.195593191	-2.792067851	-1.100161229
H	-2.430809289	-3.671179522	-1.557813244
H	-3.062480598	-2.369829449	-0.761354556
C	-0.997041146	1.336837609	0.416226530
H	-0.670272983	1.025940389	1.417492952
H	-0.795062342	2.413279535	0.319747462
C	-2.465067873	1.038324724	0.231449105
C	-3.199643695	1.637633081	-0.802966158
H	-2.718321581	2.377232835	-1.446337800
C	-4.538185408	1.303799154	-1.017851012
H	-5.095518003	1.785625418	-1.821373118
C	-5.168470253	0.360482207	-0.200843353
H	-6.215600427	0.104789538	-0.363832306
C	-4.449366750	-0.238272502	0.836957140
H	-4.937484970	-0.961855038	1.490701232
C	-3.109127533	0.098761923	1.049785804
H	-2.553059153	-0.368280748	1.864804949

## ——— 245\_GFA06: PBE+TS ———

O	0.756369461	5.511526619	0.561071458
C	0.835066722	4.454831637	-0.040718048
O	2.000621049	4.005872773	-0.551494845
H	1.848053758	3.121897262	-1.018928954



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C -0.397384767  3.549705001 -0.325551808
C -1.670526979  4.112022301  0.293270180
H -2.535265393  3.490389723  0.026788824
H -1.588480590  4.154489104  1.386798068
H -1.844165639  5.133109006 -0.062009408
H -0.492850953  3.517572553 -1.426517710
N -0.197949653  2.164056047  0.134728114
H -0.859271754  1.777520632  0.829063471
C  0.578058743  1.268715766 -0.511551011
O  1.376092626  1.581986453 -1.425273177
C  0.407926672 -0.188351017 -0.026189586
H  0.497003240 -0.170338601  1.073608081
N -0.934872654 -0.683638194 -0.330490122
H -1.088341336 -1.385982970 -1.060291639
C -2.016105063 -0.427807714  0.440360313
O -2.022150352  0.384206827  1.387983444
C -3.272730384 -1.206919796  0.048293140
H -3.970165936 -0.478653901 -0.390431014
H -3.735026383 -1.550692707  0.988171846
N -2.998043865 -2.267709784 -0.930808855
H -2.775315850 -3.153376334 -0.475519181
H -3.793764446 -2.426709165 -1.546182790
C  1.474964589 -1.117542658 -0.622280971
H  1.432922873 -1.055582346 -1.718922354
H  2.459211732 -0.721493413 -0.336267509
C  1.320776371 -2.551394784 -0.166907572
C  1.604474385 -2.925031221  1.155934557
H  1.970273552 -2.176839367  1.862369037
C  1.436035657 -4.244394234  1.579108330
H  1.668745539 -4.516602225  2.608988146
C  0.981725817 -5.218978842  0.685091171
H  0.862142445 -6.252656551  1.009861011
C  0.700508315 -4.861188670 -0.634837967
H  0.360235353 -5.616761424 -1.343564327
C  0.868737581 -3.538183493 -1.053958613
H  0.660076517 -3.269964291 -2.091741729

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———— 246\_GFA16: PBE+TS ————

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O -5.286024405  0.305922320 -1.320956557
C -4.380434626  0.486292993 -0.522151702
O -4.151672019  1.683589310  0.046603793
H -3.376678280  1.612876509  0.703271794
C -3.491829394 -0.700229011 -0.069285862
C -4.024666834 -1.284905059  1.251734226
H -3.471769004 -2.198899035  1.503386451
H -3.920343763 -0.572146202  2.078854104
H -5.086325749 -1.537674378  1.138695245
H -3.614953723 -1.446586061 -0.862522829
N -2.042823958 -0.435005248 -0.013108984
H -1.416830813 -1.027633126 -0.594281228
C -1.426626606  0.442036508  0.797944696
O -2.019589886  1.302418548  1.498032945
C  0.108915332  0.432654228  0.805926645
H  0.370889302  0.899232888  1.763425830
N  0.749593052 -0.888192580  0.827279763
H  1.537057163 -1.009132199  1.475357378

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C 0.828210798 -1.769053594 -0.200025167  
O 0.049120705 -1.808456654 -1.174835803  
C 1.982984108 -2.766196657 -0.078028962  
H 2.358815053 -2.915872612 -1.103370925  
H 1.555908145 -3.727110757 0.244422548  
N 2.992874050 -2.330869576 0.894132835  
H 3.672553743 -1.700832396 0.462594373  
H 3.502339135 -3.119829991 1.288823456  
C 0.660161645 1.338914780 -0.341077758  
H 0.244188468 1.006289490 -1.301014494  
H 0.287843940 2.356110234 -0.154748866  
C 2.168204050 1.299302489 -0.393107630  
C 2.820936283 0.569046259 -1.396659838  
H 2.227718558 0.091111437 -2.178320232  
C 4.213512909 0.443897135 -1.402909933  
H 4.704044217 -0.117974904 -2.198237287  
C 4.977327039 1.044645983 -0.398622452  
H 6.063539963 0.950416177 -0.403352452  
C 4.336933897 1.782882246 0.601910483  
H 4.925805475 2.266143912 1.381627809  
C 2.946570893 1.910805806 0.601913212  
H 2.459652138 2.492635785 1.387650377

———— 247\_GFA03: PBE+TS ————

O -3.021601151 0.615088002 -1.538196829  
C -3.006745972 1.349031358 -0.564110555  
O -4.140359223 1.767119241 0.069609177  
H -4.885733645 1.368387008 -0.426116514  
C -1.751574193 1.932848268 0.065929422  
C -1.629947723 3.438117299 -0.242768342  
H -2.484606414 3.987445813 0.171247282  
H -0.710375748 3.818468417 0.216093622  
H -1.585635478 3.607833797 -1.326423907  
H -1.810525168 1.801584872 1.157859360  
N -0.626806330 1.152356582 -0.435099070  
H -0.856157520 0.496041923 -1.181560987  
C 0.497052305 0.963847189 0.310956709  
O 0.763457242 1.633419354 1.319260219  
C 1.388910548 -0.197168690 -0.137286143  
H 1.244755914 -0.422726833 -1.204689046  
N 2.771101232 0.185165852 0.059723212  
H 2.998930699 0.870595016 0.784280366  
C 3.796573042 -0.372507061 -0.635950653  
O 3.658547355 -1.240470953 -1.509837974  
C 5.184712866 0.148403298 -0.242440280  
H 5.757321391 0.244814372 -1.180300121  
H 5.661608114 -0.659230082 0.332446611  
N 5.138661134 1.358762113 0.589615926  
H 5.949456635 1.427265387 1.202367171  
H 5.108499026 2.204763165 0.020199038  
C 1.026456484 -1.472769448 0.692798685  
H 1.683157887 -2.277261717 0.334401934  
H 1.281373272 -1.265790400 1.741404734  
C -0.423892482 -1.861982649 0.568986269  
C -0.887301542 -2.557044165 -0.558391460  
H -0.174366163 -2.873777180 -1.322160316

C -2.244980318 -2.842728793 -0.713867261  
H -2.588110611 -3.378918207 -1.598780818  
C -3.163042566 -2.440424485 0.258766765  
H -4.223149987 -2.662008144 0.135479192  
C -2.713934731 -1.753882897 1.389517070  
H -3.422190394 -1.441789676 2.157866102  
C -1.355887126 -1.466934753 1.540705616  
H -1.009124663 -0.919565194 2.419073794

———— 248\_GFA01: PBE+TS ————

O -1.534685909 -0.550675785 -3.041748402  
C -0.573329976 -1.301383787 -3.035844626  
O 0.052922380 -1.714639970 -4.175531781  
H -0.436949657 -1.297162185 -4.914507091  
C 0.044051306 -1.915506784 -1.788776199  
C -0.280867303 -3.419165876 -1.695731264  
H 0.166110043 -3.816800256 -0.777638624  
H -1.366547042 -3.577617777 -1.661733438  
H 0.134196369 -3.960360295 -2.554955811  
H 1.137757608 -1.793948888 -1.838267467  
N -0.455541196 -1.155476539 -0.649968578  
H -1.197867666 -0.490278376 -0.866687575  
C 0.288519086 -0.996035903 0.479925904  
O 1.293630082 -1.675430523 0.733434937  
C -0.160040622 0.148062695 1.392169677  
H -1.226855354 0.375824055 1.247841531  
N 0.032271502 -0.254127214 2.769723913  
H 0.736206535 -0.962787804 2.990193706  
C -0.678801195 0.282904418 3.795541934  
O -1.554447440 1.149693483 3.659521379  
C -0.333328698 -0.288010391 5.177093658  
H -1.184097252 -0.921798492 5.467074527  
H -0.331540832 0.567281277 5.872900831  
N 0.894335736 -1.096000870 5.188143854  
H 1.716915954 -0.529387496 5.394682729  
H 0.850400490 -1.840804597 5.881260330  
C 0.668272232 1.431218841 1.051874596  
H 0.298505745 2.227041198 1.712850588  
H 1.715597810 1.227073561 1.314678389  
C 0.559868670 1.838732408 -0.395057800  
C 1.539775300 1.450348206 -1.321514656  
H 2.409226526 0.890143775 -0.972564353  
C 1.407628566 1.759614538 -2.676698321  
H 2.181372779 1.450284981 -3.380394413  
C 0.288556263 2.463214223 -3.129053075  
H 0.182357421 2.706083242 -4.186559225  
C -0.692776810 2.857726970 -2.216718109  
H -1.570137312 3.404742559 -2.562233738  
C -0.556639136 2.549176018 -0.861600958  
H -1.326857003 2.861522358 -0.153563980

———— 249\_GFA14: PBE+TS ————

O 0.431479679 -3.152508928 -0.780046704  
C 0.123642482 -2.664886302 -1.857006385  
O 0.676893384 -3.078207183 -3.032717369  
H 1.326236139 -3.771865142 -2.793024475

C -0.976048069 -1.604683106 -2.057625724  
C -0.902338920 -0.831256907 -3.378846930  
H -0.962145335 -1.512748768 -4.235000546  
H -1.744085981 -0.129913401 -3.427693232  
H 0.031945828 -0.263462731 -3.441547147  
H -1.915110596 -2.182803127 -2.041076315  
N -1.027408987 -0.729965209 -0.888126068  
H -1.721265822 -0.939542604 -0.162910087  
C 0.115396849 -0.116852358 -0.446440119  
O 1.156516484 -0.056896225 -1.110505549  
C 0.016394957 0.366755565 1.018002811  
H -1.012723409 0.692871463 1.225296330  
N 0.256096198 -0.818986886 1.844589952  
H 1.205194144 -1.195822323 1.937522677  
C -0.721778892 -1.739657529 2.069661047  
O -1.923728142 -1.554490111 1.805466278  
C -0.218980064 -3.051609283 2.673496010  
H -0.897997054 -3.835727009 2.300387506  
H -0.357294790 -2.994107638 3.764135672  
N 1.204544197 -3.267405955 2.380662127  
H 1.316242703 -3.606425564 1.422214842  
H 1.615408913 -3.952981943 3.012613102  
C 1.003004740 1.496421981 1.332949189  
H 1.055433375 1.601552357 2.426086310  
H 1.999972559 1.208196173 0.970073783  
C 0.577922623 2.804907527 0.704731708  
C -0.379896816 3.614120215 1.334596533  
H -0.789076949 3.308771315 2.300011365  
C -0.813455807 4.802862081 0.745463798  
H -1.557744992 5.418845425 1.250875114  
C -0.291460085 5.203441635 -0.487352906  
H -0.630159250 6.130342315 -0.950793882  
C 0.664907102 4.407475266 -1.121936416  
H 1.079482367 4.713510951 -2.082876069  
C 1.094948578 3.217054430 -0.531379943  
H 1.828353659 2.587715535 -1.035764287

———— 250\_GFA05: PBE+TS ————

O -2.142892531 1.485071297 -1.773781536  
C -2.295903621 0.438142392 -2.376441401  
O -2.789509623 0.374064624 -3.650060998  
H -2.951255466 1.300727015 -3.924464359  
C -2.041008109 -0.971575532 -1.823049071  
C -3.344459165 -1.538025149 -1.244364651  
H -3.178850899 -2.558629571 -0.876642908  
H -3.699540152 -0.916272655 -0.410135839  
H -4.124736866 -1.566466378 -2.013896390  
H -1.699230941 -1.590471641 -2.664615339  
N -1.009855602 -0.957650924 -0.798735728  
H -1.313976084 -0.916762004 0.173214802  
C 0.250938776 -0.513408073 -1.091784647  
O 0.622915602 -0.293788438 -2.250861858  
C 1.163284362 -0.284979139 0.119243696  
H 1.156713122 -1.175673324 0.768654880  
N 2.505160268 -0.083281929 -0.378138240  
H 2.637507518 0.089881844 -1.378486129

```
C 3.595775109 -0.225422959 0.416275424
O 3.541474496 -0.512847479 1.622931652
C 4.938429037 -0.014589223 -0.293444697
H 5.399312673 -1.009881619 -0.377715131
H 5.570744583 0.562714435 0.402278077
N 4.804964862 0.564280333 -1.637670329
H 4.795196465 1.584167922 -1.606947631
H 5.574061339 0.284073997 -2.244079151
C 0.677524689 0.932633329 0.975643322
H 1.544209277 1.239075621 1.576941638
H 0.416729902 1.760412197 0.301765260
C -0.476052183 0.603283505 1.889765766
C -1.765943599 1.097003463 1.640735460
H -1.932192839 1.736356672 0.773031779
C -2.833421729 0.756315762 2.476780843
H -3.828097413 1.153387989 2.271192448
C -2.627081792 -0.086444867 3.571167977
H -3.459667029 -0.353737027 4.222050711
C -1.344773047 -0.580869747 3.830617332
H -1.174898310 -1.232693707 4.688006591
C -0.278190251 -0.238520237 2.998212395
H 0.723928173 -0.619109776 3.206927978
```

———— 251\_GFA04: PBE+TS ————

```
O 1.746979000 1.477543000 -2.169293000
C 2.361673000 0.435461000 -2.304132000
O 3.632997000 0.377499000 -2.804433000
H 3.894816000 1.303397000 -2.989793000
C 1.830162000 -0.975819000 -2.011239000
C 1.280237000 -1.599740000 -3.300309000
H 0.435549000 -1.013345000 -3.688130000
H 2.059357000 -1.636144000 -4.070229000
H 0.936170000 -2.623061000 -3.105080000
H 2.679498000 -1.565373000 -1.639957000
N 0.798382000 -0.948871000 -0.987659000
H -0.171343000 -0.909398000 -1.298782000
C 1.085653000 -0.476879000 0.265065000
O 2.244357000 -0.252755000 0.635460000
C -0.127551000 -0.223488000 1.168668000
H -0.772715000 -1.116287000 1.193847000
N 0.362151000 0.018208000 2.507473000
H 1.348147000 0.258595000 2.637379000
C -0.426367000 -0.150077000 3.599556000
O -1.618835000 -0.491381000 3.544499000
C 0.257661000 0.140690000 4.940686000
H -0.113108000 -0.619922000 5.648429000
H -0.143275000 1.105473000 5.285513000
N 1.719763000 0.243066000 4.843013000
H 2.167881000 -0.668959000 4.934637000
H 2.103447000 0.849083000 5.566480000
C -0.991207000 0.972979000 0.643776000
H -1.599087000 1.297577000 1.498905000
H -0.322800000 1.799859000 0.368270000
C -1.898266000 0.611476000 -0.506558000
C -1.645224000 1.072981000 -1.808009000
H -0.779274000 1.711045000 -1.987545000
```

```

C -2.474413000  0.700820000 -2.870447000
H -2.265721000  1.072893000 -3.873997000
C -3.567441000 -0.139470000 -2.648269000
H -4.215223000 -0.428411000 -3.476207000
C -3.831142000 -0.600664000 -1.354653000
H -4.687972000 -1.249225000 -1.171373000
C -3.005571000 -0.227869000 -0.293019000
H -3.218802000 -0.583036000  0.717416000

```

**11.2.8 GGF: PBE+TS**

## ——— 221\_GGF14: PBE+TS ———

```

O -4.328286961 -0.617415876 -1.227713985
C -3.532803360 -0.160123120 -0.423779797
O -3.925361204  0.492800427  0.686770612
H -3.113100275  0.772958346  1.230213132
C -2.008561344 -0.371503652 -0.606332595
H -1.885306304 -0.637323772 -1.662041496
N -1.182690770  0.828148206 -0.410339369
H -0.521256664  1.083256923 -1.165449062
C -0.986305422  1.466683986  0.760507375
O -1.679167427  1.281407149  1.790143749
C  0.150323591  2.497370739  0.751518368
H  0.196282184  2.937484535  1.751791492
H -0.104638903  3.291733118  0.031480578
N  1.457213379  1.946193275  0.416234086
H  2.184462622  1.820175292  1.125488889
C  1.834074534  1.595898808 -0.834960052
O  1.080553696  1.640771591 -1.829642700
C  3.284343462  1.130561780 -0.956989896
H  3.805368487  1.896116839 -1.549947176
H  3.267709491  0.215841564 -1.570445544
N  3.945308577  0.971195799  0.345404053
H  4.927881821  1.236789009  0.303186931
H  3.895426323  0.001331160  0.659307265
C -1.551669308 -1.572133304  0.272084236
H -1.865574042 -1.406995491  1.310750334
H -2.098450079 -2.454662143 -0.092094491
C -0.061814106 -1.817044895  0.236948187
C  0.587362626 -2.232090220 -0.935869541
H  0.011097810 -2.375825560 -1.851330988
C  1.959843570 -2.482519915 -0.943821359
H  2.443943435 -2.815292772 -1.861868352
C  2.710166368 -2.329904478  0.227041618
H  3.775649858 -2.563848403  0.227564133
C  2.079023203 -1.897783710  1.396099690
H  2.651292720 -1.777598313  2.316802066
C  0.706713242 -1.633561348  1.393970098
H  0.216166174 -1.295688574  2.307876511

```

## ——— 222\_GGF13: PBE+TS ———

```

O -4.323447267 -1.145899204  0.700916323
C -3.531819315 -0.362099291  0.203868968
O -3.929956709  0.709248869 -0.508811472
H -3.120324108  1.239288538 -0.817721694
C -2.007801160 -0.524045045  0.428327281
H -1.878822490 -1.560194590  0.760326280

```

N -1.182006548 -0.398221030 -0.780793422  
H -0.536299740 -1.175212633 -1.005471186  
C -0.988756882 0.732051299 -1.489757973  
O -1.680390544 1.771368865 -1.361792292  
C 0.145317754 0.666573200 -2.521938874  
H 0.202053697 1.647968120 -3.001374134  
H -0.121535391 -0.079910364 -3.287451734  
N 1.449600841 0.334728008 -1.964467125  
H 2.179905899 1.040543130 -1.836254716  
C 1.809345928 -0.906909569 -1.569225263  
O 1.045827928 -1.894706615 -1.587858849  
C 3.245417186 -1.024994079 -1.059839148  
H 3.717444698 -1.837638456 -1.630919373  
H 3.169010829 -1.380730698 -0.023046213  
N 4.000772486 0.234955935 -1.141806661  
H 4.804157887 0.157164334 -1.762661584  
H 4.342121609 0.522990227 -0.226755699  
C -1.550427585 0.424661684 1.575558795  
H -1.822368402 1.458474954 1.326564521  
H -2.128803616 0.143218960 2.467444074  
C -0.068655138 0.344305512 1.851487030  
C 0.785662297 1.373960401 1.434544905  
H 0.364550537 2.237355415 0.917019424  
C 2.158995787 1.313561357 1.684091576  
H 2.802081564 2.134877120 1.365945253  
C 2.702643413 0.210755992 2.346534441  
H 3.772109992 0.165696364 2.557289230  
C 1.863474362 -0.831800536 2.752468788  
H 2.278935763 -1.695952718 3.271257546  
C 0.491102624 -0.762707307 2.508005610  
H -0.155766185 -1.576507151 2.840498367

———— 223\_GGF07: PBE+TS ————

O 4.142994390 1.484515685 0.524436482  
C 3.459999016 0.482445803 0.389653675  
O 3.919592792 -0.771323565 0.678802329  
H 4.844125176 -0.645965423 0.978685420  
C 2.021901715 0.492765579 -0.129960043  
H 2.112981294 0.692537876 -1.211995782  
N 1.344307587 -0.780519136 -0.025755269  
H 0.936566111 -1.074338061 0.873222062  
C 0.926707961 -1.454223282 -1.137719593  
O 1.236143554 -1.150215567 -2.295909033  
C -0.015584189 -2.625890304 -0.814131215  
H 0.454060990 -3.291215248 -0.074233015  
H -0.190179439 -3.181265525 -1.739995647  
N -1.294339674 -2.165425903 -0.286153298  
H -2.108703795 -2.034690440 -0.891301015  
C -1.471746420 -1.756201523 0.991822382  
O -0.572107327 -1.749425881 1.856095206  
C -2.893553758 -1.297523649 1.314121137  
H -2.795119843 -0.420817526 1.974386279  
H -3.354214882 -2.097088358 1.912882701  
N -3.696705119 -1.066099665 0.105901725  
H -3.581640658 -0.102913512 -0.218863480  
H -4.688251932 -1.215440935 0.286092303

C	1.229924959	1.628502555	0.557257625
H	1.226685578	1.454188420	1.643926813
H	1.788656031	2.563352915	0.400357302
C	-0.198923124	1.785166429	0.082358886
C	-1.211081184	2.048293499	1.017159608
H	-0.961102069	2.080973924	2.078641735
C	-2.528016290	2.278819623	0.612638261
H	-3.293577520	2.498055935	1.357903681
C	-2.861786185	2.229523928	-0.743878522
H	-3.885062194	2.423577149	-1.067322098
C	-1.868216808	1.938266862	-1.683570230
H	-2.117317445	1.885670389	-2.743485657
C	-0.551344664	1.720801783	-1.274887812
H	0.202837365	1.490205150	-2.027482905

———— 224\_GGF12: PBE+TS ————

O	1.489484887	-3.135985610	-0.039225990
C	0.977349245	-1.910513777	0.284400261
O	1.679515381	-0.933978423	0.479440958
H	2.462864072	-3.025354382	-0.062578394
C	-0.557509214	-1.949361274	0.325800261
H	-0.833754171	-2.871122326	0.856008854
N	-1.076621093	-0.817724350	1.067106916
H	-1.263657117	0.051811211	0.559529637
C	-0.808478958	-0.710609105	2.411754747
O	-0.418041982	-1.659241572	3.097731050
C	-0.958454764	0.714611269	2.969655055
H	-0.797785936	0.672682114	4.051088440
H	-1.958841047	1.116835187	2.758550096
N	0.025018624	1.595789021	2.351124330
H	1.015529932	1.515885273	2.597911814
C	-0.198564773	2.162636846	1.134880945
O	-1.313365710	2.185322987	0.581726357
C	1.044177782	2.742502972	0.460870335
H	1.019823491	3.833957502	0.598483123
H	0.911169774	2.549505437	-0.617422196
N	2.283094252	2.207168727	1.040788339
H	3.080715613	2.805837811	0.832387602
H	2.475015884	1.273422581	0.669858921
C	-1.144427317	-2.008503732	-1.111255519
H	-0.823483291	-2.956330324	-1.563242040
H	-2.237726802	-2.049174692	-1.006915800
C	-0.740354663	-0.847050451	-1.990999679
C	0.444921487	-0.898838766	-2.742129427
H	1.048752561	-1.808150878	-2.731655832
C	0.858621237	0.195659268	-3.501755987
H	1.780114377	0.135569260	-4.081202561
C	0.091909741	1.364502637	-3.523125302
H	0.415804607	2.222029239	-4.113828841
C	-1.094760003	1.423766242	-2.790928586
H	-1.698504800	2.330297824	-2.792206065
C	-1.509515165	0.323309242	-2.037984877
H	-2.438256140	0.386365013	-1.469064943

———— 225\_GGF10: PBE+TS ————

O	-1.249928000	4.254146000	0.167235000
---	--------------	-------------	-------------



```
C -0.173260000  3.456976000  0.474036000
O  0.762450000  3.842098000  1.147674000
H -1.078355000  5.113326000  0.605194000
C -0.355619000  2.060298000 -0.115999000
H -0.637222000  2.188338000 -1.171979000
N  0.883108000  1.317035000 -0.108253000
H  1.236241000  0.916911000  0.772403000
C  1.432390000  0.843710000 -1.265824000
O  1.053809000  1.158272000 -2.400666000
C  2.562654000 -0.171928000 -1.024157000
H  3.317950000  0.264435000 -0.353615000
H  3.022244000 -0.395627000 -1.991036000
N  2.070369000 -1.411720000 -0.434286000
H  1.849110000 -2.228347000 -1.008971000
C  1.761272000 -1.545680000  0.876986000
O  1.877891000 -0.634282000  1.719838000
C  1.252671000 -2.933938000  1.269094000
H  0.422652000 -2.772251000  1.975403000
H  2.062046000 -3.415378000  1.837506000
N  0.905876000 -3.760896000  0.105497000
H  1.068659000 -4.749896000  0.286201000
H -0.079258000 -3.643014000 -0.140824000
C -1.478812000  1.318052000  0.655177000
H -1.220595000  1.301664000  1.725109000
H -2.402509000  1.910910000  0.565028000
C -1.739743000 -0.100570000  0.192701000
C -2.027547000 -1.090184000  1.143688000
H -2.000926000 -0.834548000  2.204038000
C -2.356109000 -2.390987000  0.755339000
H -2.594519000 -3.138194000  1.512967000
C -2.380451000 -2.731361000 -0.600258000
H -2.651588000 -3.741304000 -0.910090000
C -2.065643000 -1.761004000 -1.556191000
H -2.067635000 -2.016753000 -2.615805000
C -1.752831000 -0.458375000 -1.164012000
H -1.503840000  0.277319000 -1.928740000
```

———— 226\_GGF15: PBE+TS ————

```
O  3.898647000 -1.512414000 -0.971106000
C  3.386546000 -0.693886000 -0.229566000
O  4.099307000  0.285911000  0.368971000
H  3.480573000  0.854890000  0.928662000
C  1.880215000 -0.693921000  0.139978000
H  1.843371000 -0.763864000  1.241377000
N  1.229175000  0.571357000 -0.215716000
H  0.569609000  0.610929000 -1.007111000
C  1.329832000  1.671135000  0.560257000
O  2.165470000  1.774635000  1.488248000
C  0.350560000  2.802153000  0.234151000
H  0.631213000  3.238317000 -0.737670000
H  0.467728000  3.568213000  1.006645000
N -1.043157000  2.383961000  0.176366000
H -1.671826000  2.495669000  0.975283000
C -1.585122000  1.742411000 -0.888310000
O -0.932896000  1.412892000 -1.898221000
C -3.080423000  1.457413000 -0.763103000
```

H -3.265810000 0.511263000 -1.293834000  
H -3.599836000 2.248919000 -1.324329000  
N -3.532594000 1.475997000 0.634776000  
H -4.516668000 1.732206000 0.703897000  
H -3.427588000 0.548095000 1.051830000  
C 1.125652000 -1.870286000 -0.483724000  
H 1.197487000 -1.805044000 -1.578583000  
H 1.659730000 -2.790598000 -0.205945000  
C -0.326533000 -1.948433000 -0.059997000  
C -0.692379000 -2.002643000 1.295013000  
H 0.078122000 -1.983621000 2.068044000  
C -2.032457000 -2.089913000 1.674809000  
H -2.292749000 -2.136928000 2.732702000  
C -3.037997000 -2.134776000 0.702544000  
H -4.084372000 -2.225470000 0.996310000  
C -2.687077000 -2.085677000 -0.648847000  
H -3.459943000 -2.132144000 -1.416846000  
C -1.344292000 -1.982290000 -1.022479000  
H -1.080709000 -1.922577000 -2.079221000

———— 227\_GGF04: PBE+TS ————

O -0.361632322 1.247266401 3.873250679  
C 0.424056987 0.421850190 3.450210043  
O 1.451149559 -0.086556828 4.207940330  
H 1.385912688 0.362281720 5.076267344  
C 0.445795398 -0.172516202 2.043535607  
H 0.497241549 -1.266532815 2.155720615  
N -0.782389298 0.109423484 1.338061758  
H -0.943712382 1.042228589 0.935387570  
C -1.607631948 -0.894550967 0.918646029  
O -1.476423167 -2.084389219 1.229448967  
C -2.719752133 -0.405183734 -0.025317818  
H -3.245260708 0.448429364 0.427990158  
H -3.423964191 -1.229937801 -0.169094644  
N -2.195987872 0.005884787 -1.322306159  
H -2.181687287 -0.631702327 -2.121735258  
C -1.587828210 1.196783631 -1.538931618  
O -1.425305355 2.069304383 -0.663840394  
C -1.114617714 1.408841197 -2.978098907  
H -0.147180571 1.931958059 -2.914412297  
H -1.824089670 2.109838328 -3.442431534  
N -1.084488962 0.159037172 -3.749681470  
H -0.182495209 -0.309337296 -3.637122664  
H -1.228203059 0.326731799 -4.744270301  
C 1.687231127 0.346455778 1.271396163  
H 1.672865771 1.447209987 1.273830373  
H 2.586075084 0.042781289 1.830120941  
C 1.782437411 -0.143675144 -0.158797082  
C 2.143316871 0.750444017 -1.176418213  
H 2.293968862 1.803258951 -0.932059925  
C 2.314884337 0.313669427 -2.492357956  
H 2.615369334 1.025823817 -3.261758190  
C 2.102765725 -1.029052561 -2.819186730  
H 2.247774226 -1.376130630 -3.843567372  
C 1.716116680 -1.925178927 -1.817042519  
H 1.542116826 -2.974487808 -2.056790366

C 1.560867101 -1.486587387 -0.501002264  
H 1.252225521 -2.201519722 0.262260104

———— 228\_GGF08: PBE+TS ————

O -4.063909000 -0.737330000 -0.550243000  
C -2.876544000 -0.932736000 0.109639000  
O -2.428313000 -2.039650000 0.342964000  
H -4.401525000 -1.634247000 -0.752269000  
C -2.227050000 0.388640000 0.485803000  
H -2.965745000 0.956738000 1.075421000  
N -1.072289000 0.099749000 1.311841000  
H -0.670602000 -0.849429000 1.288319000  
C -0.400228000 1.079974000 1.974162000  
O -0.768796000 2.262246000 2.020611000  
C 0.883959000 0.593056000 2.672081000  
H 0.633729000 -0.221825000 3.368798000  
H 1.285782000 1.439299000 3.237233000  
N 1.899760000 0.114230000 1.743329000  
H 2.679841000 0.703402000 1.447089000  
C 1.861445000 -1.116519000 1.177306000  
O 0.958661000 -1.947696000 1.383973000  
C 3.031027000 -1.433831000 0.244456000  
H 2.588867000 -1.870023000 -0.665204000  
H 3.604886000 -2.235572000 0.730987000  
N 3.902555000 -0.277318000 -0.013170000  
H 3.641036000 0.181024000 -0.886462000  
H 4.880564000 -0.552347000 -0.083511000  
C -1.898488000 1.269486000 -0.765889000  
H -2.764381000 1.234172000 -1.441498000  
H -1.802339000 2.300199000 -0.405192000  
C -0.631261000 0.879781000 -1.488430000  
C 0.491355000 1.715944000 -1.414646000  
H 0.433039000 2.625791000 -0.815638000  
C 1.666085000 1.406210000 -2.104158000  
H 2.513320000 2.092497000 -2.059662000  
C 1.746677000 0.232865000 -2.858764000  
H 2.656681000 -0.008274000 -3.409997000  
C 0.643881000 -0.625011000 -2.916196000  
H 0.697273000 -1.543932000 -3.500219000  
C -0.535035000 -0.299309000 -2.244011000  
H -1.391100000 -0.971424000 -2.316442000

———— 229\_GGF11: PBE+TS ————

O -0.589937418 3.622335813 -0.964507967  
C 0.461330829 3.074491067 -0.326091504  
O 1.610450263 3.403988311 -0.566569509  
H -1.456148063 3.246181868 -0.595260127  
C 0.080884900 2.045478840 0.777589101  
H -0.493074868 2.624782836 1.522458191  
N -0.799356057 0.985511907 0.281278280  
H -0.402048431 0.049562979 0.202635513  
C -2.104714012 1.142808800 -0.015795561  
O -2.669719879 2.260631601 -0.034069774  
C -2.882864501 -0.135258082 -0.323932186  
H -3.580653578 0.091393920 -1.140174506  
H -3.473470650 -0.378595863 0.573837789

N -2.065880167 -1.287076929 -0.642295963  
H -1.688952753 -1.449535542 -1.580075107  
C -1.825088672 -2.298860518 0.250076947  
O -2.212666488 -2.292917457 1.422333664  
C -1.030145126 -3.466799635 -0.346204665  
H -1.752509245 -4.280653270 -0.508953592  
H -0.340677485 -3.812740925 0.439960209  
N -0.385571804 -3.127787208 -1.623234237  
H 0.557927585 -2.764062407 -1.469756962  
H -0.304920252 -3.944071814 -2.228011795  
C 1.307662596 1.420992805 1.476905895  
H 2.071820775 2.206120880 1.544642961  
H 1.013567033 1.147692912 2.499256037  
C 1.879891140 0.196535155 0.791770999  
C 2.666249687 0.302070108 -0.368590798  
H 2.866308085 1.289435283 -0.784371007  
C 3.186913975 -0.839368037 -0.979242533  
H 3.801633752 -0.738316161 -1.874056564  
C 2.941555564 -2.106901725 -0.439446356  
H 3.371933388 -2.994793190 -0.903803401  
C 2.158429040 -2.224855147 0.710988984  
H 1.972981979 -3.204985570 1.151425342  
C 1.623640010 -1.082085369 1.313557576  
H 1.009878849 -1.184740236 2.210436628

———— 230\_GGF09: PBE+TS ————

O -0.351234568 -2.083803725 -2.241179230  
C -0.227108586 -0.992111444 -2.763960004  
O 0.353859029 -0.821381304 -3.995581400  
H 0.606698606 -1.720704257 -4.290187895  
C -0.665868859 0.334756153 -2.167244751  
H -1.331631890 0.821746721 -2.899351711  
N -1.403671525 0.054795497 -0.950971938  
H -1.325785568 -0.883564156 -0.534474247  
C -2.078548007 1.026453066 -0.277526801  
O -2.221259722 2.184527600 -0.694703356  
C -2.645792928 0.572258940 1.080715822  
H -3.348365583 -0.259785208 0.923302236  
H -3.185670680 1.422823215 1.507224716  
N -1.621677460 0.130796440 2.017890175  
H -1.175096596 0.775356233 2.672485550  
C -1.072214843 -1.108692060 1.966099824  
O -1.416050411 -1.982808040 1.151011480  
C 0.054483350 -1.358114704 2.967308237  
H 0.972385866 -1.426697880 2.365853436  
H -0.113577199 -2.358206220 3.397828232  
N 0.204424061 -0.283883701 3.962627221  
H 1.186056714 -0.112247242 4.173841807  
H -0.265331615 -0.514033755 4.838012050  
C 0.541655018 1.308040886 -1.955637646  
H 1.110977416 1.344202878 -2.893958444  
H 0.110553904 2.302450756 -1.789425209  
C 1.431735223 0.941863168 -0.794176931  
C 2.403475279 -0.065023788 -0.897014909  
H 2.534055163 -0.596526526 -1.840817057  
C 3.216269849 -0.390179277 0.190140681

H	3.968932469	-1.172065804	0.089146721
C	3.076827912	0.294985045	1.400562974
H	3.726501399	0.054892081	2.242897049
C	2.111229842	1.297501636	1.516930945
H	1.992828278	1.841211506	2.454204225
C	1.292344721	1.609796949	0.430709566
H	0.537590945	2.391890321	0.523945582

———— 231\_GGF01: PBE+TS ————

O	2.023685461	-3.076563413	0.961349953
C	1.074963898	-2.341593854	0.740492643
O	0.293978388	-1.893018592	1.740278059
H	-0.423510646	-1.257457300	1.468447753
C	0.781519580	-1.898325314	-0.719372570
H	0.705432030	-2.839008999	-1.281712843
N	-0.450154574	-1.156093608	-0.896878681
H	-0.396985170	-0.142441015	-0.825403834
C	-1.689547170	-1.729130641	-0.894251856
O	-1.894509333	-2.941362589	-0.965205443
C	-2.859637706	-0.737609628	-0.762693848
H	-3.535084651	-1.180956116	-0.017427992
H	-3.395738023	-0.698579181	-1.718942744
N	-2.491149700	0.617483158	-0.377877451
H	-2.689966746	1.431849964	-0.965559958
C	-1.949451467	0.922078030	0.829197104
O	-1.639369283	0.072488732	1.685173676
C	-1.714353943	2.413342593	1.067807201
H	-0.715833717	2.500860318	1.524578576
H	-2.439645917	2.724358755	1.833738685
N	-1.890761928	3.220349781	-0.148193547
H	-0.990302700	3.382428124	-0.602306035
H	-2.298132812	4.130354917	0.061457969
C	1.971107035	-1.070067016	-1.269123013
H	2.891341506	-1.598500643	-0.987891133
H	1.908298189	-1.066610323	-2.365691923
C	1.983942917	0.355502556	-0.759626007
C	2.366283197	0.657371637	0.558856811
H	2.698173468	-0.142427100	1.221670590
C	2.326495503	1.969517987	1.031322371
H	2.625840594	2.181056146	2.057780085
C	1.917175506	3.011650722	0.193021374
H	1.904882140	4.038311136	0.559469280
C	1.543686167	2.728547379	-1.122831767
H	1.253889852	3.535788711	-1.797666447
C	1.569870601	1.410073336	-1.589122792
H	1.283047455	1.195543351	-2.620300247

———— 232\_GGF06: PBE+TS ————

O	-0.522033000	1.556823000	4.113830000
C	-0.385763000	0.525814000	3.485143000
O	-0.640355000	-0.692471000	4.036532000
H	-0.475093000	-1.351266000	3.320394000
C	0.113276000	0.484468000	2.027252000
H	1.194893000	0.687189000	2.092791000
N	-0.013771000	-0.845638000	1.430695000
H	-0.882259000	-1.063527000	0.905714000

C 1.108096000 -1.512504000 0.970958000  
O 2.259912000 -1.230690000 1.301586000  
C 0.780048000 -2.640765000 -0.020479000  
H 0.026349000 -3.316967000 0.411490000  
H 1.700538000 -3.201927000 -0.205742000  
N 0.277262000 -2.119796000 -1.286175000  
H 0.878703000 -2.023328000 -2.109159000  
C -0.985965000 -1.669482000 -1.464362000  
O -1.845547000 -1.626532000 -0.559083000  
C -1.301695000 -1.214490000 -2.887733000  
H -1.901313000 -0.295005000 -2.797252000  
H -1.961146000 -1.981831000 -3.319468000  
N -0.096616000 -1.072589000 -3.714194000  
H 0.255873000 -0.113881000 -3.669606000  
H -0.285014000 -1.291629000 -4.691075000  
C -0.589406000 1.565831000 1.191252000  
H -1.668819000 1.351844000 1.163477000  
H -0.486460000 2.512027000 1.744334000  
C -0.085469000 1.732204000 -0.226949000  
C -0.988667000 2.123990000 -1.227401000  
H -2.043046000 2.248270000 -0.973928000  
C -0.561644000 2.363912000 -2.534683000  
H -1.280576000 2.680637000 -3.291104000  
C 0.785002000 2.196563000 -2.873179000  
H 1.127699000 2.398126000 -3.889047000  
C 1.690296000 1.781749000 -1.892244000  
H 2.740875000 1.636047000 -2.144081000  
C 1.260471000 1.555105000 -0.582533000  
H 1.989925000 1.231761000 0.160654000

———— 233\_GGF03: PBE+TS ————

O -1.498425284 -2.234326485 0.743980690  
C -2.120139276 -1.297177584 1.214563031  
O -3.466963436 -1.340045343 1.444715777  
H -3.759295523 -2.228529487 1.152473736  
C -1.526203425 0.052403447 1.582428095  
H -1.815582134 0.306167000 2.613248874  
N -0.085142162 -0.068933235 1.527336252  
H 0.303834648 -0.706703889 0.836778949  
C 0.750086570 0.732562056 2.244038929  
O 0.362868084 1.554087442 3.082183864  
C 2.248734499 0.553286004 1.949636429  
H 2.731453611 0.230823434 2.882195179  
H 2.637015206 1.549060649 1.696207838  
N 2.578228461 -0.351007844 0.866330187  
H 2.652041305 -1.363449464 0.991879630  
C 2.843118025 0.084449766 -0.402538942  
O 2.864645218 1.272160942 -0.744194297  
C 3.063311493 -1.045685046 -1.414390239  
H 3.886771319 -0.731184495 -2.074181896  
H 2.154879283 -1.064481847 -2.035463399  
N 3.257280129 -2.362735652 -0.786354564  
H 4.245194046 -2.605202068 -0.721585307  
H 2.792523690 -3.103449914 -1.308616474  
C -2.068255939 1.185687361 0.646828579  
H -3.157376044 1.244561386 0.775930890

```

H -1.636720088  2.122344299  1.024754803
C -1.702935114  0.968693291 -0.800568761
C -0.455409252  1.384280944 -1.291217285
H  0.235474618  1.924896983 -0.644039199
C -0.075558175  1.108392150 -2.606581598
H  0.904422611  1.435230505 -2.954275139
C -0.945102896  0.422885516 -3.459040354
H -0.652062845  0.210713023 -4.487817526
C -2.197418006  0.018717659 -2.987874202
H -2.885674640 -0.508339391 -3.649178328
C -2.569922853  0.287424653 -1.669194522
H -3.548544724 -0.033899764 -1.306979700

```

———— 234\_GGF02: PBE+TS ————

```

O  1.888672000 -2.669362000  0.762169000
C  0.821835000 -2.991343000 -0.025862000
O  0.887943000 -3.819637000 -0.919341000
H  2.636683000 -3.213604000  0.439578000
C -0.448703000 -2.237253000  0.352141000
H -1.057310000 -2.964573000  0.919496000
N -0.167549000 -1.109988000  1.223944000
H  0.766038000 -0.671923000  1.227819000
C -1.157890000 -0.482549000  1.913886000
O -2.329820000 -0.880337000  1.964371000
C -0.688749000  0.787885000  2.651993000
H  0.076220000  0.509625000  3.393965000
H -1.558216000  1.196187000  3.175015000
N -0.142708000  1.818235000  1.775524000
H -0.684691000  2.646514000  1.520516000
C  1.096862000  1.770713000  1.235616000
O  1.893018000  0.824427000  1.396560000
C  1.477289000  2.985866000  0.389041000
H  1.924855000  2.589604000 -0.536296000
H  2.282704000  3.501678000  0.931581000
N  0.355413000  3.908761000  0.163102000
H -0.098839000  3.709036000 -0.728661000
H  0.664629000  4.878935000  0.146925000
C -1.281230000 -1.859279000 -0.909266000
H -1.206114000 -2.698018000 -1.614885000
H -2.327388000 -1.776193000 -0.592806000
C -0.854933000 -0.564765000 -1.559063000
C -1.662050000  0.574431000 -1.436757000
H -2.585473000  0.507328000 -0.859669000
C -1.307918000  1.777677000 -2.051972000
H -1.973921000  2.639048000 -1.973324000
C -0.118857000  1.868759000 -2.780266000
H  0.154629000  2.800488000 -3.277664000
C  0.710160000  0.747203000 -2.885196000
H  1.638685000  0.806679000 -3.453549000
C  0.340622000 -0.459114000 -2.287576000
H  0.981303000 -1.334231000 -2.403381000

```

———— 235\_GGF05: PBE+TS ————

```

O -2.072892661  0.751795949  1.820916860
C -2.477359275  1.165860059  0.747586465
O -3.802844300  1.345519726  0.469943882

```

H	-4.289085284	1.072497208	1.275733541
C	-1.602220737	1.499318596	-0.449549131
H	-1.882931861	2.486995453	-0.842388038
N	-0.230445127	1.555853816	0.005087765
H	0.032065574	0.906789279	0.742269847
C	0.731676816	2.291423639	-0.621990293
O	0.497594502	3.070391044	-1.551674726
C	2.158628192	2.101514422	-0.078228248
H	2.477458971	3.056754215	0.362984256
H	2.806356079	1.899226939	-0.940895848
N	2.324577074	1.010406746	0.860609920
H	1.884609660	1.024985023	1.782829418
C	2.829196617	-0.208095813	0.487992208
O	3.366249316	-0.432209591	-0.601555590
C	2.676055450	-1.290877702	1.562982390
H	3.589625034	-1.278992954	2.176708238
H	2.657736470	-2.253875661	1.029426803
N	1.517049997	-1.037578445	2.432610107
H	0.659137176	-1.387180934	1.998561265
H	1.614669568	-1.511730533	3.329781777
C	-1.802910548	0.452126240	-1.599542672
H	-2.869064591	0.427322296	-1.862794033
H	-1.252744578	0.840644687	-2.466825435
C	-1.296601101	-0.916484991	-1.218196799
C	0.038865463	-1.272393665	-1.462788942
H	0.698658854	-0.578436250	-1.984915915
C	0.542183643	-2.504721736	-1.040337874
H	1.583565859	-2.752189674	-1.245870856
C	-0.283567857	-3.401607402	-0.357427726
H	0.105297239	-4.366298611	-0.029524855
C	-1.617359716	-3.061624824	-0.111278768
H	-2.271264904	-3.759013049	0.412742857
C	-2.118242253	-1.831193842	-0.541080796
H	-3.162244762	-1.577251661	-0.347630052

**11.2.9 WGG: PBE+TS**

———— 206\_WGG06: PBE+TS ————

O	-1.710223000	-3.571970000	-0.053708000
C	-0.576005000	-3.256988000	0.285945000
O	0.456199000	-3.289652000	-0.570770000
H	1.277868000	-2.889339000	-0.118901000
C	-0.245577000	-2.803943000	1.718339000
H	0.461400000	-3.528313000	2.157425000
H	-1.173935000	-2.827166000	2.294195000
N	0.310416000	-1.455412000	1.815559000
H	-0.207974000	-0.711097000	2.317082000
C	1.540111000	-1.133823000	1.369323000
O	2.271051000	-1.925474000	0.726329000
C	2.047663000	0.263261000	1.754035000
H	3.017009000	0.390648000	1.263610000
H	2.205973000	0.273274000	2.844975000
N	1.195539000	1.385119000	1.381975000
H	1.474564000	2.007544000	0.621379000
C	0.005949000	1.682020000	1.953384000
O	-0.534693000	0.986556000	2.839963000
C	-0.685608000	2.927993000	1.391514000



H	-1.194678000	3.393681000	2.253422000
N	0.291365000	3.823662000	0.747529000
H	0.797265000	4.374769000	1.443263000
H	-0.186044000	4.483531000	0.131937000
C	-1.793621000	2.490135000	0.380707000
H	-2.048890000	3.378975000	-0.222053000
H	-2.691807000	2.251093000	0.965392000
C	-1.476170000	1.312501000	-0.492057000
C	-2.100520000	0.085161000	-0.386880000
H	-2.896370000	-0.225387000	0.283223000
N	-1.570870000	-0.802493000	-1.299084000
H	-1.810749000	-1.790273000	-1.346687000
C	-0.559777000	-0.176022000	-2.000212000
C	0.300995000	-0.683561000	-2.978918000
H	0.240774000	-1.724680000	-3.293715000
C	1.246772000	0.183920000	-3.515508000
H	1.935766000	-0.178540000	-4.278284000
C	1.330997000	1.524731000	-3.084807000
H	2.081696000	2.179644000	-3.527797000
C	0.480946000	2.023180000	-2.102684000
H	0.577758000	3.053796000	-1.765427000
C	-0.484216000	1.170943000	-1.531162000

———— 207\_WGG08: PBE+TS ————

O	0.475916667	3.343122917	1.994565764
C	0.701757465	3.136264806	0.809728617
O	-0.225010779	3.363760774	-0.137642325
H	0.122713072	3.024683048	-1.033455368
C	2.053332324	2.595181284	0.307660000
H	2.705998589	2.472222994	1.175939609
H	2.500025605	3.342330442	-0.369317716
N	1.961881933	1.306848966	-0.380721811
H	2.398899844	0.466623419	0.027639150
C	1.374851297	1.159741100	-1.586527458
O	0.781357739	2.091538830	-2.180091868
C	1.493603421	-0.230970174	-2.220674644
H	2.555664648	-0.443341642	-2.414923003
H	0.960900983	-0.191652930	-3.175418202
N	0.944077377	-1.326107452	-1.427557488
H	-0.022421615	-1.598550193	-1.598090545
C	1.577295353	-1.855335544	-0.346860198
O	2.665581270	-1.412297833	0.074277171
C	0.871229085	-3.025720522	0.339701288
H	0.117553355	-3.429875390	-0.353709398
N	1.875923913	-4.068124514	0.563629937
H	2.692411632	-3.651353303	1.019635549
H	1.507965020	-4.797249486	1.177326660
C	0.139691769	-2.520436553	1.626593502
H	0.904602191	-2.338938328	2.396311572
H	-0.486579678	-3.354428442	1.986534788
C	-0.669057144	-1.275245696	1.424073351
C	-0.451828199	-0.061261876	2.044416494
H	0.267632219	0.204909341	2.812254664
N	-1.316295806	0.893219474	1.546411636
H	-1.277746289	1.880056906	1.789894759
C	-2.086569026	0.327205433	0.552094531

C -3.035620743 0.905861380 -0.296481349  
H -3.277196658 1.966507807 -0.230056354  
C -3.642689551 0.083023227 -1.241260396  
H -4.381212032 0.504673634 -1.922816939  
C -3.320809575 -1.287786712 -1.330959662  
H -3.829247513 -1.906980418 -2.070200549  
C -2.373449525 -1.861880316 -0.486679698  
H -2.155544951 -2.929103208 -0.555860391  
C -1.724317689 -1.052507246 0.467850319

———— 208\_WGG04: PBE+TS ————

O -1.462798239 2.380894589 -1.949853593  
C -0.844005910 2.631904595 -0.927534404  
O -1.413024946 3.286972115 0.104814371  
H -0.722162193 3.420611846 0.831595742  
C 0.642918150 2.261526110 -0.739597832  
H 1.222391213 3.199103354 -0.716751079  
H 0.957634115 1.672699002 -1.604449930  
N 0.939182125 1.484309110 0.466849842  
H 1.208237697 0.506185055 0.348016545  
C 0.866421601 2.001299882 1.715167431  
O 0.494298777 3.177805329 1.935632150  
C 1.201473592 1.046556127 2.865385950  
H 1.124908921 1.618209286 3.796004146  
H 2.223601719 0.656474488 2.756175131  
N 0.293519504 -0.087460096 2.886544444  
H -0.676072258 0.004271301 3.200168944  
C 0.577997704 -1.250501827 2.236140562  
O 1.682221074 -1.489699548 1.723605304  
C -0.595250950 -2.248581863 2.181386127  
H -0.381384627 -3.006127629 2.952990557  
N -1.850707251 -1.577428906 2.562948550  
H -2.255496788 -1.114628456 1.743036100  
H -2.534942016 -2.253596370 2.902905319  
C -0.628001197 -2.967727473 0.804010656  
H -1.429299499 -3.721251867 0.850000144  
H 0.314593588 -3.516677819 0.678698244  
C -0.832074844 -2.047691846 -0.365981668  
C -2.018556030 -1.473341952 -0.787202105  
H -3.025260186 -1.592665126 -0.398353431  
N -1.805748746 -0.712444778 -1.924197953  
H -2.455687753 -0.031357140 -2.301814748  
C -0.466864008 -0.765318272 -2.255605755  
C 0.221292910 -0.167051725 -3.317804535  
H -0.291759734 0.480007268 -4.027892580  
C 1.587225118 -0.413521295 -3.412707615  
H 2.155824173 0.032332085 -4.228911192  
C 2.250766565 -1.226701345 -2.467288053  
H 3.323060693 -1.392685190 -2.569160596  
C 1.564231187 -1.817950034 -1.412633647  
H 2.089871958 -2.419356426 -0.672893633  
C 0.178053791 -1.596405555 -1.294061911

———— 209\_WGG03: PBE+TS ————

O -1.997216631 3.330789530 0.478371164  
C -0.809741517 3.134112144 0.699540611

```

O  0.132402156  3.376843723 -0.228501965
H  1.031486711  3.041210202  0.112978930
C -0.300545289  2.591368559  2.047772412
H -1.168302576  2.455810640  2.698579648
H  0.367290542  3.344280821  2.498599774
N  0.400881391  1.310548974  1.950788852
H  0.001771016  0.464713825  2.387194133
C  1.602473482  1.173012918  1.353273492
O  2.188467417  2.109523534  0.759356653
C  2.242712592 -0.216090244  1.458302008
H  2.458122712 -0.428446405  2.516371929
H  3.187324411 -0.172782408  0.907811644
N  1.443160528 -1.313931002  0.920974252
H  1.579810193 -1.559952652 -0.058853698
C  0.363320384 -1.841703101  1.561786600
O -0.041385143 -1.402557655  2.658965964
C -0.323625977 -3.029353786  0.865532997
H  0.367215632 -3.438938132  0.113882169
N -0.651198796 -4.113101895  1.794376354
H  0.200479007 -4.569553097  2.127097352
H -1.113089348 -3.718447033  2.619194784
C -1.613274327 -2.546278552  0.147839941
H -2.382784384 -2.378327525  0.916137122
H -1.965088747 -3.384658906 -0.472623237
C -1.425722695 -1.291862375 -0.650079677
C -2.059397384 -0.086212143 -0.428312118
H -2.830700742  0.166694813  0.292158546
N -1.572861105  0.877649984 -1.289401843
H -1.826815085  1.861883122 -1.246039199
C -0.573965266  0.325105355 -2.063314952
C  0.267477313  0.916313282 -3.010602129
H  0.192181140  1.978266950 -3.243469830
C  1.216639234  0.104163999 -3.625331832
H  1.892727349  0.535544498 -4.363080551
C  1.317654993 -1.267863217 -3.312420831
H  2.059220375 -1.878253099 -3.827793947
C  0.481961406 -1.853933940 -2.364779598
H  0.556683976 -2.922461823 -2.155826677
C -0.475945949 -1.055174884 -1.707400244

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———— 210\_WGG05: PBE+TS ————

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O -0.883480367 -1.816377939  0.282711025
C -1.818225655 -1.292520028 -0.297277505
O -2.561372806 -1.946582319 -1.243076545
H -2.184455906 -2.848531048 -1.299979957
C -2.333366445  0.128802725 -0.094408804
H -3.412138079  0.068720868  0.104133403
H -2.193722712  0.684339809 -1.031427398
N -1.663167260  0.811925440  0.984846882
H -0.790697978  1.297452510  0.773837027
C -1.901938698  0.443613230  2.285834210
O -2.880099559 -0.225856011  2.629971650
C -0.803531577  0.875493263  3.271398901
H -1.128781557  0.598095874  4.279086679
H -0.632756453  1.959798776  3.221555701
N  0.450126584  0.208486364  2.945062960

```

H	0.546062363	-0.801765572	3.077263886
C	1.330891734	0.737129022	2.053436383
O	1.255727707	1.903971264	1.629400815
C	2.450201347	-0.230545301	1.620204685
H	3.287876871	-0.034993660	2.311689814
N	2.019838884	-1.616670249	1.844125616
H	2.814387301	-2.255678259	1.825681118
H	1.360106093	-1.904659940	1.113375049
C	2.963350246	0.103481822	0.188871499
H	3.919505414	-0.426108318	0.060302917
H	3.185347394	1.178664031	0.151847483
C	2.035638883	-0.273773663	-0.927718803
C	1.975783133	-1.509635442	-1.538970739
H	2.571026254	-2.398785510	-1.356127024
N	1.006257753	-1.508578819	-2.527839276
H	0.798442614	-2.283986585	-3.143833107
C	0.421435650	-0.258665391	-2.586023492
C	-0.582783795	0.229438313	-3.428474854
H	-1.048476519	-0.403526646	-4.184052506
C	-0.968240246	1.556956682	-3.263624189
H	-1.748793177	1.970781695	-3.901468140
C	-0.362815423	2.374654571	-2.284208367
H	-0.687177118	3.410209900	-2.183315685
C	0.636645855	1.886316618	-1.448251073
H	1.088022730	2.518216651	-0.684616295
C	1.045096518	0.545267276	-1.584486946

## ——— 211\_WGG02: PBE+TS ———

O	2.022390000	-1.127289000	-2.869427000
C	2.546252000	-0.338030000	-2.092024000
O	3.792547000	-0.515692000	-1.626391000
H	3.977092000	0.178417000	-0.912531000
C	1.828817000	0.923236000	-1.573647000
H	0.874131000	1.030532000	-2.095063000
H	2.455815000	1.802187000	-1.789307000
N	1.570017000	0.868963000	-0.137184000
H	0.636610000	0.624434000	0.190618000
C	2.556061000	0.990685000	0.779678000
O	3.758348000	1.135765000	0.460856000
C	2.140389000	0.925432000	2.247970000
H	2.566738000	1.804410000	2.750971000
H	2.614813000	0.028624000	2.674471000
N	0.716236000	0.828085000	2.469913000
H	0.093656000	1.641250000	2.493203000
C	0.094999000	-0.361990000	2.744114000
O	0.691537000	-1.436749000	2.866183000
C	-1.440794000	-0.250408000	2.840874000
H	-1.693147000	-0.499245000	3.883529000
N	-1.887255000	1.133200000	2.583164000
H	-2.707458000	1.361748000	3.143318000
H	-2.149685000	1.251910000	1.601134000
C	-2.075836000	-1.329113000	1.917840000
H	-3.168563000	-1.289123000	2.046676000
H	-1.743348000	-2.312083000	2.275829000
C	-1.704082000	-1.166123000	0.471798000
C	-0.667766000	-1.814862000	-0.175967000

H 0.031947000 -2.543418000 0.220111000  
N -0.594412000 -1.406385000 -1.494278000  
H 0.177999000 -1.610196000 -2.133114000  
C -1.564525000 -0.450517000 -1.720930000  
C -1.849458000 0.287461000 -2.875672000  
H -1.269010000 0.149994000 -3.788180000  
C -2.906441000 1.191731000 -2.817143000  
H -3.156324000 1.782344000 -3.698039000  
C -3.672009000 1.344252000 -1.642001000  
H -4.507523000 2.043860000 -1.638809000  
C -3.384880000 0.612224000 -0.494413000  
H -4.006183000 0.727083000 0.395600000  
C -2.300664000 -0.288435000 -0.506509000

———— 212\_WGG14: PBE+TS ————

O -1.292989814 -3.668137141 -0.222189933  
C -0.709270312 -2.956696396 -1.026566688  
O -1.368937559 -2.229570815 -1.945349553  
H -0.696006230 -1.708746520 -2.499598357  
C 0.830199841 -2.843597800 -1.070038000  
H 1.180224686 -3.263152684 -2.026279315  
H 1.232757139 -3.441693218 -0.249143193  
N 1.349030549 -1.479750610 -0.936007130  
H 1.709628756 -1.202533277 -0.021606231  
C 1.194514716 -0.547240730 -1.899705702  
O 0.565599056 -0.781416501 -2.961776689  
C 1.755277880 0.839917126 -1.634230150  
H 2.383118161 1.122413039 -2.494709862  
H 2.370716311 0.890149392 -0.725915634  
N 0.622773512 1.737133342 -1.471747452  
H -0.292513440 1.489406260 -1.857280509  
C 0.617907308 2.769777172 -0.587688377  
O 1.621478615 3.201046383 -0.004191955  
C -0.789968806 3.313581710 -0.293295865  
H -0.681741244 4.405987425 -0.181412972  
N -1.741578955 2.928813288 -1.350280285  
H -2.702063051 2.965766710 -1.007001320  
H -1.679227867 3.562397568 -2.148499465  
C -1.249557861 2.756184232 1.083826691  
H -2.264738451 3.141945697 1.270811550  
H -0.602350388 3.210479382 1.846759284  
C -1.231039447 1.262032846 1.235411271  
C -2.266341424 0.384759367 0.984597905  
H -3.265693971 0.585123098 0.612951722  
N -1.886585344 -0.908980666 1.293211120  
H -2.410383180 -1.750029806 1.070432417  
C -0.579597238 -0.898963776 1.735534097  
C 0.238114664 -1.954375068 2.154541826  
H -0.131600024 -2.978696697 2.171699350  
C 1.549654580 -1.644705214 2.508460924  
H 2.216980772 -2.440323861 2.839120525  
C 2.025136426 -0.314225955 2.460161418  
H 3.056016144 -0.106891173 2.746188671  
C 1.197794386 0.737334743 2.074676728  
H 1.583201138 1.755253566 2.028715924  
C -0.130471033 0.455886561 1.702466215

## ——— 213\_WGG15: PBE+TS ———

O -1.595209863 -3.326053212 0.765570079  
C -2.314182390 -2.425358270 0.347555929  
O -3.343553752 -1.950058645 1.061066179  
H -3.788313353 -1.190853695 0.545747532  
C -2.109804855 -1.796755900 -1.044989770  
H -2.971489058 -2.085653654 -1.670899420  
H -1.205680407 -2.233988195 -1.476323380  
N -1.955838939 -0.342822811 -1.065575221  
H -1.057501405 0.074322960 -1.365160311  
C -2.939284902 0.518561069 -0.738228487  
O -4.061155953 0.157486631 -0.305163224  
C -2.612183311 2.005253345 -0.937254228  
H -3.497288800 2.570593067 -0.632354278  
H -2.424093731 2.183796419 -2.008331680  
N -1.463481240 2.471652707 -0.168736056  
H -1.577655241 3.137499638 0.596308489  
C -0.181325509 2.213559438 -0.536180390  
O 0.111487674 1.487905568 -1.505593036  
C 0.887544010 2.817049079 0.377113648  
H 1.783233757 2.926193347 -0.257395956  
N 0.411183465 4.079343240 0.971568875  
H 0.522434642 4.862956687 0.326032607  
H 0.945848773 4.303229668 1.812760616  
C 1.209517233 1.829785057 1.539127501  
H 0.387104372 1.909572971 2.267276393  
H 2.117101969 2.210029037 2.038936263  
C 1.382451037 0.400521679 1.141158969  
C 0.484964727 -0.617375672 1.388742871  
H -0.453580363 -0.593850381 1.933990716  
N 0.934149413 -1.796623575 0.826357725  
H 0.389051735 -2.658613637 0.820625562  
C 2.137070952 -1.558950273 0.188154098  
C 2.967402455 -2.422478035 -0.534821975  
H 2.711774425 -3.473756098 -0.670033019  
C 4.135150396 -1.889802906 -1.074214550  
H 4.803951613 -2.535127171 -1.643583171  
C 4.470523543 -0.530911816 -0.896153394  
H 5.395218128 -0.150805824 -1.330270359  
C 3.642016006 0.325804817 -0.179569848  
H 3.913063216 1.375072646 -0.053559468  
C 2.453533532 -0.179729299 0.375437168

## ——— 214\_WGG01: PBE+TS ———

O -3.115468000 -1.131867000 -1.374307000  
C -2.476290000 -0.318443000 -2.031025000  
O -2.572635000 1.002304000 -1.813809000  
H -1.919970000 1.490042000 -2.420845000  
C -1.512686000 -0.741373000 -3.155663000  
H -1.878984000 -0.323513000 -4.107635000  
H -1.529419000 -1.832570000 -3.222115000  
N -0.130874000 -0.313182000 -2.942461000  
H 0.585641000 -0.985388000 -2.616716000  
C 0.250086000 0.980916000 -2.998395000  
O -0.546946000 1.924973000 -3.212683000  
C 1.744408000 1.226742000 -2.754744000

H	1.935431000	2.287529000	-2.941533000
H	2.336301000	0.623192000	-3.460220000
N	2.148924000	0.907676000	-1.391858000
H	2.364673000	1.632946000	-0.700193000
C	2.329633000	-0.353794000	-0.937765000
O	2.106579000	-1.372714000	-1.626853000
C	2.846862000	-0.437884000	0.511399000
H	3.892910000	-0.774535000	0.419108000
N	2.852796000	0.900359000	1.130646000
H	3.621035000	0.991572000	1.794028000
H	1.982875000	1.049959000	1.650872000
C	2.055729000	-1.517685000	1.299062000
H	2.563075000	-1.670494000	2.263822000
H	2.128236000	-2.462828000	0.744913000
C	0.618510000	-1.142710000	1.508936000
C	-0.433411000	-1.451291000	0.667583000
H	-0.437624000	-2.055740000	-0.232839000
N	-1.601916000	-0.884994000	1.131861000
H	-2.479848000	-0.909209000	0.613183000
C	-1.333421000	-0.177337000	2.284169000
C	-2.181785000	0.574393000	3.104247000
H	-3.240393000	0.685971000	2.869415000
C	-1.625366000	1.174362000	4.229939000
H	-2.258488000	1.769803000	4.887585000
C	-0.256656000	1.021589000	4.538339000
H	0.141728000	1.493481000	5.436561000
C	0.587150000	0.276564000	3.720926000
H	1.639850000	0.157200000	3.983689000
C	0.061122000	-0.330134000	2.562232000

———— 215\_WGG07: PBE+TS ————

O	1.296363000	0.233077000	3.671481000
C	0.708624000	1.034188000	2.959756000
O	1.363728000	1.958047000	2.234859000
H	0.689174000	2.509853000	1.713414000
C	-0.831592000	1.070644000	2.846095000
H	-1.186155000	2.023210000	3.270802000
H	-1.230997000	0.246113000	3.441262000
N	-1.350808000	0.937977000	1.481887000
H	-1.715617000	0.025283000	1.205520000
C	-1.198167000	1.900763000	0.548019000
O	-0.571792000	2.964375000	0.780984000
C	-1.758580000	1.633730000	-0.839177000
H	-2.388903000	2.492083000	-1.122726000
H	-2.372927000	0.725116000	-0.888962000
N	-0.626306000	1.471393000	-1.736578000
H	0.289538000	1.855487000	-1.489132000
C	-0.620915000	0.588825000	-2.770488000
O	-1.623865000	0.004849000	-3.202367000
C	0.788430000	0.297659000	-3.314208000
H	0.681450000	0.183759000	-4.406726000
N	1.737104000	1.358563000	-2.930584000
H	1.675508000	2.153141000	-3.569030000
H	2.698021000	1.015976000	-2.963453000
C	1.253220000	-1.078236000	-2.756588000
H	2.269428000	-1.260839000	-3.141914000

H 0.611095000 -1.843684000 -3.213492000  
C 1.234062000 -1.235001000 -1.262855000  
C 2.268816000 -0.983960000 -0.384836000  
H 3.266743000 -0.607427000 -0.583953000  
N 1.889569000 -1.296999000 0.907999000  
H 2.414700000 -1.078891000 1.749239000  
C 0.583354000 -1.741924000 0.897381000  
C -0.234278000 -2.163120000 1.952361000  
H 0.135886000 -2.183777000 2.976686000  
C -1.545647000 -2.518001000 1.641716000  
H -2.213293000 -2.850273000 2.436716000  
C -2.020589000 -2.469252000 0.310919000  
H -3.051103000 -2.756574000 0.102284000  
C -1.192985000 -2.081643000 -0.739887000  
H -1.577247000 -2.035307000 -1.758342000  
C 0.134551000 -1.707404000 -0.457581000

———— 216\_WGG11: PBE+TS ————

O -4.676992000 -0.029939000 0.019901000  
C -3.370095000 0.315236000 0.188839000  
O -2.989394000 1.475767000 0.158138000  
H -5.166275000 0.807506000 -0.123091000  
C -2.503629000 -0.930319000 0.353172000  
H -2.299303000 -1.314047000 -0.657872000  
H -3.093606000 -1.682424000 0.893420000  
N -1.252846000 -0.711161000 1.037934000  
H -0.401302000 -0.540995000 0.509694000  
C -1.204027000 -0.702464000 2.407462000  
O -2.213305000 -0.825155000 3.107629000  
C 0.185842000 -0.549425000 3.036868000  
H 0.209105000 -1.224192000 3.904941000  
H 0.285278000 0.478684000 3.417817000  
N 1.295366000 -0.781027000 2.137098000  
H 1.471902000 -1.693454000 1.707342000  
C 2.267530000 0.144766000 1.884159000  
O 2.336046000 1.253122000 2.428740000  
C 3.256223000 -0.282127000 0.777401000  
H 4.255751000 -0.276834000 1.238248000  
N 2.973019000 -1.651976000 0.305241000  
H 2.378818000 -1.635102000 -0.527356000  
H 3.832778000 -2.138066000 0.055286000  
C 3.219233000 0.804836000 -0.338862000  
H 3.926327000 0.510741000 -1.129447000  
H 3.584863000 1.745481000 0.092787000  
C 1.836046000 0.997394000 -0.889337000  
C 0.886263000 1.861686000 -0.378187000  
H 0.977141000 2.562245000 0.445358000  
N -0.311798000 1.712473000 -1.049771000  
H -1.211778000 2.031643000 -0.689753000  
C -0.174938000 0.709236000 -1.989168000  
C -1.113402000 0.169575000 -2.876526000  
H -2.136728000 0.544691000 -2.911344000  
C -0.688160000 -0.847139000 -3.728024000  
H -1.392762000 -1.285943000 -4.434086000  
C 0.646219000 -1.305027000 -3.705111000  
H 0.950153000 -2.089636000 -4.397693000



C 1.579036000 -0.766270000 -2.824188000  
H 2.611364000 -1.120445000 -2.837095000  
C 1.177219000 0.247606000 -1.931219000

———— 217\_WGG09: PBE+TS ————

O -1.474758649 -0.772033021 -3.738891408  
C -0.210137837 -0.653389207 -3.298948683  
O 0.607980573 -1.557237530 -3.415926130  
H -1.996723079 0.041292802 -3.446521330  
C 0.122013944 0.695409287 -2.634693579  
H -0.142347425 1.509027641 -3.327256572  
H 1.193194104 0.739068817 -2.423798266  
N -0.604124616 0.893092687 -1.383172845  
H -0.128156224 0.699665910 -0.501675089  
C -1.921349514 1.196858025 -1.374251406  
O -2.595044040 1.285778249 -2.425183519  
C -2.571965159 1.452225534 -0.019040885  
H -3.453178184 0.799416629 0.041999750  
H -2.921897405 2.494500674 -0.014823559  
N -1.743829351 1.176045490 1.139829716  
H -1.074864528 1.868513103 1.462405361  
C -1.895444831 0.014432087 1.869187641  
O -2.732345403 -0.842870001 1.572477956  
C -0.951597192 -0.145619792 3.070834410  
H -0.380660780 0.785755805 3.217056951  
N -1.668886818 -0.426355048 4.319430279  
H -2.248399422 0.371537528 4.588779920  
H -2.308122839 -1.211962399 4.165107759  
C 0.034223408 -1.301652235 2.779205629  
H -0.549047032 -2.233986885 2.755610109  
H 0.712269123 -1.369910702 3.643287166  
C 0.797538319 -1.159982293 1.498195097  
C 0.681574059 -1.962972377 0.381406602  
H 0.019994465 -2.805851909 0.209921625  
N 1.573936223 -1.562158897 -0.597667048  
H 1.537380922 -1.862107451 -1.574346202  
C 2.260627663 -0.452086676 -0.143783621  
C 3.238118486 0.328082468 -0.773883178  
H 3.592001110 0.088182377 -1.777145290  
C 3.756898285 1.407980548 -0.064123785  
H 4.520861227 2.033600128 -0.525045160  
C 3.325172630 1.695822485 1.248122806  
H 3.766576149 2.538919321 1.779331073  
C 2.360303568 0.915241094 1.876667472  
H 2.055738278 1.136590321 2.900487274  
C 1.798967791 -0.172711587 1.179762958

———— 218\_WGG13: PBE+TS ————

O -1.636290973 2.421194892 1.698058664  
C -0.824671293 3.109684499 0.874151203  
O 0.103700526 3.782798742 1.294391061  
H -2.323500943 1.924210040 1.141553311  
C -1.156364077 2.994202303 -0.630715197  
H -0.408403207 3.567109621 -1.184194546  
H -2.149463345 3.437003823 -0.804861919  
N -1.152701261 1.622255386 -1.148000579

H -0.321576425 1.317397798 -1.657804719  
C -2.089740493 0.715277059 -0.803699590  
O -3.019504296 0.983558922 -0.001625586  
C -1.953748376 -0.691774947 -1.359878056  
H -1.159625742 -0.787664831 -2.111297986  
H -2.911991809 -0.969979105 -1.826961006  
N -1.625571818 -1.558692362 -0.233850235  
H -1.893232920 -1.242463992 0.693639230  
C -0.835799495 -2.662941173 -0.355835160  
O -0.508394519 -3.144275469 -1.448710629  
C -0.297105661 -3.215027719 0.964833958  
H -0.897159654 -2.817023591 1.801267808  
N -0.433999923 -4.669652715 0.934119861  
H 0.164636463 -5.111188727 1.634025070  
H -0.143152936 -5.006744637 0.011801757  
C 1.175268243 -2.706087400 1.147288234  
H 1.782688321 -3.198930939 0.372911674  
H 1.526693216 -3.088247028 2.118207391  
C 1.375134140 -1.220916154 1.077901369  
C 1.332820680 -0.321419417 2.125082830  
H 1.143158485 -0.498799719 3.179044107  
N 1.605586725 0.957994459 1.671127832  
H 1.499818554 1.813393056 2.208061735  
C 1.805633518 0.916401004 0.306420566  
C 2.092038446 1.947761368 -0.595157185  
H 2.209349232 2.974983636 -0.253265404  
C 2.182445454 1.612129984 -1.944838109  
H 2.398064550 2.389869923 -2.677582500  
C 2.017309308 0.276453589 -2.378532719  
H 2.099142346 0.047865142 -3.441300847  
C 1.774927599 -0.752866621 -1.472164825  
H 1.649365577 -1.777265092 -1.821163429  
C 1.657994782 -0.442891608 -0.103743433

———— 219\_WGG10: PBE+TS ————

O 1.542772533 -0.750897652 3.342682166  
C 2.270819135 -0.348818501 2.441945504  
O 3.283239530 -1.085946761 1.965375561  
H 3.748132793 -0.573241368 1.216268675  
C 2.098615608 1.049225464 1.814187534  
H 2.969084109 1.658265318 2.113303187  
H 1.198493299 1.497657128 2.242542060  
N 1.961537300 1.075942181 0.358628414  
H 1.068335299 1.374388015 -0.070581077  
C 2.951525951 0.735208718 -0.489708329  
O 4.063270234 0.290405449 -0.111623537  
C 2.643853372 0.927937191 -1.981144932  
H 3.533185250 0.610797740 -2.533410971  
H 2.466867121 1.999272168 -2.170487754  
N 1.495155335 0.162352541 -2.453475658  
H 1.611716925 -0.606063289 -3.115466428  
C 0.211303178 0.534420332 -2.212003410  
O -0.089693128 1.507189848 -1.494331459  
C -0.852451450 -0.376903872 -2.827988721  
H -1.741029744 0.263641324 -2.956605480  
N -0.359545511 -0.979169791 -4.080754377

H -0.895372015 -1.818647550 -4.308905283  
H -0.457873775 -0.336423097 -4.868547212  
C -1.200341673 -1.532136395 -1.840930971  
H -0.386358604 -2.271220761 -1.907951934  
H -2.109603851 -2.021488163 -2.230194602  
C -1.385412564 -1.130796103 -0.414135552  
C -0.496613715 -1.383123262 0.610237985  
H 0.441354735 -1.930106823 0.592298666  
N -0.955869224 -0.825228857 1.787542334  
H -0.416512360 -0.818175211 2.653124237  
C -2.155851451 -0.185067877 1.542209869  
C -2.993828790 0.532012018 2.403214739  
H -2.746515415 0.659269631 3.457460499  
C -4.158133186 1.072768716 1.864742994  
H -4.834739408 1.635422318 2.507931998  
C -4.481757035 0.902666948 0.501882468  
H -5.403346953 1.338663181 0.116199187  
C -3.645659967 0.191775172 -0.352389602  
H -3.907518913 0.072047976 -1.404649701  
C -2.460896975 -0.365861046 0.159509912

———— 220\_WGG12: PBE+TS ————

O -1.371487042 -3.584864433 -0.152086856  
C -0.812327481 -2.901122199 -0.994539416  
O -1.499125964 -2.158314608 -1.883948092  
H -0.839653554 -1.682685916 -2.490276444  
C 0.725251196 -2.839111746 -1.130823971  
H 1.004162613 -3.279987224 -2.100704408  
H 1.158706238 -3.440801141 -0.328726917  
N 1.291037658 -1.489494715 -1.043803952  
H 1.710730508 -1.211332568 -0.154275808  
C 1.111430424 -0.567034430 -2.010957755  
O 0.424779467 -0.800194481 -3.038471342  
C 1.691398503 0.820839265 -1.790254207  
H 2.268430490 1.099293154 -2.686354606  
H 2.350980477 0.886633573 -0.915079285  
N 0.556565265 1.708074343 -1.571393408  
H -0.339099895 1.431945307 -1.965718888  
C 0.569644761 2.727953286 -0.664674150  
O 1.606980926 3.155154970 -0.141815968  
C -0.821841209 3.258930204 -0.257520807  
H -0.729199544 4.354997055 -0.235623383  
N -1.967617541 2.915279939 -1.098494900  
H -1.858643331 3.192499887 -2.073142883  
H -2.216529908 1.925875809 -1.042205680  
C -1.094848569 2.789735303 1.201556063  
H -2.062674226 3.219395420 1.495018568  
H -0.326138327 3.234297727 1.847228752  
C -1.110093580 1.298067236 1.382790092  
C -2.199512671 0.455504518 1.266257191  
H -3.234613295 0.695802894 1.043692292  
N -1.826239600 -0.851408746 1.530291982  
H -2.400740897 -1.673754530 1.374876994  
C -0.475994328 -0.885285092 1.810937229  
C 0.349894688 -1.966558695 2.138941915  
H -0.048498500 -2.977890181 2.205062771

C	1.701745202	-1.700253166	2.343888691
H	2.375842901	-2.517694779	2.600076264
C	2.211688278	-0.385332726	2.240810017
H	3.273333730	-0.210695888	2.415631979
C	1.379999443	0.692145002	1.945510216
H	1.786669254	1.699385109	1.863213336
C	0.010883441	0.453526263	1.719734772

**11.2.10 WG: PBE+TS**

## ——— 191\_WG03: PBE+TS ———

O	0.947740363	-3.081887564	-0.688439247
C	1.662145756	-2.100361740	-0.570773100
O	2.426647861	-1.894149199	0.520722811
H	2.839128758	-0.966137721	0.465951580
C	1.788022576	-1.029351939	-1.677674218
H	1.156456089	-1.344149540	-2.512307346
H	2.836219157	-1.005376449	-2.017634109
N	1.379562875	0.314580580	-1.276528542
H	0.512320759	0.721687955	-1.634477005
C	1.997178997	1.043890216	-0.325965463
O	3.012647154	0.650744518	0.299152564
C	1.319785410	2.369955299	0.020621615
H	2.130388563	3.063061239	0.305835370
N	0.510807032	2.846689435	-1.112308581
H	-0.152191143	3.557471822	-0.801573638
H	1.099196637	3.276135859	-1.828704406
C	0.424753167	2.146859748	1.285675795
H	-0.210837793	3.041009465	1.396694340
H	1.094782219	2.130019261	2.155424264
C	-0.385280742	0.885506662	1.264688689
C	-0.001355182	-0.290823758	1.874922538
H	0.861616552	-0.489331604	2.501214463
N	-0.874996798	-1.307361149	1.543616323
H	-0.705586775	-2.290106042	1.725111482
C	-1.837548943	-0.813173706	0.683296369
C	-2.900514222	-1.465391581	0.050825727
H	-3.070470278	-2.533052966	0.188585097
C	-3.728377574	-0.702123592	-0.766805151
H	-4.561251104	-1.180038873	-1.282359330
C	-3.505437944	0.680160488	-0.940061440
H	-4.180499532	1.251834946	-1.576846651
C	-2.439602093	1.322131454	-0.318319062
H	-2.279462481	2.388116273	-0.475309731
C	-1.572248319	0.578031203	0.503219991

## ——— 192\_WG10: PBE+TS ———

O	2.215182592	-2.494116679	0.638414166
C	1.044186946	-1.914405678	1.028670329
O	0.955982486	-1.157922921	1.981238727
H	2.903709913	-2.142234197	1.239906644
C	-0.108918928	-2.361263005	0.155010262
H	-0.289668497	-3.431975470	0.356972978
H	0.165117239	-2.284565279	-0.906581786
N	-1.273721222	-1.544651521	0.408661616
H	-1.308266106	-1.010387904	1.280873854
C	-2.027768500	-1.061692622	-0.620289556

O -1.966316640 -1.484478853 -1.782401647  
 C -2.923549462 0.127703850 -0.247447529  
 H -3.831480307 0.027446666 -0.868063116  
 N -3.194784373 0.164019346 1.198848382  
 H -3.596021142 1.064374791 1.466127029  
 H -3.866408594 -0.558929832 1.462603500  
 C -2.208148080 1.438409706 -0.691598674  
 H -2.872997812 2.279237833 -0.434109941  
 H -2.144919043 1.418153744 -1.788349524  
 C -0.846252594 1.651073630 -0.099459917  
 C -0.557665772 2.242439813 1.111806196  
 H -1.227653234 2.683344443 1.842517025  
 N 0.806754696 2.214884257 1.341806966  
 H 1.260133795 2.514688437 2.195432423  
 C 1.431626021 1.578765925 0.287765572  
 C 2.781708133 1.275487482 0.086601412  
 H 3.540736131 1.558291538 0.817020844  
 C 3.118966166 0.592707620 -1.078971211  
 H 4.161529805 0.336543750 -1.268335356  
 C 2.133271235 0.225604810 -2.019608480  
 H 2.431625400 -0.312729604 -2.919100029  
 C 0.791072123 0.530370672 -1.817178029  
 H 0.038676496 0.216024527 -2.540447649  
 C 0.416483132 1.215591724 -0.645663479

———— 193\_WG06: PBE+TS ————

O -2.044398567 2.289501411 -0.561342630  
 C -1.100764624 2.471071236 0.388175100  
 O -0.219696884 3.306227565 0.276181321  
 H -2.609000876 1.489400120 -0.311100809  
 C -1.232204155 1.560663003 1.627731169  
 H -2.215495783 1.731067641 2.092261937  
 H -0.450723853 1.847664581 2.336599849  
 N -1.085009483 0.132563742 1.339787673  
 H -0.169601318 -0.285182174 1.496805476  
 C -1.971588854 -0.569495132 0.594596610  
 O -3.031726314 -0.058743748 0.160704013  
 C -1.578854123 -1.999982090 0.239438477  
 H -0.869052865 -2.366511499 0.998708627  
 N -2.781974092 -2.827410748 0.288814257  
 H -2.634899333 -3.712927140 -0.197904028  
 H -3.546183397 -2.332329763 -0.179382491  
 C -0.840538124 -1.976946382 -1.150729253  
 H -1.594126653 -1.766318443 -1.923796292  
 H -0.463594459 -2.996802839 -1.330874597  
 C 0.256895472 -0.962116806 -1.219331591  
 C 0.195032129 0.244741109 -1.883176627  
 H -0.579743810 0.631891418 -2.536266402  
 N 1.298570757 1.017939793 -1.571597843  
 H 1.390063248 2.001975557 -1.797596070  
 C 2.084199253 0.337384445 -0.661987355  
 C 3.261563587 0.723371180 -0.014688897  
 H 3.712005982 1.699251608 -0.196048397  
 C 3.829715533 -0.179958629 0.879227037  
 H 4.744487969 0.091948465 1.405028151  
 C 3.243425192 -1.441008244 1.117260176

H 3.721113580 -2.125595685 1.817987947  
C 2.071404340 -1.823968138 0.471223661  
H 1.636035704 -2.806972581 0.657937300  
C 1.465705825 -0.929440834 -0.433005498

———— 194\_WG02: PBE+TS ————

O -1.972459460 2.345673964 -0.564807362  
C -1.012737711 2.497750094 0.373374215  
O -0.093865417 3.287780216 0.239272960  
H -2.562422358 1.567792500 -0.302532411  
C -1.175846017 1.608909610 1.624354677  
H -2.155164336 1.812008171 2.083498692  
H -0.389016301 1.879980359 2.333309368  
N -1.070386814 0.173642923 1.347500140  
H -0.155225295 -0.256077443 1.475127833  
C -1.975554512 -0.505896888 0.599310637  
O -3.026126125 0.032544973 0.174980739  
C -1.629007147 -1.960888064 0.250878289  
H -0.945303752 -2.353418195 1.018538054  
N -2.794388528 -2.839963169 0.193809905  
H -3.185650899 -2.975100308 1.128093566  
H -3.525744249 -2.389469121 -0.364157853  
C -0.890006299 -1.980045598 -1.124431522  
H -1.635838167 -1.772479498 -1.906042332  
H -0.539417790 -3.010766525 -1.279486736  
C 0.220983485 -0.980327348 -1.207629256  
C 0.183513790 0.217441894 -1.888848031  
H -0.585530218 0.614354066 -2.543128825  
N 1.304959157 0.971133287 -1.592631101  
H 1.408187045 1.953734964 -1.820708802  
C 2.077353647 0.288037755 -0.673037140  
C 3.263153789 0.657697298 -0.031644703  
H 3.734379602 1.621713365 -0.224042431  
C 3.813333557 -0.246497556 0.873057392  
H 4.734649825 0.013315034 1.393695236  
C 3.201646431 -1.491826389 1.128624771  
H 3.667264436 -2.178008223 1.836076982  
C 2.020806682 -1.858603344 0.488785995  
H 1.567065247 -2.831217427 0.685225087  
C 1.432775700 -0.962206377 -0.425736034

———— 195\_WG01: PBE+TS ————

O -3.071544774 -0.982389766 1.214551424  
C -3.169859367 0.346955349 1.436998576  
O -3.221702350 0.819275214 2.558401656  
H -3.001994188 -1.147414118 0.214381676  
C -3.249363493 1.221163365 0.165646004  
H -3.302364360 2.265314790 0.485852964  
H -4.180848813 0.968594870 -0.368629575  
N -2.110564403 1.070334149 -0.735516492  
H -1.462866953 1.841983658 -0.924283000  
C -1.840072018 -0.044634143 -1.436654164  
O -2.523348066 -1.096180734 -1.353282820  
C -0.586668933 0.029449722 -2.323147061  
H -0.942767600 -0.117500824 -3.355302657  
N 0.045699725 1.356434831 -2.219210459

```
H 0.376429731 1.683859226 -3.124675622
H 0.848581517 1.324613772 -1.584917388
C 0.349442421 -1.156691239 -1.950943370
H 1.150578246 -1.210205142 -2.702677958
H -0.235917573 -2.082092949 -2.030356743
C 0.925550260 -1.010885822 -0.572613274
C 0.331110593 -1.414057102 0.607051241
H -0.599096861 -1.947477807 0.768711151
N 1.105427312 -1.021465002 1.682411980
H 0.862998894 -1.172975905 2.653857768
C 2.221388213 -0.348186222 1.224938399
C 3.280237383 0.236885950 1.926166560
H 3.322587772 0.211220628 3.015343518
C 4.282854226 0.852132745 1.181962173
H 5.122245413 1.318707613 1.696975670
C 4.234046135 0.875807244 -0.227846823
H 5.040540571 1.358970802 -0.778879057
C 3.180770877 0.291015317 -0.923448721
H 3.168107175 0.306261970 -2.014518511
C 2.142203287 -0.329591442 -0.200727067
```

———— 196\_WG14: PBE+TS ————

```
O 0.437344000 2.333858000 2.629065000
C 0.968688000 1.283576000 1.946305000
O 1.878769000 1.395885000 1.140711000
H 0.903411000 3.133115000 2.306441000
C 0.312898000 -0.024464000 2.333642000
H -0.781192000 0.074073000 2.307426000
H 0.582855000 -0.250396000 3.379892000
N 0.743415000 -1.063414000 1.420694000
H 1.517158000 -0.805888000 0.808280000
C -0.103035000 -2.060776000 1.032679000
O -1.171436000 -2.300545000 1.612606000
C 0.329699000 -2.844772000 -0.210949000
H 1.424294000 -2.758024000 -0.326587000
N -0.028539000 -4.246180000 0.000751000
H -0.918037000 -4.273106000 0.509590000
H -0.157782000 -4.729274000 -0.889581000
C -0.329964000 -2.200782000 -1.479734000
H -1.421729000 -2.296018000 -1.374889000
H -0.036726000 -2.823813000 -2.339256000
C 0.051006000 -0.773513000 -1.726822000
C 1.160311000 -0.323448000 -2.413375000
H 1.918969000 -0.888462000 -2.945758000
N 1.214835000 1.060149000 -2.370870000
H 1.948347000 1.629559000 -2.773062000
C 0.143100000 1.535031000 -1.641436000
C -0.208209000 2.843017000 -1.294027000
H 0.391742000 3.696006000 -1.612731000
C -1.347942000 3.013578000 -0.513528000
H -1.653051000 4.018721000 -0.223214000
C -2.117200000 1.908083000 -0.091514000
H -3.001951000 2.079602000 0.521133000
C -1.764777000 0.608340000 -0.438674000
H -2.359688000 -0.236839000 -0.091041000
C -0.615214000 0.402441000 -1.223998000
```

## ———— 197\_WG07: PBE+TS ————

O	2.271441720	0.567939687	2.719420577
C	1.125893992	0.946773390	2.076754796
O	1.100714310	1.788069123	1.196853758
H	2.994114671	1.073530425	2.292591905
C	-0.085192655	0.220229305	2.636860601
H	-0.219962200	0.545146448	3.683299104
H	0.098921751	-0.863052377	2.660928834
N	-1.247292446	0.466484378	1.822384404
H	-1.406208064	1.393951078	1.423072706
C	-1.940979318	-0.544151338	1.230124022
O	-1.846795950	-1.737065166	1.553585933
C	-2.824742102	-0.096682677	0.049772880
H	-3.834655474	-0.475358740	0.265176148
N	-2.876033378	1.368474990	-0.073208906
H	-2.226354849	1.685666113	-0.799680704
H	-3.810388486	1.691293391	-0.317905738
C	-2.312802153	-0.811471010	-1.244535829
H	-3.073954483	-0.669227377	-2.026240779
H	-2.251483180	-1.888427044	-1.036220225
C	-0.992716953	-0.281336717	-1.717989508
C	-0.812463513	0.731669744	-2.641069023
H	-1.547961341	1.250404266	-3.249021536
N	0.535888399	1.022784265	-2.769538159
H	0.926876135	1.731907159	-3.376605358
C	1.259329659	0.200971756	-1.926143356
C	2.637692921	0.127682146	-1.701750780
H	3.333984034	0.780706134	-2.228705410
C	3.087757344	-0.813837303	-0.781277761
H	4.156749036	-0.902362580	-0.584658876
C	2.185165733	-1.665063585	-0.109050475
H	2.572313000	-2.393698283	0.603164056
C	0.815210259	-1.592253690	-0.336602348
H	0.127607097	-2.248618351	0.196428655
C	0.326597486	-0.639398561	-1.251283607

## ———— 198\_WG09: PBE+TS ————

O	0.434086499	2.360136287	2.618643634
C	0.965743771	1.306956007	1.939573952
O	1.869515276	1.417569788	1.126716213
H	0.892451414	3.158888528	2.284555460
C	0.318120347	0.001519869	2.344553062
H	-0.776535532	0.093361720	2.311992224
H	0.585069161	-0.203522860	3.395698832
N	0.750294220	-1.054237686	1.450058097
H	1.518261152	-0.799949875	0.828111418
C	-0.120941473	-2.031455162	1.052151553
O	-1.202287146	-2.235384663	1.621651464
C	0.308407419	-2.849390021	-0.178238436
H	1.404509383	-2.811022734	-0.280379545
N	-0.095567390	-4.256556562	-0.089560831
H	-1.065980119	-4.283590625	0.242000345
H	0.453584026	-4.725455334	0.634805936
C	-0.314181036	-2.220361394	-1.458097162
H	-1.408724164	-2.312794994	-1.378912178
H	-0.005115210	-2.858222605	-2.297310984



```

C  0.067309099 -0.791674297 -1.702515803
C  1.180441876 -0.347544385 -2.386206660
H  1.947122328 -0.917382860 -2.901836382
N  1.227882232  1.036858731 -2.367103997
H  1.970817326  1.601680899 -2.758464408
C  0.148144339  1.518382390 -1.654034657
C -0.211994489  2.829980266 -1.329977236
H  0.383484315  3.680875726 -1.662318197
C -1.356020496  3.008291551 -0.557358045
H -1.666755627  4.017134348 -0.285712762
C -2.123441127  1.906330583 -0.122242294
H -3.012033317  2.083740413  0.483589135
C -1.764191638  0.603165920 -0.449764871
H -2.357182316 -0.239566077 -0.093644518
C -0.608674102  0.389100109 -1.224678358

```

———— 199\_WG15: PBE+TS ————

```

O -2.880749255  0.819424039  0.336735699
C -2.293979698  0.259252342 -0.572722140
O -1.585787786  0.917908592 -1.535307467
H -1.491549140  1.854877632 -1.251259886
C -2.240292308 -1.248076360 -0.797896763
H -2.883326613 -1.496268605 -1.659066159
H -2.632126223 -1.754881165  0.090554809
N -0.877012009 -1.701906288 -1.014025871
H -0.264382180 -1.178384917 -1.643642827
C -0.228248288 -2.493536832 -0.109046663
O -0.776951372 -3.100613230  0.818241208
C  1.298209671 -2.519917585 -0.288650192
H  1.612860919 -3.560298228 -0.094181683
N  1.695258926 -2.037232818 -1.624009115
H  2.692789251 -1.820140234 -1.638307033
H  1.538537126 -2.756884259 -2.332442805
C  1.920954143 -1.627761242  0.830566171
H  2.976836926 -1.446753938  0.569424356
H  1.928908762 -2.228833950  1.748885091
C  1.202654990 -0.339795517  1.109532866
C  0.308312617 -0.162766167  2.145124288
H -0.008871453 -0.873762538  2.900772375
N -0.220783652  1.113120299  2.107873255
H -1.016836393  1.423564300  2.651479397
C  0.291506458  1.780561019  1.013704203
C -0.006321658  3.054572702  0.517433971
H -0.719616490  3.705921659  1.022530307
C  0.641342970  3.457493752 -0.649983645
H  0.437013558  4.445063330 -1.063515424
C  1.565318230  2.609271294 -1.297455861
H  2.054524073  2.954262326 -2.208163076
C  1.852944187  1.342431373 -0.800630007
H  2.548066516  0.693265694 -1.330525524
C  1.208067192  0.896443521  0.366974146

```

———— 200\_WG13: PBE+TS ————

```

O -2.560542268 -0.610244704 -2.419899106
C -1.936542727 -0.986283148 -1.269383087
O -1.060817674 -1.834965985 -1.226707545

```

H -2.127596039 -1.114337731 -3.139955540  
C -2.491734054 -0.255977159 -0.064643980  
H -3.542813026 -0.565490299 0.070480259  
H -2.504963055 0.828519911 -0.242188846  
N -1.674123320 -0.547606997 1.093204687  
H -1.061715428 -1.357111554 0.994221221  
C -1.287624922 0.446394119 1.952223900  
O -1.820027671 1.563983540 1.968057129  
C -0.106645574 0.109944540 2.885973738  
H -0.356473237 0.596000852 3.841262650  
N 0.187485166 -1.299813444 3.147542331  
H -0.642539746 -1.829935403 3.412386244  
H 0.626524046 -1.749116937 2.340053889  
C 1.173982880 0.808680276 2.340320290  
H 1.955232037 0.679561233 3.102351055  
H 0.963947713 1.883790111 2.260065963  
C 1.642576891 0.266611521 1.022253270  
C 2.528251114 -0.776044818 0.830237428  
H 3.090690647 -1.346129605 1.563259812  
N 2.672984440 -1.031334850 -0.523837634  
H 3.254329239 -1.756841052 -0.923601492  
C 1.877145250 -0.157397255 -1.238965570  
C 1.672015164 -0.041286110 -2.617268492  
H 2.177981046 -0.698919941 -3.324685611  
C 0.791103686 0.944281873 -3.052904623  
H 0.609368887 1.066309669 -4.120897008  
C 0.137093610 1.795539043 -2.136581126  
H -0.542842951 2.559399607 -2.513460172  
C 0.342956159 1.676797785 -0.766077399  
H -0.177055019 2.334655339 -0.069284848  
C 1.218607736 0.681244572 -0.293221785

———— 201\_WG12: PBE+TS ————

O 1.812615885 -2.894820362 -0.483666528  
C 2.304349389 -1.780109769 -0.429918514  
O 3.001756427 -1.349212461 0.642037497  
H 3.183577275 -0.357028524 0.531052794  
C 2.193000461 -0.762890898 -1.586891602  
H 1.708667276 -1.266176759 -2.427946710  
H 3.205707464 -0.454887219 -1.889279519  
N 1.413843717 0.430167976 -1.253925238  
H 0.450443716 0.476876451 -1.577051454  
C 1.807003244 1.344022085 -0.333840124  
O 2.906103223 1.252279237 0.264347677  
C 0.822746816 2.476552187 -0.000816656  
H 1.461061973 3.340008949 0.241391911  
N -0.114982752 2.884014289 -1.045588869  
H -0.870383025 2.213792698 -1.198102496  
H 0.345250553 3.085057911 -1.932905813  
C 0.053181972 2.079739046 1.301154280  
H -0.690635436 2.869701299 1.481250454  
H 0.768467671 2.105388735 2.133693213  
C -0.576698551 0.719909427 1.222850500  
C 0.004320095 -0.445225081 1.680650425  
H 0.925109410 -0.584247347 2.237103622  
N -0.740254038 -1.538783926 1.282324699

```

H -0.433180215 -2.501120377 1.370684589
C -1.818860891 -1.105216961 0.536241317
C -2.830987168 -1.831599609 -0.099722817
H -2.851636823 -2.921116509 -0.067715131
C -3.811575791 -1.112494763 -0.776960412
H -4.612983045 -1.648161030 -1.285145363
C -3.793751850 0.297817040 -0.805418043
H -4.590905587 0.829245647 -1.325082223
C -2.786298767 1.019385885 -0.172690177
H -2.806307043 2.110493320 -0.179402415
C -1.760657584 0.322389414 0.499196127

```

———— 202\_WG08: PBE+TS ————

```

O 0.617709834 -0.846314942 3.747906394
C 1.102886071 0.336527147 3.319021116
O 1.760533115 1.073484802 4.033497788
H 0.120855455 -1.302683639 2.991212423
C 0.826270394 0.678025536 1.841705780
H 1.439949845 0.007833065 1.214742900
H 1.163322196 1.704482323 1.676316682
N -0.569760070 0.585140751 1.416813015
H -1.038936166 1.394034394 1.001613810
C -1.241737312 -0.572162914 1.263301902
O -0.833623402 -1.678410143 1.692316432
C -2.539631211 -0.466928658 0.460016889
H -3.238250607 -1.192651643 0.909692991
N -3.044448044 0.916335584 0.478263125
H -3.670825067 1.088369615 -0.308799801
H -3.568191600 1.105739146 1.334360169
C -2.267877418 -0.939658006 -1.000836002
H -3.228885115 -0.904936731 -1.538863348
H -1.981719725 -1.999514954 -0.950311502
C -1.227262288 -0.157414264 -1.745135979
C -1.437408990 0.966765466 -2.516130881
H -2.365290074 1.468671135 -2.771091545
N -0.230345006 1.448855661 -2.992079358
H -0.121454403 2.235634725 -3.619825938
C 0.792610655 0.630584672 -2.547568841
C 2.171196715 0.702996362 -2.772325967
H 2.607462360 1.495976153 -3.380538276
C 2.967360205 -0.279428634 -2.191131187
H 4.045719381 -0.255854515 -2.347384217
C 2.401811823 -1.308861410 -1.409635803
H 3.055420976 -2.064684201 -0.974006615
C 1.030093815 -1.376607996 -1.185772996
H 0.612268392 -2.170390996 -0.567010786
C 0.196666266 -0.395140891 -1.756528374

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———— 203\_WG11: PBE+TS ————

```

O 1.623774828 -0.373258520 -1.515991872
C 2.639698021 0.176849727 -0.790912995
O 3.629245775 -0.440184152 -0.440064363
H 1.801307864 -1.337041823 -1.555958490
C 2.413866075 1.658997304 -0.496927297
H 3.040838860 2.233713141 -1.196351777
H 2.788340053 1.844157948 0.517580573

```

N 1.040644776 2.097478703 -0.556700502  
H 0.528275967 2.176535784 -1.436736999  
C 0.275867095 2.226000676 0.561920406  
O 0.713593422 2.149756507 1.718817176  
C -1.221724222 2.464241267 0.285508468  
H -1.445423168 3.444154961 0.733649257  
N -1.507750846 2.529500180 -1.157224524  
H -2.210615993 3.237339158 -1.364496151  
H -1.868496492 1.625699795 -1.479983284  
C -2.063347743 1.394009001 1.050559406  
H -3.106372712 1.742413646 1.075552257  
H -1.701005619 1.363217520 2.087101096  
C -1.999124875 0.036428102 0.418521858  
C -2.890450334 -0.460381157 -0.513335783  
H -3.817057771 -0.029067606 -0.880541596  
N -2.474998927 -1.707639189 -0.951095839  
H -2.972831536 -2.291909641 -1.610621455  
C -1.301042101 -2.046280562 -0.303517775  
C -0.501373343 -3.188045831 -0.423463574  
H -0.765102232 -3.998405054 -1.104112570  
C 0.641094623 -3.255861357 0.371280610  
H 1.285513235 -4.132661628 0.308302412  
C 0.970952161 -2.214232107 1.264944406  
H 1.876475837 -2.297178864 1.864873814  
C 0.177392881 -1.077965909 1.375495787  
H 0.458607366 -0.268385820 2.048280562  
C -0.976287929 -0.971578200 0.575473758

———— 204\_WG04: PBE+TS ————

O 0.873333121 -0.300753688 -4.016765899  
C -0.328533263 -0.856710777 -3.763691553  
O -1.012652849 -1.365079247 -4.635178414  
H 1.275175208 0.049193174 -3.153238072  
C -0.766842209 -0.854166113 -2.284236751  
H -0.124729901 -1.563323517 -1.734124190  
H -1.794318124 -1.226139760 -2.245157317  
N -0.721864364 0.443197377 -1.616231704  
H -1.573248223 0.902070774 -1.279320220  
C 0.406413505 1.100467928 -1.298334761  
O 1.549001797 0.751951685 -1.690174908  
C 0.220765681 2.327487259 -0.396487480  
H 0.674899837 3.162200272 -0.951220684  
N -1.204724639 2.608031979 -0.165795931  
H -1.463421621 2.351880262 0.791866729  
H -1.425366964 3.591924950 -0.306571679  
C 1.037394360 2.139584559 0.921687512  
H 1.141839609 3.129285215 1.389635263  
H 2.046248129 1.800034651 0.648192761  
C 0.392632314 1.192572893 1.887516401  
C -0.391559776 1.549209638 2.968603771  
H -0.622256871 2.536262235 3.357788778  
N -0.871777506 0.415330012 3.601241399  
H -1.425920153 0.408492131 4.448747193  
C -0.399994340 -0.706041472 2.942490194  
C -0.605087460 -2.063872669 3.210186008  
H -1.219159831 -2.391895795 4.049430824

C	0.013130873	-2.982347420	2.367351106
H	-0.122598014	-4.048678256	2.547606706
C	0.822759710	-2.557090568	1.292455216
H	1.304800576	-3.304743888	0.662308302
C	1.026290638	-1.206775634	1.029914898
H	1.663856308	-0.893794415	0.203102179
C	0.401978443	-0.251173775	1.854645324

———— 205\_WG05: PBE+TS ————

O	-4.634913875	-0.748225537	0.028988096
C	-4.480370396	0.411808817	0.697732571
O	-5.423281842	1.094473956	1.058357467
H	-3.725632260	-1.163418956	-0.142241421
C	-3.023833950	0.800924303	1.032094962
H	-2.661491220	0.101202141	1.804607709
H	-3.046568816	1.805566844	1.462448837
N	-2.090363559	0.800473463	-0.090136717
H	-1.637745850	1.660225944	-0.415852164
C	-1.671707225	-0.307412874	-0.728203211
O	-2.143742574	-1.450020288	-0.505447379
C	-0.583171669	-0.079058658	-1.789270824
H	-1.089846724	-0.236766717	-2.755621740
N	-0.105303332	1.313929886	-1.747443075
H	0.143696079	1.642481623	-2.679406839
H	0.734270766	1.381624416	-1.164494933
C	0.521914324	-1.158450437	-1.639309668
H	1.172834386	-1.105478368	-2.524567054
H	0.036321029	-2.143171833	-1.651928102
C	1.332977879	-0.986664788	-0.388798616
C	1.033710714	-1.498995124	0.857585518
H	0.206035154	-2.133977890	1.156597977
N	1.984751822	-1.086392313	1.775590856
H	2.011117766	-1.356722546	2.750713538
C	2.927203419	-0.299707009	1.138884975
C	4.072535951	0.329622241	1.638031094
H	4.354204468	0.249071043	2.688450717
C	4.848819152	1.056987459	0.740579422
H	5.752348487	1.554218655	1.092212785
C	4.493462817	1.151852169	-0.621531683
H	5.133680761	1.718542799	-1.297461351
C	3.353542805	0.525961550	-1.114557782
H	3.100919706	0.599279912	-2.173435817
C	2.542166809	-0.214832882	-0.232249147

———— 206\_WGG06: PBE+TS ————

O	-1.710223000	-3.571970000	-0.053708000
C	-0.576005000	-3.256988000	0.285945000
O	0.456199000	-3.289652000	-0.570770000
H	1.277868000	-2.889339000	-0.118901000
C	-0.245577000	-2.803943000	1.718339000
H	0.461400000	-3.528313000	2.157425000
H	-1.173935000	-2.827166000	2.294195000
N	0.310416000	-1.455412000	1.815559000
H	-0.207974000	-0.711097000	2.317082000
C	1.540111000	-1.133823000	1.369323000
O	2.271051000	-1.925474000	0.726329000

C	2.047663000	0.263261000	1.754035000
H	3.017009000	0.390648000	1.263610000
H	2.205973000	0.273274000	2.844975000
N	1.195539000	1.385119000	1.381975000
H	1.474564000	2.007544000	0.621379000
C	0.005949000	1.682020000	1.953384000
O	-0.534693000	0.986556000	2.839963000
C	-0.685608000	2.927993000	1.391514000
H	-1.194678000	3.393681000	2.253422000
N	0.291365000	3.823662000	0.747529000
H	0.797265000	4.374769000	1.443263000
H	-0.186044000	4.483531000	0.131937000
C	-1.793621000	2.490135000	0.380707000
H	-2.048890000	3.378975000	-0.222053000
H	-2.691807000	2.251093000	0.965392000
C	-1.476170000	1.312501000	-0.492057000
C	-2.100520000	0.085161000	-0.386880000
H	-2.896370000	-0.225387000	0.283223000
N	-1.570870000	-0.802493000	-1.299084000
H	-1.810749000	-1.790273000	-1.346687000
C	-0.559777000	-0.176022000	-2.000212000
C	0.300995000	-0.683561000	-2.978918000
H	0.240774000	-1.724680000	-3.293715000
C	1.246772000	0.183920000	-3.515508000
H	1.935766000	-0.178540000	-4.278284000
C	1.330997000	1.524731000	-3.084807000
H	2.081696000	2.179644000	-3.527797000
C	0.480946000	2.023180000	-2.102684000
H	0.577758000	3.053796000	-1.765427000
C	-0.484216000	1.170943000	-1.531162000

## ——— 207\_WGG08: PBE+TS ———

O	0.475916667	3.343122917	1.994565764
C	0.701757465	3.136264806	0.809728617
O	-0.225010779	3.363760774	-0.137642325
H	0.122713072	3.024683048	-1.033455368
C	2.053332324	2.595181284	0.307660000
H	2.705998589	2.472222994	1.175939609
H	2.500025605	3.342330442	-0.369317716
N	1.961881933	1.306848966	-0.380721811
H	2.398899844	0.466623419	0.027639150
C	1.374851297	1.159741100	-1.586527458
O	0.781357739	2.091538830	-2.180091868
C	1.493603421	-0.230970174	-2.220674644
H	2.555664648	-0.443341642	-2.414923003
H	0.960900983	-0.191652930	-3.175418202
N	0.944077377	-1.326107452	-1.427557488
H	-0.022421615	-1.598550193	-1.598090545
C	1.577295353	-1.855335544	-0.346860198
O	2.665581270	-1.412297833	0.074277171
C	0.871229085	-3.025720522	0.339701288
H	0.117553355	-3.429875390	-0.353709398
N	1.875923913	-4.068124514	0.563629937
H	2.692411632	-3.651353303	1.019635549
H	1.507965020	-4.797249486	1.177326660
C	0.139691769	-2.520436553	1.626593502

H 0.904602191 -2.338938328 2.396311572  
H -0.486579678 -3.354428442 1.986534788  
C -0.669057144 -1.275245696 1.424073351  
C -0.451828199 -0.061261876 2.044416494  
H 0.267632219 0.204909341 2.812254664  
N -1.316295806 0.893219474 1.546411636  
H -1.277746289 1.880056906 1.789894759  
C -2.086569026 0.327205433 0.552094531  
C -3.035620743 0.905861380 -0.296481349  
H -3.277196658 1.966507807 -0.230056354  
C -3.642689551 0.083023227 -1.241260396  
H -4.381212032 0.504673634 -1.922816939  
C -3.320809575 -1.287786712 -1.330959662  
H -3.829247513 -1.906980418 -2.070200549  
C -2.373449525 -1.861880316 -0.486679698  
H -2.155544951 -2.929103208 -0.555860391  
C -1.724317689 -1.052507246 0.467850319

———— 208\_WGG04: PBE+TS ————

O -1.462798239 2.380894589 -1.949853593  
C -0.844005910 2.631904595 -0.927534404  
O -1.413024946 3.286972115 0.104814371  
H -0.722162193 3.420611846 0.831595742  
C 0.642918150 2.261526110 -0.739597832  
H 1.222391213 3.199103354 -0.716751079  
H 0.957634115 1.672699002 -1.604449930  
N 0.939182125 1.484309110 0.466849842  
H 1.208237697 0.506185055 0.348016545  
C 0.866421601 2.001299882 1.715167431  
O 0.494298777 3.177805329 1.935632150  
C 1.201473592 1.046556127 2.865385950  
H 1.124908921 1.618209286 3.796004146  
H 2.223601719 0.656474488 2.756175131  
N 0.293519504 -0.087460096 2.886544444  
H -0.676072258 0.004271301 3.200168944  
C 0.577997704 -1.250501827 2.236140562  
O 1.682221074 -1.489699548 1.723605304  
C -0.595250950 -2.248581863 2.181386127  
H -0.381384627 -3.006127629 2.952990557  
N -1.850707251 -1.577428906 2.562948550  
H -2.255496788 -1.114628456 1.743036100  
H -2.534942016 -2.253596370 2.902905319  
C -0.628001197 -2.967727473 0.804010656  
H -1.429299499 -3.721251867 0.850000144  
H 0.314593588 -3.516677819 0.678698244  
C -0.832074844 -2.047691846 -0.365981668  
C -2.018556030 -1.473341952 -0.787202105  
H -3.025260186 -1.592665126 -0.398353431  
N -1.805748746 -0.712444778 -1.924197953  
H -2.455687753 -0.031357140 -2.301814748  
C -0.466864008 -0.765318272 -2.255605755  
C 0.221292910 -0.167051725 -3.317804535  
H -0.291759734 0.480007268 -4.027892580  
C 1.587225118 -0.413521295 -3.412707615  
H 2.155824173 0.032332085 -4.228911192  
C 2.250766565 -1.226701345 -2.467288053

H 3.323060693 -1.392685190 -2.569160596  
C 1.564231187 -1.817950034 -1.412633647  
H 2.089871958 -2.419356426 -0.672893633  
C 0.178053791 -1.596405555 -1.294061911

———— 209\_WGG03: PBE+TS ————

O -1.997216631 3.330789530 0.478371164  
C -0.809741517 3.134112144 0.699540611  
O 0.132402156 3.376843723 -0.228501965  
H 1.031486711 3.041210202 0.112978930  
C -0.300545289 2.591368559 2.047772412  
H -1.168302576 2.455810640 2.698579648  
H 0.367290542 3.344280821 2.498599774  
N 0.400881391 1.310548974 1.950788852  
H 0.001771016 0.464713825 2.387194133  
C 1.602473482 1.173012918 1.353273492  
O 2.188467417 2.109523534 0.759356653  
C 2.242712592 -0.216090244 1.458302008  
H 2.458122712 -0.428446405 2.516371929  
H 3.187324411 -0.172782408 0.907811644  
N 1.443160528 -1.313931002 0.920974252  
H 1.579810193 -1.559952652 -0.058853698  
C 0.363320384 -1.841703101 1.561786600  
O -0.041385143 -1.402557655 2.658965964  
C -0.323625977 -3.029353786 0.865532997  
H 0.367215632 -3.438938132 0.113882169  
N -0.651198796 -4.113101895 1.794376354  
H 0.200479007 -4.569553097 2.127097352  
H -1.113089348 -3.718447033 2.619194784  
C -1.613274327 -2.546278552 0.147839941  
H -2.382784384 -2.378327525 0.916137122  
H -1.965088747 -3.384658906 -0.472623237  
C -1.425722695 -1.291862375 -0.650079677  
C -2.059397384 -0.086212143 -0.428312118  
H -2.830700742 0.166694813 0.292158546  
N -1.572861105 0.877649984 -1.289401843  
H -1.826815085 1.861883122 -1.246039199  
C -0.573965266 0.325105355 -2.063314952  
C 0.267477313 0.916313282 -3.010602129  
H 0.192181140 1.978266950 -3.243469830  
C 1.216639234 0.104163999 -3.625331832  
H 1.892727349 0.535544498 -4.363080551  
C 1.317654993 -1.267863217 -3.312420831  
H 2.059220375 -1.878253099 -3.827793947  
C 0.481961406 -1.853933940 -2.364779598  
H 0.556683976 -2.922461823 -2.155826677  
C -0.475945949 -1.055174884 -1.707400244

———— 210\_WGG05: PBE+TS ————

O -0.883480367 -1.816377939 0.282711025  
C -1.818225655 -1.292520028 -0.297277505  
O -2.561372806 -1.946582319 -1.243076545  
H -2.184455906 -2.848531048 -1.299979957  
C -2.333366445 0.128802725 -0.094408804  
H -3.412138079 0.068720868 0.104133403  
H -2.193722712 0.684339809 -1.031427398



N	-1.663167260	0.811925440	0.984846882
H	-0.790697978	1.297452510	0.773837027
C	-1.901938698	0.443613230	2.285834210
O	-2.880099559	-0.225856011	2.629971650
C	-0.803531577	0.875493263	3.271398901
H	-1.128781557	0.598095874	4.279086679
H	-0.632756453	1.959798776	3.221555701
N	0.450126584	0.208486364	2.945062960
H	0.546062363	-0.801765572	3.077263886
C	1.330891734	0.737129022	2.053436383
O	1.255727707	1.903971264	1.629400815
C	2.450201347	-0.230545301	1.620204685
H	3.287876871	-0.034993660	2.311689814
N	2.019838884	-1.616670249	1.844125616
H	2.814387301	-2.255678259	1.825681118
H	1.360106093	-1.904659940	1.113375049
C	2.963350246	0.103481822	0.188871499
H	3.919505414	-0.426108318	0.060302917
H	3.185347394	1.178664031	0.151847483
C	2.035638883	-0.273773663	-0.927718803
C	1.975783133	-1.509635442	-1.538970739
H	2.571026254	-2.398785510	-1.356127024
N	1.006257753	-1.508578819	-2.527839276
H	0.798442614	-2.283986585	-3.143833107
C	0.421435650	-0.258665391	-2.586023492
C	-0.582783795	0.229438313	-3.428474854
H	-1.048476519	-0.403526646	-4.184052506
C	-0.968240246	1.556956682	-3.263624189
H	-1.748793177	1.970781695	-3.901468140
C	-0.362815423	2.374654571	-2.284208367
H	-0.687177118	3.410209900	-2.183315685
C	0.636645855	1.886316618	-1.448251073
H	1.088022730	2.518216651	-0.684616295
C	1.045096518	0.545267276	-1.584486946

———— 211\_WGG02: PBE+TS ————

O	2.022390000	-1.127289000	-2.869427000
C	2.546252000	-0.338030000	-2.092024000
O	3.792547000	-0.515692000	-1.626391000
H	3.977092000	0.178417000	-0.912531000
C	1.828817000	0.923236000	-1.573647000
H	0.874131000	1.030532000	-2.095063000
H	2.455815000	1.802187000	-1.789307000
N	1.570017000	0.868963000	-0.137184000
H	0.636610000	0.624434000	0.190618000
C	2.556061000	0.990685000	0.779678000
O	3.758348000	1.135765000	0.460856000
C	2.140389000	0.925432000	2.247970000
H	2.566738000	1.804410000	2.750971000
H	2.614813000	0.028624000	2.674471000
N	0.716236000	0.828085000	2.469913000
H	0.093656000	1.641250000	2.493203000
C	0.094999000	-0.361990000	2.744114000
O	0.691537000	-1.436749000	2.866183000
C	-1.440794000	-0.250408000	2.840874000
H	-1.693147000	-0.499245000	3.883529000

```
N -1.887255000  1.133200000  2.583164000
H -2.707458000  1.361748000  3.143318000
H -2.149685000  1.251910000  1.601134000
C -2.075836000 -1.329113000  1.917840000
H -3.168563000 -1.289123000  2.046676000
H -1.743348000 -2.312083000  2.275829000
C -1.704082000 -1.166123000  0.471798000
C -0.667766000 -1.814862000 -0.175967000
H  0.031947000 -2.543418000  0.220111000
N -0.594412000 -1.406385000 -1.494278000
H  0.177999000 -1.610196000 -2.133114000
C -1.564525000 -0.450517000 -1.720930000
C -1.849458000  0.287461000 -2.875672000
H -1.269010000  0.149994000 -3.788180000
C -2.906441000  1.191731000 -2.817143000
H -3.156324000  1.782344000 -3.698039000
C -3.672009000  1.344252000 -1.642001000
H -4.507523000  2.043860000 -1.638809000
C -3.384880000  0.612224000 -0.494413000
H -4.006183000  0.727083000  0.395600000
C -2.300664000 -0.288435000 -0.506509000
```

———— 212\_WGG14: PBE+TS ————

```
O -1.292989814 -3.668137141 -0.222189933
C -0.709270312 -2.956696396 -1.026566688
O -1.368937559 -2.229570815 -1.945349553
H -0.696006230 -1.708746520 -2.499598357
C  0.830199841 -2.843597800 -1.070038000
H  1.180224686 -3.263152684 -2.026279315
H  1.232757139 -3.441693218 -0.249143193
N  1.349030549 -1.479750610 -0.936007130
H  1.709628756 -1.202533277 -0.021606231
C  1.194514716 -0.547240730 -1.899705702
O  0.565599056 -0.781416501 -2.961776689
C  1.755277880  0.839917126 -1.634230150
H  2.383118161  1.122413039 -2.494709862
H  2.370716311  0.890149392 -0.725915634
N  0.622773512  1.737133342 -1.471747452
H -0.292513440  1.489406260 -1.857280509
C  0.617907308  2.769777172 -0.587688377
O  1.621478615  3.201046383 -0.004191955
C -0.789968806  3.313581710 -0.293295865
H -0.681741244  4.405987425 -0.181412972
N -1.741578955  2.928813288 -1.350280285
H -2.702063051  2.965766710 -1.007001320
H -1.679227867  3.562397568 -2.148499465
C -1.249557861  2.756184232  1.083826691
H -2.264738451  3.141945697  1.270811550
H -0.602350388  3.210479382  1.846759284
C -1.231039447  1.262032846  1.235411271
C -2.266341424  0.384759367  0.984597905
H -3.265693971  0.585123098  0.612951722
N -1.886585344 -0.908980666  1.293211120
H -2.410383180 -1.750029806  1.070432417
C -0.579597238 -0.898963776  1.735534097
C  0.238114664 -1.954375068  2.154541826
```

H	-0.131600024	-2.978696697	2.171699350
C	1.549654580	-1.644705214	2.508460924
H	2.216980772	-2.440323861	2.839120525
C	2.025136426	-0.314225955	2.460161418
H	3.056016144	-0.106891173	2.746188671
C	1.197794386	0.737334743	2.074676728
H	1.583201138	1.755253566	2.028715924
C	-0.130471033	0.455886561	1.702466215

———— 213\_WGG15: PBE+TS ————

O	-1.595209863	-3.326053212	0.765570079
C	-2.314182390	-2.425358270	0.347555929
O	-3.343553752	-1.950058645	1.061066179
H	-3.788313353	-1.190853695	0.545747532
C	-2.109804855	-1.796755900	-1.044989770
H	-2.971489058	-2.085653654	-1.670899420
H	-1.205680407	-2.233988195	-1.476323380
N	-1.955838939	-0.342822811	-1.065575221
H	-1.057501405	0.074322960	-1.365160311
C	-2.939284902	0.518561069	-0.738228487
O	-4.061155953	0.157486631	-0.305163224
C	-2.612183311	2.005253345	-0.937254228
H	-3.497288800	2.570593067	-0.632354278
H	-2.424093731	2.183796419	-2.008331680
N	-1.463481240	2.471652707	-0.168736056
H	-1.577655241	3.137499638	0.596308489
C	-0.181325509	2.213559438	-0.536180390
O	0.111487674	1.487905568	-1.505593036
C	0.887544010	2.817049079	0.377113648
H	1.783233757	2.926193347	-0.257395956
N	0.411183465	4.079343240	0.971568875
H	0.522434642	4.862956687	0.326032607
H	0.945848773	4.303229668	1.812760616
C	1.209517233	1.829785057	1.539127501
H	0.387104372	1.909572971	2.267276393
H	2.117101969	2.210029037	2.038936263
C	1.382451037	0.400521679	1.141158969
C	0.484964727	-0.617375672	1.388742871
H	-0.453580363	-0.593850381	1.933990716
N	0.934149413	-1.796623575	0.826357725
H	0.389051735	-2.658613637	0.820625562
C	2.137070952	-1.558950273	0.188154098
C	2.967402455	-2.422478035	-0.534821975
H	2.711774425	-3.473756098	-0.670033019
C	4.135150396	-1.889802906	-1.074214550
H	4.803951613	-2.535127171	-1.643583171
C	4.470523543	-0.530911816	-0.896153394
H	5.395218128	-0.150805824	-1.330270359
C	3.642016006	0.325804817	-0.179569848
H	3.913063216	1.375072646	-0.053559468
C	2.453533532	-0.179729299	0.375437168

———— 214\_WGG01: PBE+TS ————

O	-3.115468000	-1.131867000	-1.374307000
C	-2.476290000	-0.318443000	-2.031025000
O	-2.572635000	1.002304000	-1.813809000

```
H -1.919970000  1.490042000 -2.420845000
C -1.512686000 -0.741373000 -3.155663000
H -1.878984000 -0.323513000 -4.107635000
H -1.529419000 -1.832570000 -3.222115000
N -0.130874000 -0.313182000 -2.942461000
H  0.585641000 -0.985388000 -2.616716000
C  0.250086000  0.980916000 -2.998395000
O -0.546946000  1.924973000 -3.212683000
C  1.744408000  1.226742000 -2.754744000
H  1.935431000  2.287529000 -2.941533000
H  2.336301000  0.623192000 -3.460220000
N  2.148924000  0.907676000 -1.391858000
H  2.364673000  1.632946000 -0.700193000
C  2.329633000 -0.353794000 -0.937765000
O  2.106579000 -1.372714000 -1.626853000
C  2.846862000 -0.437884000  0.511399000
H  3.892910000 -0.774535000  0.419108000
N  2.852796000  0.900359000  1.130646000
H  3.621035000  0.991572000  1.794028000
H  1.982875000  1.049959000  1.650872000
C  2.055729000 -1.517685000  1.299062000
H  2.563075000 -1.670494000  2.263822000
H  2.128236000 -2.462828000  0.744913000
C  0.618510000 -1.142710000  1.508936000
C -0.433411000 -1.451291000  0.667583000
H -0.437624000 -2.055740000 -0.232839000
N -1.601916000 -0.884994000  1.131861000
H -2.479848000 -0.909209000  0.613183000
C -1.333421000 -0.177337000  2.284169000
C -2.181785000  0.574393000  3.104247000
H -3.240393000  0.685971000  2.869415000
C -1.625366000  1.174362000  4.229939000
H -2.258488000  1.769803000  4.887585000
C -0.256656000  1.021589000  4.538339000
H  0.141728000  1.493481000  5.436561000
C  0.587150000  0.276564000  3.720926000
H  1.639850000  0.157200000  3.983689000
C  0.061122000 -0.330134000  2.562232000
```

———— 215\_WGG07: PBE+TS ————

```
O  1.296363000  0.233077000  3.671481000
C  0.708624000  1.034188000  2.959756000
O  1.363728000  1.958047000  2.234859000
H  0.689174000  2.509853000  1.713414000
C -0.831592000  1.070644000  2.846095000
H -1.186155000  2.023210000  3.270802000
H -1.230997000  0.246113000  3.441262000
N -1.350808000  0.937977000  1.481887000
H -1.715617000  0.025283000  1.205520000
C -1.198167000  1.900763000  0.548019000
O -0.571792000  2.964375000  0.780984000
C -1.758580000  1.633730000 -0.839177000
H -2.388903000  2.492083000 -1.122726000
H -2.372927000  0.725116000 -0.888962000
N -0.626306000  1.471393000 -1.736578000
H  0.289538000  1.855487000 -1.489132000
```

```

C -0.620915000  0.588825000 -2.770488000
O -1.623865000  0.004849000 -3.202367000
C  0.788430000  0.297659000 -3.314208000
H  0.681450000  0.183759000 -4.406726000
N  1.737104000  1.358563000 -2.930584000
H  1.675508000  2.153141000 -3.569030000
H  2.698021000  1.015976000 -2.963453000
C  1.253220000 -1.078236000 -2.756588000
H  2.269428000 -1.260839000 -3.141914000
H  0.611095000 -1.843684000 -3.213492000
C  1.234062000 -1.235001000 -1.262855000
C  2.268816000 -0.983960000 -0.384836000
H  3.266743000 -0.607427000 -0.583953000
N  1.889569000 -1.296999000  0.907999000
H  2.414700000 -1.078891000  1.749239000
C  0.583354000 -1.741924000  0.897381000
C -0.234278000 -2.163120000  1.952361000
H  0.135886000 -2.183777000  2.976686000
C -1.545647000 -2.518001000  1.641716000
H -2.213293000 -2.850273000  2.436716000
C -2.020589000 -2.469252000  0.310919000
H -3.051103000 -2.756574000  0.102284000
C -1.192985000 -2.081643000 -0.739887000
H -1.577247000 -2.035307000 -1.758342000
C  0.134551000 -1.707404000 -0.457581000

```

———— 216\_WGG11: PBE+TS ————

```

O -4.676992000 -0.029939000  0.019901000
C -3.370095000  0.315236000  0.188839000
O -2.989394000  1.475767000  0.158138000
H -5.166275000  0.807506000 -0.123091000
C -2.503629000 -0.930319000  0.353172000
H -2.299303000 -1.314047000 -0.657872000
H -3.093606000 -1.682424000  0.893420000
N -1.252846000 -0.711161000  1.037934000
H -0.401302000 -0.540995000  0.509694000
C -1.204027000 -0.702464000  2.407462000
O -2.213305000 -0.825155000  3.107629000
C  0.185842000 -0.549425000  3.036868000
H  0.209105000 -1.224192000  3.904941000
H  0.285278000  0.478684000  3.417817000
N  1.295366000 -0.781027000  2.137098000
H  1.471902000 -1.693454000  1.707342000
C  2.267530000  0.144766000  1.884159000
O  2.336046000  1.253122000  2.428740000
C  3.256223000 -0.282127000  0.777401000
H  4.255751000 -0.276834000  1.238248000
N  2.973019000 -1.651976000  0.305241000
H  2.378818000 -1.635102000 -0.527356000
H  3.832778000 -2.138066000  0.055286000
C  3.219233000  0.804836000 -0.338862000
H  3.926327000  0.510741000 -1.129447000
H  3.584863000  1.745481000  0.092787000
C  1.836046000  0.997394000 -0.889337000
C  0.886263000  1.861686000 -0.378187000
H  0.977141000  2.562245000  0.445358000

```

N -0.311798000 1.712473000 -1.049771000  
H -1.211778000 2.031643000 -0.689753000  
C -0.174938000 0.709236000 -1.989168000  
C -1.113402000 0.169575000 -2.876526000  
H -2.136728000 0.544691000 -2.911344000  
C -0.688160000 -0.847139000 -3.728024000  
H -1.392762000 -1.285943000 -4.434086000  
C 0.646219000 -1.305027000 -3.705111000  
H 0.950153000 -2.089636000 -4.397693000  
C 1.579036000 -0.766270000 -2.824188000  
H 2.611364000 -1.120445000 -2.837095000  
C 1.177219000 0.247606000 -1.931219000

———— 217\_WGG09: PBE+TS ————

O -1.474758649 -0.772033021 -3.738891408  
C -0.210137837 -0.653389207 -3.298948683  
O 0.607980573 -1.557237530 -3.415926130  
H -1.996723079 0.041292802 -3.446521330  
C 0.122013944 0.695409287 -2.634693579  
H -0.142347425 1.509027641 -3.327256572  
H 1.193194104 0.739068817 -2.423798266  
N -0.604124616 0.893092687 -1.383172845  
H -0.128156224 0.699665910 -0.501675089  
C -1.921349514 1.196858025 -1.374251406  
O -2.595044040 1.285778249 -2.425183519  
C -2.571965159 1.452225534 -0.019040885  
H -3.453178184 0.799416629 0.041999750  
H -2.921897405 2.494500674 -0.014823559  
N -1.743829351 1.176045490 1.139829716  
H -1.074864528 1.868513103 1.462405361  
C -1.895444831 0.014432087 1.869187641  
O -2.732345403 -0.842870001 1.572477956  
C -0.951597192 -0.145619792 3.070834410  
H -0.380660780 0.785755805 3.217056951  
N -1.668886818 -0.426355048 4.319430279  
H -2.248399422 0.371537528 4.588779920  
H -2.308122839 -1.211962399 4.165107759  
C 0.034223408 -1.301652235 2.779205629  
H -0.549047032 -2.233986885 2.755610109  
H 0.712269123 -1.369910702 3.643287166  
C 0.797538319 -1.159982293 1.498195097  
C 0.681574059 -1.962972377 0.381406602  
H 0.019994465 -2.805851909 0.209921625  
N 1.573936223 -1.562158897 -0.597667048  
H 1.537380922 -1.862107451 -1.574346202  
C 2.260627663 -0.452086676 -0.143783621  
C 3.238118486 0.328082468 -0.773883178  
H 3.592001110 0.088182377 -1.777145290  
C 3.756898285 1.407980548 -0.064123785  
H 4.520861227 2.033600128 -0.525045160  
C 3.325172630 1.695822485 1.248122806  
H 3.766576149 2.538919321 1.779331073  
C 2.360303568 0.915241094 1.876667472  
H 2.055738278 1.136590321 2.900487274  
C 1.798967791 -0.172711587 1.179762958

———— 218\_WGG13: PBE+TS ————

O	-1.636290973	2.421194892	1.698058664
C	-0.824671293	3.109684499	0.874151203
O	0.103700526	3.782798742	1.294391061
H	-2.323500943	1.924210040	1.141553311
C	-1.156364077	2.994202303	-0.630715197
H	-0.408403207	3.567109621	-1.184194546
H	-2.149463345	3.437003823	-0.804861919
N	-1.152701261	1.622255386	-1.148000579
H	-0.321576425	1.317397798	-1.657804719
C	-2.089740493	0.715277059	-0.803699590
O	-3.019504296	0.983558922	-0.001625586
C	-1.953748376	-0.691774947	-1.359878056
H	-1.159625742	-0.787664831	-2.111297986
H	-2.911991809	-0.969979105	-1.826961006
N	-1.625571818	-1.558692362	-0.233850235
H	-1.893232920	-1.242463992	0.693639230
C	-0.835799495	-2.662941173	-0.355835160
O	-0.508394519	-3.144275469	-1.448710629
C	-0.297105661	-3.215027719	0.964833958
H	-0.897159654	-2.817023591	1.801267808
N	-0.433999923	-4.669652715	0.934119861
H	0.164636463	-5.111188727	1.634025070
H	-0.143152936	-5.006744637	0.011801757
C	1.175268243	-2.706087400	1.147288234
H	1.782688321	-3.198930939	0.372911674
H	1.526693216	-3.088247028	2.118207391
C	1.375134140	-1.220916154	1.077901369
C	1.332820680	-0.321419417	2.125082830
H	1.143158485	-0.498799719	3.179044107
N	1.605586725	0.957994459	1.671127832
H	1.499818554	1.813393056	2.208061735
C	1.805633518	0.916401004	0.306420566
C	2.092038446	1.947761368	-0.595157185
H	2.209349232	2.974983636	-0.253265404
C	2.182445454	1.612129984	-1.944838109
H	2.398064550	2.389869923	-2.677582500
C	2.017309308	0.276453589	-2.378532719
H	2.099142346	0.047865142	-3.441300847
C	1.774927599	-0.752866621	-1.472164825
H	1.649365577	-1.777265092	-1.821163429
C	1.657994782	-0.442891608	-0.103743433

———— 219\_WGG10: PBE+TS ————

O	1.542772533	-0.750897652	3.342682166
C	2.270819135	-0.348818501	2.441945504
O	3.283239530	-1.085946761	1.965375561
H	3.748132793	-0.573241368	1.216268675
C	2.098615608	1.049225464	1.814187534
H	2.969084109	1.658265318	2.113303187
H	1.198493299	1.497657128	2.242542060
N	1.961537300	1.075942181	0.358628414
H	1.068335299	1.374388015	-0.070581077
C	2.951525951	0.735208718	-0.489708329
O	4.063270234	0.290405449	-0.111623537
C	2.643853372	0.927937191	-1.981144932
H	3.533185250	0.610797740	-2.533410971

H 2.466867121 1.999272168 -2.170487754  
N 1.495155335 0.162352541 -2.453475658  
H 1.611716925 -0.606063289 -3.115466428  
C 0.211303178 0.534420332 -2.212003410  
O -0.089693128 1.507189848 -1.494331459  
C -0.852451450 -0.376903872 -2.827988721  
H -1.741029744 0.263641324 -2.956605480  
N -0.359545511 -0.979169791 -4.080754377  
H -0.895372015 -1.818647550 -4.308905283  
H -0.457873775 -0.336423097 -4.868547212  
C -1.200341673 -1.532136395 -1.840930971  
H -0.386358604 -2.271220761 -1.907951934  
H -2.109603851 -2.021488163 -2.230194602  
C -1.385412564 -1.130796103 -0.414135552  
C -0.496613715 -1.383123262 0.610237985  
H 0.441354735 -1.930106823 0.592298666  
N -0.955869224 -0.825228857 1.787542334  
H -0.416512360 -0.818175211 2.653124237  
C -2.155851451 -0.185067877 1.542209869  
C -2.993828790 0.532012018 2.403214739  
H -2.746515415 0.659269631 3.457460499  
C -4.158133186 1.072768716 1.864742994  
H -4.834739408 1.635422318 2.507931998  
C -4.481757035 0.902666948 0.501882468  
H -5.403346953 1.338663181 0.116199187  
C -3.645659967 0.191775172 -0.352389602  
H -3.907518913 0.072047976 -1.404649701  
C -2.460896975 -0.365861046 0.159509912

———— 220\_WGG12: PBE+TS ————

O -1.371487042 -3.584864433 -0.152086856  
C -0.812327481 -2.901122199 -0.994539416  
O -1.499125964 -2.158314608 -1.883948092  
H -0.839653554 -1.682685916 -2.490276444  
C 0.725251196 -2.839111746 -1.130823971  
H 1.004162613 -3.279987224 -2.100704408  
H 1.158706238 -3.440801141 -0.328726917  
N 1.291037658 -1.489494715 -1.043803952  
H 1.710730508 -1.211332568 -0.154275808  
C 1.111430424 -0.567034430 -2.010957755  
O 0.424779467 -0.800194481 -3.038471342  
C 1.691398503 0.820839265 -1.790254207  
H 2.268430490 1.099293154 -2.686354606  
H 2.350980477 0.886633573 -0.915079285  
N 0.556565265 1.708074343 -1.571393408  
H -0.339099895 1.431945307 -1.965718888  
C 0.569644761 2.727953286 -0.664674150  
O 1.606980926 3.155154970 -0.141815968  
C -0.821841209 3.258930204 -0.257520807  
H -0.729199544 4.354997055 -0.235623383  
N -1.967617541 2.915279939 -1.098494900  
H -1.858643331 3.192499887 -2.073142883  
H -2.216529908 1.925875809 -1.042205680  
C -1.094848569 2.789735303 1.201556063  
H -2.062674226 3.219395420 1.495018568  
H -0.326138327 3.234297727 1.847228752



C	-1.110093580	1.298067236	1.382790092
C	-2.199512671	0.455504518	1.266257191
H	-3.234613295	0.695802894	1.043692292
N	-1.826239600	-0.851408746	1.530291982
H	-2.400740897	-1.673754530	1.374876994
C	-0.475994328	-0.885285092	1.810937229
C	0.349894688	-1.966558695	2.138941915
H	-0.048498500	-2.977890181	2.205062771
C	1.701745202	-1.700253166	2.343888691
H	2.375842901	-2.517694779	2.600076264
C	2.211688278	-0.385332726	2.240810017
H	3.273333730	-0.210695888	2.415631979
C	1.379999443	0.692145002	1.945510216
H	1.786669254	1.699385109	1.863213336
C	0.010883441	0.453526263	1.719734772

**11.2.11 FGG: PBE+D3**

———— 252\_FGG55: PBE+D3 ————

O	-3.202244359	0.141196826	-2.266992528
C	-3.097559873	-0.028181342	-1.070810376
O	-3.165877308	0.985423354	-0.190998855
H	-2.971384353	0.634518586	0.736149058
C	-2.903082260	-1.423556004	-0.442293466
H	-2.910079322	-2.158443008	-1.254395643
H	-3.755930019	-1.623716115	0.230176514
N	-1.659635047	-1.576750438	0.304158617
H	-0.899786814	-2.166900089	-0.064787249
C	-1.426152226	-0.957301974	1.477244388
O	-2.224774299	-0.161607035	2.007380758
C	-0.090120620	-1.312205636	2.144926133
H	-0.047510558	-2.400202753	2.311546750
H	-0.066309968	-0.798853548	3.112488934
N	1.087560972	-0.924026760	1.378100909
H	1.484152603	-0.000385952	1.545250445
C	1.514229127	-1.609026429	0.284990584
O	0.926208431	-2.618049669	-0.136734414
C	2.774062967	-1.062464182	-0.415162098
N	3.520920987	-2.090862795	-1.127982696
H	2.870541131	-2.604185698	-1.732608115
H	3.875595627	-2.783669497	-0.463382140
H	3.438410393	-0.628649483	0.351535988
C	2.380613369	0.065228872	-1.404392512
H	3.311679970	0.364716990	-1.911259658
H	1.713438032	-0.359543036	-2.172653216
C	1.718588737	1.249178999	-0.743679502
C	2.432701609	2.043781261	0.170084201
H	3.491526825	1.837318615	0.352612721
C	1.810773208	3.101499853	0.837792766
H	2.382807898	3.710789859	1.541346458
C	0.463256009	3.386381003	0.597011818
H	-0.024636513	4.211666693	1.118952663
C	-0.253485567	2.615347332	-0.320458500
H	-1.306436604	2.822400453	-0.517056084
C	0.371556939	1.554150569	-0.981283659
H	-0.198619122	0.953982179	-1.695818994

———— 253\_FGG99: PBE+D3 ————

O 1.200920591 -0.004100722 -1.278231297  
C 2.167709300 0.075027129 -0.550128977  
O 3.303302131 -0.646048505 -0.733973102  
H 3.137988532 -1.218757128 -1.512009402  
C 2.299907982 0.984085755 0.669960343  
H 3.127201437 1.684393748 0.475865914  
H 2.577187485 0.369437550 1.538683562  
N 1.099212706 1.730144559 0.934728843  
H 0.312650669 1.248700044 1.376710327  
C 0.804381135 2.837272604 0.179487461  
O 1.631924046 3.436315222 -0.499354047  
C -0.681861506 3.230997215 0.222282332  
H -0.799231088 4.163226759 -0.342740730  
H -1.014528697 3.381710530 1.260644335  
N -1.502322549 2.186836990 -0.369094161  
H -1.507095733 2.049443457 -1.383484646  
C -1.917678176 1.110123989 0.341907310  
O -1.787634787 1.013905183 1.570597029  
C -2.593017384 0.018967556 -0.514043681  
N -2.033625864 0.054404656 -1.867005987  
H -1.076555146 -0.314458808 -1.865793261  
H -2.591906478 -0.509532604 -2.508985287  
H -3.652640274 0.326823592 -0.594459949  
C -2.588177380 -1.352716041 0.214787515  
H -2.999235314 -1.194611526 1.222814225  
H -3.286194090 -2.010306166 -0.328890183  
C -1.239502615 -2.021906535 0.307382430  
C -0.780250119 -2.852616341 -0.725902574  
H -1.423682944 -3.036434396 -1.590746005  
C 0.474003282 -3.465232380 -0.657311587  
H 0.806019372 -4.113741131 -1.471560119  
C 1.291285091 -3.263021981 0.456456046  
H 2.268178869 -3.746621553 0.519216226  
C 0.841507932 -2.446810579 1.499395376  
H 1.466002304 -2.299466737 2.384159555  
C -0.409630378 -1.832376538 1.424965666  
H -0.761612342 -1.196056868 2.238670499

———— 254\_FGG300: PBE+D3 ————

O -1.332105062 -1.748882940 0.215529971  
C -2.347449702 -2.155269394 -0.314113238  
O -2.627971748 -3.474167515 -0.470986900  
H -1.879311698 -3.966815176 -0.073908178  
C -3.469180700 -1.296171631 -0.889714421  
H -4.384389400 -1.510463703 -0.314636567  
H -3.651993609 -1.607934716 -1.929715671  
N -3.193450625 0.111070642 -0.803191943  
H -2.431457648 0.504733406 -1.366500504  
C -3.551663340 0.815063851 0.318497533  
O -4.342823645 0.403184467 1.161507917  
C -2.816412964 2.160044199 0.448122185  
H -3.265232887 2.715748746 1.279835507  
H -2.907925694 2.743866199 -0.480744022  
N -1.404216655 1.935640359 0.713508142  
H -1.083041008 1.703774208 1.657026291  
C -0.526975491 1.622179931 -0.271276861

O -0.811247043 1.666787273 -1.476892186  
C 0.864860917 1.202112608 0.236959708  
N 0.749724852 0.664515342 1.598019948  
H 1.676581162 0.569319545 2.018390701  
H 0.339149664 -0.274876876 1.555855443  
H 1.462288349 2.130152870 0.304382258  
C 1.542113723 0.269317266 -0.794423787  
H 0.947246180 -0.655726269 -0.862382111  
H 1.494812936 0.757595503 -1.779045553  
C 2.965735220 -0.040358884 -0.417410586  
C 3.291064888 -1.198038094 0.305389721  
H 2.500881365 -1.912374133 0.552494090  
C 4.607108136 -1.455859338 0.698624591  
H 4.839300296 -2.365971406 1.256092291  
C 5.624298382 -0.555951084 0.374547431  
H 6.653575912 -0.756559037 0.678295675  
C 5.316263035 0.600433925 -0.348454937  
H 6.106463221 1.305815655 -0.614969554  
C 4.000164466 0.853278668 -0.737657685  
H 3.768216215 1.756785534 -1.309054698

———— 255\_FGG252: PBE+D3 ————

O -2.858989479 -1.363703693 -0.603322095  
C -3.888516830 -0.825319616 -0.249623064  
O -5.120824703 -1.347177217 -0.484129043  
H -4.979231960 -2.184766392 -0.973261183  
C -4.002264537 0.497493766 0.503730281  
H -4.604609536 0.335117402 1.411122391  
H -4.554388630 1.202188909 -0.138416257  
N -2.721703187 1.067783125 0.819980740  
H -2.123164804 0.589862709 1.504028891  
C -2.081097351 1.862171248 -0.097484850  
O -2.637579107 2.381868949 -1.060082286  
C -0.569961871 1.983075722 0.163429760  
H -0.376138514 2.288217732 1.203478150  
H -0.158800989 2.730986114 -0.524137605  
N 0.068897733 0.699077309 -0.068710442  
H 0.327204785 0.405365101 -1.014369927  
C 0.064276869 -0.291517002 0.849723520  
O -0.342917060 -0.153904520 2.014443435  
C 0.608559104 -1.633705461 0.344479279  
N 0.480851437 -1.709383408 -1.114673535  
H -0.497072098 -1.881142772 -1.364280662  
H 1.042880045 -2.474193463 -1.492497016  
H 0.005544229 -2.392509077 0.877597556  
C 2.075620910 -1.827259082 0.801916558  
H 2.072451357 -1.809880157 1.902884993  
H 2.389387391 -2.840226384 0.495654077  
C 3.047424454 -0.803540608 0.270353198  
C 3.736207307 -1.010250216 -0.932625903  
H 3.595560578 -1.945973078 -1.480244670  
C 4.605555520 -0.041960109 -1.439240768  
H 5.130726533 -0.221553376 -2.379544624  
C 4.804738087 1.152671932 -0.743509912  
H 5.486915717 1.910163880 -1.135148946  
C 4.132235506 1.368095793 0.461996972

H	4.288311062	2.294752458	1.018662314
C	3.262295876	0.398040318	0.962092176
H	2.736616159	0.573033165	1.904728500

## ———— 256\_FGG366: PBE+D3 ————

O	-2.013777674	1.824956305	0.370468649
C	-3.144782525	1.990947113	-0.038905114
O	-3.771996139	3.196062791	-0.030938206
H	-3.142927841	3.833792705	0.367086118
C	-4.057939610	0.916260179	-0.623046280
H	-4.430059502	1.260625996	-1.599825001
H	-4.926529878	0.815014153	0.047170106
N	-3.409675230	-0.362437279	-0.728780558
H	-2.638146325	-0.472484450	-1.397398775
C	-3.413393509	-1.221885065	0.339976327
O	-4.176742922	-1.124671010	1.296340398
C	-2.315098728	-2.295191179	0.252585990
H	-2.346168237	-2.807654272	-0.721421384
H	-2.480022556	-3.021475371	1.057277673
N	-1.006216191	-1.679231342	0.406312574
H	-0.657748931	-1.425849412	1.335290309
C	-0.385774477	-1.035729972	-0.611820231
O	-0.778434725	-1.059606249	-1.787945461
C	0.876561685	-0.270429131	-0.199966336
N	0.805943519	0.107754001	1.214688217
H	1.729395008	0.394799169	1.548457536
H	0.169424335	0.901609389	1.328411093
H	0.923863592	0.595210553	-0.886894572
C	2.114464472	-1.157503582	-0.465561116
H	2.051987199	-2.047894893	0.180521363
H	2.062017965	-1.496344974	-1.511688014
C	3.407004561	-0.423694983	-0.211056055
C	4.139006404	-0.636738349	0.966151888
H	3.785683063	-1.376862640	1.689851012
C	5.316682747	0.073055678	1.218068281
H	5.875435794	-0.110362892	2.138378542
C	5.781224039	1.008331914	0.292014405
H	6.703994732	1.559547754	0.482375827
C	5.061983379	1.228560461	-0.886859786
H	5.423090242	1.952487865	-1.620834502
C	3.886556757	0.519468103	-1.133700582
H	3.331115507	0.691562916	-2.059784335

## ———— 257\_FGG215: PBE+D3 ————

O	2.974239696	-1.755288656	1.418403390
C	3.004768810	-0.706213086	0.807650448
O	3.206722675	-0.652366041	-0.517206616
H	3.173336725	0.309352503	-0.821087820
C	2.837630911	0.658236177	1.505257912
H	3.782541639	1.219226359	1.393355189
H	2.663097139	0.468413124	2.570031642
N	1.739080623	1.469233254	0.995215274
H	0.864253656	1.568984014	1.535700768
C	1.759949320	2.048292118	-0.220623349
O	2.691393845	1.907503858	-1.036366662
C	0.537694558	2.919483915	-0.542193823

H	0.735554336	3.411677188	-1.501081260
H	0.424238155	3.687499580	0.242458291
N	-0.697410058	2.162105888	-0.648185686
H	-1.171192019	2.019972766	-1.545499096
C	-1.383342940	1.702990885	0.418165218
O	-0.983280479	1.797953207	1.591523577
C	-2.747579832	1.072456814	0.077494757
N	-2.942189118	0.991709414	-1.375005992
H	-3.912878543	1.172200199	-1.629097827
H	-2.706039428	0.051249613	-1.707912488
H	-3.481045355	1.789723231	0.485443954
C	-2.933906514	-0.267924136	0.840194948
H	-2.649033358	-0.098053714	1.889224996
H	-4.005985134	-0.522834845	0.819892386
C	-2.128897886	-1.394672549	0.242495241
C	-2.693721355	-2.237371333	-0.728809136
H	-3.747535638	-2.116119381	-0.997965088
C	-1.937812665	-3.245834467	-1.333937227
H	-2.398109064	-3.893760783	-2.083390197
C	-0.602738293	-3.429892018	-0.970830237
H	-0.009814841	-4.218419939	-1.438378329
C	-0.028635428	-2.608730848	0.004182985
H	1.010505596	-2.754220897	0.305997482
C	-0.786853687	-1.600251854	0.601381253
H	-0.336006048	-0.968309558	1.370501120

———— 258\_FGG224: PBE+D3 ————

O	3.378459490	-1.214631137	1.506626826
C	3.188290721	-0.413004367	0.614664466
O	3.242972462	-0.754925714	-0.680869188
H	2.992196097	0.043044282	-1.248064842
C	2.895523486	1.075543288	0.892155299
H	3.716403927	1.673850947	0.457752431
H	2.891539400	1.214942498	1.978731402
N	1.623220991	1.553491862	0.364716516
H	0.854617548	1.814634321	1.004839684
C	1.388075261	1.705877649	-0.950905634
O	2.198566770	1.383836890	-1.841318784
C	0.043748938	2.359291852	-1.303348744
H	0.000782842	2.427631204	-2.396601850
H	0.034531901	3.379053606	-0.881675117
N	-1.133978670	1.648064987	-0.833043975
H	-1.737365018	1.138915135	-1.483399482
C	-1.553175596	1.648343873	0.450372021
O	-0.915144553	2.153651547	1.389012797
C	-2.899320546	0.953374230	0.690877159
N	-3.647367532	0.823041726	-0.566053565
H	-4.101563988	1.706643493	-0.807703590
H	-4.384826324	0.122105921	-0.473869003
H	-3.411489533	1.584101545	1.442659433
C	-2.665908154	-0.428324905	1.355362295
H	-2.200987634	-0.239338297	2.334221465
H	-3.659040832	-0.868844992	1.552364492
C	-1.811086032	-1.389397133	0.563464703
C	-0.455212847	-1.554573856	0.883604221
H	-0.031303842	-0.998015598	1.723704892

C 0.356824600 -2.428099785 0.156921835  
H 1.405401889 -2.550105643 0.433229161  
C -0.177872420 -3.144338535 -0.915945009  
H 0.456108390 -3.823908308 -1.489063035  
C -1.527972343 -2.996249889 -1.243309529  
H -1.956591631 -3.562899883 -2.072955617  
C -2.337468271 -2.131657644 -0.504251807  
H -3.396588948 -2.043125169 -0.758902329

———— 259\_FGG380: PBE+D3 ————

O -2.635792855 -2.624959966 0.648812985  
C -2.836178777 -1.452165379 0.407188280  
O -3.379242259 -0.618299128 1.306079732  
H -3.493242685 0.295524124 0.889126255  
C -2.525186887 -0.834902998 -0.971638349  
H -3.490424919 -0.609432844 -1.460796148  
H -2.002413160 -1.595394759 -1.561792511  
N -1.702099930 0.369735992 -0.953690576  
H -0.753027420 0.345236268 -1.354967148  
C -2.132416440 1.552690138 -0.477471394  
O -3.241348172 1.714307419 0.069193517  
C -1.157571595 2.725535988 -0.652617366  
H -1.645550769 3.613677532 -0.235507656  
H -0.979509231 2.881284757 -1.730301873  
N 0.121180284 2.529490618 0.008859761  
H 0.362934545 3.034515102 0.863483962  
C 1.104823301 1.758514851 -0.513217784  
O 0.977883734 1.108038338 -1.560004288  
C 2.385269816 1.700773781 0.327838631  
N 2.517166646 2.913730281 1.147722577  
H 2.895124359 3.689121957 0.598897252  
H 3.158255544 2.753046193 1.927252701  
H 3.205754217 1.554224268 -0.398450650  
C 2.342579446 0.473481709 1.271641705  
H 3.304434621 0.456955079 1.816011422  
H 1.552558454 0.646887847 2.021038314  
C 2.125043018 -0.854797258 0.592349388  
C 3.135331668 -1.433965585 -0.188501610  
H 4.094826370 -0.920252821 -0.298397992  
C 2.931271165 -2.657744678 -0.825196805  
H 3.729409850 -3.094627857 -1.429321803  
C 1.710855409 -3.325222030 -0.685649513  
H 1.553424934 -4.286988881 -1.177444651  
C 0.698744349 -2.764562543 0.096064865  
H -0.258721644 -3.274244005 0.221921947  
C 0.908965947 -1.535984558 0.728249396  
H 0.114889070 -1.106226949 1.345235428

———— 260\_FGG412: PBE+D3 ————

O 3.585189661 0.230778146 -0.305191006  
C 2.591745252 -0.423635334 -0.060599746  
O 1.619655023 -0.024858020 0.797471224  
H 1.844253775 0.897217187 1.055699487  
C 2.310418884 -1.788041100 -0.678204703  
H 2.805735423 -2.548564910 -0.050608618  
H 2.795143389 -1.797607352 -1.665294247

```

N  0.917369324 -2.150684885 -0.760764791
H  0.272300234 -1.575534296 -1.311646838
C  0.363415326 -3.049931102  0.104603960
O  1.006497345 -3.749891907  0.882533311
C -1.172606146 -3.099797665  0.024656799
H -1.511762063 -3.909287362  0.681510667
H -1.485950261 -3.312157066 -1.010072424
N -1.790403162 -1.852756607  0.441141176
H -2.018521551 -1.676861015  1.421532617
C -1.962206116 -0.796224170 -0.386150122
O -1.615073437 -0.791893658 -1.576256825
C -2.702175181  0.389921823  0.268491972
N -2.485045753  0.372275889  1.718361897
H -1.567415937  0.769195864  1.942041928
H -3.188576672  0.933482886  2.200924743
H -3.773676815  0.167957432  0.107303608
C -2.415791506  1.725386601 -0.464934045
H -2.639775196  1.574035701 -1.530945745
H -3.133380531  2.468262241 -0.077895280
C -1.011033197  2.251329276 -0.311039028
C -0.621096514  2.952447806  0.841834419
H -1.358142073  3.163571923  1.621580449
C  0.687760071  3.424227670  0.991061923
H  0.968310565  3.971289220  1.893994495
C  1.626259133  3.219310265 -0.024219310
H  2.647384948  3.589303731  0.083247178
C  1.243634438  2.542378738 -1.187584018
H  1.972500411  2.377263271 -1.983333143
C -0.056935150  2.057587561 -1.323477779
H -0.347005943  1.509503219 -2.221774182

```

———— 261\_FGG444: PBE+D3 ————

```

O  2.386940590 -2.694842216  0.926052903
C  2.665665051 -1.702651440  0.283528261
O  2.651888147 -1.687533388 -1.057264385
H  2.903318933 -0.765725882 -1.383328364
C  3.084468454 -0.379288889  0.954365764
H  4.135815363 -0.174811133  0.684569720
H  3.020338391 -0.522067032  2.038894121
N  2.267161758  0.772053870  0.591790631
H  1.571479154  1.150531810  1.254714010
C  2.295917021  1.336318577 -0.630866446
O  2.981634423  0.900346704 -1.575234715
C  1.412947245  2.582063911 -0.787460294
H  1.624939212  3.005982748 -1.775894243
H  1.683520376  3.317459081 -0.010842349
N -0.007856078  2.292544366 -0.695006375
H -0.624621866  2.340285584 -1.511443199
C -0.646403748  2.065037728  0.471431341
O -0.071138155  1.988408567  1.570456411
C -2.177610921  1.943085943  0.349026501
N -2.591948202  1.934837429 -1.058683573
H -3.489712268  2.402698411 -1.181636896
H -2.699789672  0.969313888 -1.386962838
H -2.556897747  2.871451778  0.811577391
C -2.700002281  0.752437223  1.198595893

```

```

H -2.226735932  0.815097225  2.188741010
H -3.785104118  0.884813828  1.334341923
C -2.425918434 -0.584295687  0.556655767
C -3.388138299 -1.188948760 -0.268228191
H -4.366016845 -0.712765713 -0.387711637
C -3.125239754 -2.401907428 -0.910958352
H -3.890703724 -2.859078016 -1.541978631
C -1.891371017 -3.030536125 -0.735041272
H -1.682864942 -3.980282845 -1.230711389
C -0.925849616 -2.447591296  0.090999225
H  0.037652344 -2.937627086  0.244310414
C -1.193628486 -1.235215265  0.728760350
H -0.441134357 -0.788600465  1.383441512

```

———— 262\_FGG470: PBE+D3 ————

```

O -2.588254241  0.893080104  1.727921430
C -3.040446146  0.968349519  0.604235865
O -3.880664764  1.960248871  0.202085558
H -4.020049547  2.531070900  0.986756430
C -2.756704084  0.013461038 -0.529957107
H -2.324370727  0.588237787 -1.370281417
H -3.709493669 -0.393527396 -0.909172332
N -1.880954838 -1.045785162 -0.097285751
H -1.398625378 -0.963173920  0.804360591
C -1.590466358 -2.082606499 -0.927566446
O -2.101650829 -2.227394982 -2.037906941
C -0.546185557 -3.062713965 -0.363485805
H -0.505384163 -3.921702034 -1.043380658
H -0.853946070 -3.400744606  0.639304510
N  0.775249064 -2.468355571 -0.261737763
H  1.469925457 -2.569600868 -1.004226250
C  1.156094488 -1.708180485  0.789343145
O  0.421726405 -1.454039565  1.753719286
C  2.612836500 -1.205261631  0.717960740
N  3.159819413 -1.378313098 -0.632339056
H  2.931580803 -0.560830301 -1.207765948
H  4.177102121 -1.454455215 -0.605308171
H  3.173617920 -1.878852588  1.390217372
C  2.720397005  0.227027348  1.308383453
H  2.254325848  0.212631941  2.303772553
H  3.790646086  0.457065647  1.438149533
C  2.071700823  1.276154421  0.441042914
C  0.725046610  1.631885795  0.622994953
H  0.154213233  1.170893005  1.431271209
C  0.119624417  2.575177121 -0.208991615
H -0.921900369  2.857224879 -0.038970752
C  0.841116377  3.173420622 -1.245980559
H  0.363992598  3.910709425 -1.894912701
C  2.182751711  2.836226470 -1.433328643
H  2.762112565  3.311126952 -2.228081353
C  2.791674010  1.901085220 -0.591310616
H  3.853543285  1.671460822 -0.721529659

```

———— 263\_FGG80: PBE+D3 ————

```

O  3.886918938 -1.329904310 -0.457085487
C  3.473865485 -0.213705210 -0.223215836

```



```

O  3.834807643  0.857236685 -0.950548201
H  3.386825347  1.676277004 -0.573464700
C  2.519342289  0.091279985  0.947120947
H  3.039598058  0.761673732  1.653517184
H  2.288473766 -0.852200247  1.449909206
N  1.264880954  0.716571384  0.546374123
H  0.412614429  0.156372289  0.564614471
C  1.199383706  2.016633277  0.197235443
O  2.212896908  2.731289391  0.084765387
C -0.186545601  2.614403167 -0.022773127
H -0.066581943  3.435377101 -0.745648720
H -0.519206105  3.046739125  0.936750412
N -1.210377919  1.688699994 -0.445665719
H -1.236960389  1.322889117 -1.399660721
C -2.281743044  1.359876246  0.334130029
O -2.422525387  1.712823161  1.502731414
C -3.320638805  0.467872573 -0.368130298
N -3.155987035  0.503199012 -1.829081850
H -3.679504965 -0.260205189 -2.262695820
H -3.540680585  1.372135124 -2.207738896
H -4.299633851  0.860003349 -0.033368253
C -3.213631117 -0.975440203  0.180113608
H -3.558472612 -0.943482849  1.223577148
H -3.937719871 -1.598655062 -0.374029456
C -1.842504674 -1.609716021  0.136560534
C -1.229044084 -1.988015103 -1.069193419
H -1.738769547 -1.805229453 -2.016661604
C  0.032755577 -2.586082902 -1.075761235
H  0.498754544 -2.859537438 -2.024184002
C  0.700219733 -2.841785713  0.124976567
H  1.689424261 -3.301897254  0.113675068
C  0.098985150 -2.477347952  1.331985020
H  0.603892801 -2.678391530  2.279608627
C -1.153635983 -1.855045619  1.335139267
H -1.613476070 -1.562709659  2.282122890

```

———— 264\_FGG114: PBE+D3 ————

```

O  3.830311072  1.027434109 -0.808874210
C  3.453187133 -0.052555040 -0.403493027
O  3.817913102 -1.207895584 -0.979142455
H  3.379356179 -1.975450910 -0.495393705
C  2.540387393 -0.196663103  0.831587442
H  2.310462682  0.808620724  1.200122874
H  3.094118638 -0.749146019  1.610098935
N  1.284046337 -0.887870776  0.571116203
H  0.435295224 -0.331610140  0.475228018
C  1.212835442 -2.214548706  0.342083673
O  2.218651706 -2.945618919  0.287516731
C -0.178098832 -2.804762606  0.123027499
H -0.223979593 -3.742556445  0.696730354
H -0.258019679 -3.059908796 -0.946908037
N -1.277018812 -1.928264560  0.446378196
H -1.606535346 -1.787782378  1.405063344
C -2.054694771 -1.342143630 -0.509412321
O -1.888128653 -1.485878322 -1.719131777
C -3.175266393 -0.445150722  0.059411652

```

N -3.123074231 -0.382912172 1.526697094  
H -4.059501163 -0.307084086 1.923735497  
H -2.596120071 0.442916330 1.828769206  
H -4.114708750 -0.945778880 -0.229873852  
C -3.137127547 0.934396695 -0.654719733  
H -3.180948707 0.750281908 -1.737902732  
H -4.041607946 1.493794083 -0.365545360  
C -1.903545160 1.729290722 -0.305929565  
C -0.705118901 1.549177239 -1.020634801  
H -0.689612889 0.858861333 -1.867746657  
C 0.452778746 2.246004300 -0.665698130  
H 1.376068863 2.100926932 -1.231146709  
C 0.436302884 3.131160923 0.417468029  
H 1.342842460 3.675412375 0.689392935  
C -0.748234823 3.328855079 1.129702292  
H -0.775847586 4.032972917 1.964348259  
C -1.907398292 2.635402983 0.766669992  
H -2.839969714 2.822073141 1.307404848

———— 265\_FGG357: PBE+D3 ————

O -3.743991105 1.340212149 0.795057816  
C -3.461205123 0.244658235 0.356258550  
O -3.937631344 -0.891534141 0.887466204  
H -3.562342585 -1.678667812 0.383275834  
C -2.545035720 0.058554209 -0.870555671  
H -2.222231723 1.050343511 -1.204124362  
H -3.130250037 -0.421323159 -1.673669431  
N -1.358391731 -0.746529006 -0.613052723  
H -0.468066057 -0.268773409 -0.478635777  
C -1.408302401 -2.081586598 -0.431913082  
O -2.475604789 -2.721941646 -0.421704292  
C -0.079460954 -2.799583445 -0.210467847  
H -0.110644412 -3.725684433 -0.803661900  
H -0.036150748 -3.082825760 0.854423763  
N 1.097968729 -2.019634506 -0.501598715  
H 1.441604682 -1.871814678 -1.454338154  
C 1.910928113 -1.524492955 0.475680768  
O 1.718934582 -1.683949960 1.679809261  
C 3.112211193 -0.715067846 -0.058897345  
N 3.076936641 -0.598517560 -1.523525100  
H 2.644247950 0.289270320 -1.798170766  
H 4.018339389 -0.610883150 -1.915441690  
H 3.999571074 -1.308680342 0.218146216  
C 3.192594857 0.637481064 0.701754723  
H 3.203467869 0.413042513 1.778168403  
H 4.149175385 1.119674729 0.442771070  
C 2.041069568 1.552958791 0.367283450  
C 0.821602044 1.460659395 1.062953619  
H 0.732522487 0.751245258 1.889511024  
C -0.265094626 2.268530823 0.716985606  
H -1.204738171 2.189659623 1.268447850  
C -0.155557200 3.179584717 -0.339040422  
H -1.006641855 3.809560520 -0.605589314  
C 1.051896883 3.291553607 -1.031146035  
H 1.154013830 4.014497665 -1.843603606  
C 2.140017326 2.486901440 -0.676842975

H 3.092237979 2.606101837 -1.202014955

———— 266\_FGG691: PBE+D3 ————

O 3.151368261 -1.698141826 0.101970171  
 C 4.094886965 -1.102181177 -0.371732911  
 O 5.311127493 -1.675321141 -0.588123840  
 H 5.235985256 -2.600562773 -0.273940136  
 C 4.110746107 0.358005824 -0.807582264  
 H 4.485246449 0.411844508 -1.842449441  
 H 4.826965627 0.898235391 -0.167434076  
 N 2.826403894 0.988796622 -0.675005462  
 H 2.030209250 0.630356025 -1.218160169  
 C 2.521643003 1.722791436 0.438846507  
 O 3.345915421 2.098467724 1.268296245  
 C 1.018301251 2.030369698 0.566968712  
 H 0.647230008 2.488897651 -0.363972039  
 H 0.890141057 2.734146690 1.397792830  
 N 0.241328694 0.830819971 0.826583211  
 H 0.054544663 0.505266583 1.778631785  
 C -0.099918022 -0.042975561 -0.142184862  
 O 0.160818908 0.123933758 -1.345785901  
 C -0.804825507 -1.316014833 0.359386314  
 N -1.150293299 -1.207619910 1.781138552  
 H -1.111074821 -2.118450807 2.238975262  
 H -2.104990939 -0.850837953 1.885864117  
 H -0.030958252 -2.097614445 0.259599416  
 C -1.980798973 -1.686672209 -0.582130397  
 H -1.600719248 -1.663121473 -1.614412417  
 H -2.288072557 -2.720404977 -0.356267681  
 C -3.156929734 -0.755491565 -0.428975057  
 C -4.227043752 -1.082863117 0.419124907  
 H -4.234934929 -2.055503492 0.919305475  
 C -5.290368370 -0.195946408 0.614107994  
 H -6.115890766 -0.473310780 1.273474551  
 C -5.299404009 1.037561540 -0.039342984  
 H -6.129365302 1.731735543 0.108949691  
 C -4.243551584 1.373571426 -0.892308251  
 H -4.247608787 2.333115314 -1.413799694  
 C -3.182943327 0.486926725 -1.084925261  
 H -2.358170129 0.753192017 -1.750482899

**11.2.12 GFA: PBE+D3**

———— 236\_GFA15: PBE+D3 ————

O -0.808320711 -0.361919733 5.233628661  
 C 0.039923664 -0.341753835 4.367938545  
 O 0.910609165 -1.349291217 4.193375470  
 H 1.509131179 -1.144291197 3.407759989  
 C 0.232199277 0.860358108 3.401614863  
 C -0.738866910 1.988449328 3.711350222  
 H -1.778697861 1.655367366 3.581257071  
 H -0.623261747 2.304592320 4.755509392  
 H -0.551361283 2.849323565 3.053008693  
 H 1.275229562 1.202684237 3.540801659  
 N 0.092195929 0.457395735 1.997969833  
 H -0.718793102 0.799636689 1.449852952  
 C 1.022837631 -0.250495133 1.338449423

O 2.048650245 -0.716815407 1.876537015  
C 0.814048887 -0.436456171 -0.173514541  
H 1.502130431 -1.248012800 -0.445727944  
N -0.517333140 -0.897468125 -0.562732329  
H -0.583034058 -1.720043755 -1.172696646  
C -1.654237278 -0.168220064 -0.571704839  
O -1.824516757 0.904913989 0.030239550  
C -2.782904634 -0.792071101 -1.396901379  
H -3.333676435 0.052960838 -1.847401140  
H -3.472746561 -1.272786040 -0.683638098  
N -2.289698607 -1.796555879 -2.340891160  
H -3.012399853 -2.474062866 -2.581329685  
H -1.964337662 -1.359620698 -3.206073894  
C 1.242791994 0.844209050 -0.945940123  
H 0.645311594 1.695894323 -0.591122158  
H 2.295759595 1.040789917 -0.689799559  
C 1.068334361 0.664089562 -2.431802177  
C 1.969045584 -0.116362479 -3.171345487  
H 2.847141645 -0.539643715 -2.675435509  
C 1.758887731 -0.357781241 -4.530055482  
H 2.473797066 -0.963967070 -5.090691746  
C 0.640216027 0.179441477 -5.173626442  
H 0.477065084 -0.007100052 -6.237054993  
C -0.257807935 0.969160449 -4.451060599  
H -1.125060903 1.408582529 -4.949257591  
C -0.044070900 1.207897667 -3.090382092  
H -0.748220314 1.825391431 -2.525897722

———— 237\_GFA07: PBE+D3 ————

O -0.616340336 0.917235141 5.389306167  
C -0.787309007 0.226829998 4.408166465  
O -2.011228721 -0.148023821 4.000175717  
H -1.933491256 -0.702760828 3.162695501  
C 0.384590475 -0.323475360 3.547841946  
C 1.734744406 0.101876972 4.104688802  
H 2.551014440 -0.340162466 3.514897035  
H 1.833066614 1.196765089 4.093217183  
H 1.828730974 -0.225369278 5.147653651  
H 0.290398181 -1.426091253 3.571822972  
N 0.271334534 0.090640453 2.144792592  
H 0.988083956 0.720075379 1.748318918  
C -0.603383046 -0.453739652 1.279859269  
O -1.509076410 -1.239830005 1.619575415  
C -0.413508560 -0.008251949 -0.186774986  
H -0.431706600 1.097294678 -0.187070490  
N 0.887905524 -0.406096326 -0.709826894  
H 0.958488687 -1.130374131 -1.431213667  
C 2.021060667 0.299084000 -0.504310797  
O 2.122703679 1.233997484 0.304927040  
C 3.211633433 -0.155207719 -1.350495239  
H 3.891051328 -0.698523465 -0.673329859  
H 3.743189527 0.764541812 -1.654650873  
N 2.815957192 -1.044007175 -2.446009044  
H 3.584026025 -1.652159753 -2.728782978  
H 2.522756070 -0.512957367 -3.268268087  
C -1.535169742 -0.544679538 -1.085425876

H -1.562820589 -1.642617338 -1.007395986  
H -2.492089642 -0.186265149 -0.677520809  
C -1.363480992 -0.117229257 -2.523123620  
C -0.978143150 -1.039992409 -3.505351650  
H -0.845466510 -2.090624943 -3.231294073  
C -0.770090281 -0.638589950 -4.828373765  
H -0.476374267 -1.375215318 -5.579438417  
C -0.946860871 0.698749047 -5.188419561  
H -0.788740872 1.016223093 -6.220961443  
C -1.339237340 1.628059733 -4.219981207  
H -1.489855489 2.673901564 -4.495558454  
C -1.545276816 1.222226356 -2.900967717  
H -1.854645217 1.956063650 -2.151613180

———— 238\_GFA10: PBE+D3 ————

O -0.410778859 1.850816393 -3.740274704  
C -0.270401008 2.039239053 -2.551726206  
O -1.277058963 2.475113954 -1.773954095  
H -0.967153705 2.532066238 -0.818497419  
C 1.080022485 1.820583659 -1.812494068  
C 2.182379523 1.409211735 -2.775421653  
H 2.288677198 2.158014215 -3.570078630  
H 3.140366654 1.312165818 -2.243965163  
H 1.934981162 0.452378595 -3.260207103  
H 1.333911772 2.775835595 -1.318838583  
N 0.955620099 0.814056959 -0.751664200  
H 1.255452361 -0.133036365 -0.979845589  
C 0.266483929 0.998009222 0.393198363  
O -0.296919977 2.075051737 0.674007755  
C 0.153805658 -0.219077714 1.305991032  
H 1.090069479 -0.801678806 1.295134652  
N -0.067450445 0.228401584 2.656431499  
H -0.524423336 1.126439909 2.832423542  
C 0.327107975 -0.512562631 3.723724181  
O 0.886643364 -1.607387672 3.632866022  
C 0.001761321 0.113742528 5.084347556  
H 0.871191512 -0.088434539 5.736212958  
H -0.836011900 -0.472612197 5.495497790  
N -0.399115907 1.520356689 4.994032213  
H -1.019489988 1.781635517 5.760125287  
H 0.411451846 2.139991151 5.031745990  
C -0.993689909 -1.159483189 0.808705070  
H -1.076784558 -1.953521355 1.566500103  
H -1.935282016 -0.589032344 0.804246303  
C -0.710513659 -1.743003086 -0.549983875  
C 0.277471848 -2.730695906 -0.699966549  
H 0.771408132 -3.134506782 0.188476671  
C 0.631791795 -3.196963303 -1.968091917  
H 1.400726240 -3.966404056 -2.068202300  
C 0.003473783 -2.682566337 -3.106284818  
H 0.285644632 -3.041747080 -4.097642015  
C -0.989765342 -1.709931002 -2.968627146  
H -1.478736704 -1.291544654 -3.849754792  
C -1.344002040 -1.248159305 -1.698983499  
H -2.105664454 -0.469412227 -1.601212667

———— 239\_GFA02: PBE+D3 ————

O	3.156956771	0.782888605	1.206404781
C	3.112781857	1.652258102	0.355178178
O	4.059972690	2.610709973	0.223871398
H	4.721918571	2.444120636	0.927740414
C	1.993656673	1.822941516	-0.659868982
C	1.186283628	3.103313532	-0.370027525
H	0.389807887	3.189582284	-1.120586942
H	0.729823587	3.051410043	0.629434338
H	1.832563646	3.990011392	-0.428808735
H	2.439792822	1.912973368	-1.665742101
N	1.179583192	0.629159540	-0.606468150
H	1.339729334	-0.005418587	0.173649089
C	0.328281808	0.268435815	-1.597949491
O	0.133712945	0.945079829	-2.609223141
C	-0.405106828	-1.073237260	-1.377929504
H	-0.042224355	-1.744890551	-2.174175834
N	-0.075965194	-1.714124315	-0.123447708
H	-0.507144374	-1.410422826	0.754653779
C	0.722486862	-2.818408893	-0.034901930
O	1.258614405	-3.371942393	-0.991629121
C	0.899822366	-3.338542117	1.398190700
H	1.951050370	-3.666684726	1.481584577
H	0.281307915	-4.246940144	1.474634759
N	0.465044220	-2.376152448	2.417227356
H	0.176102289	-2.847219922	3.274299912
H	1.223404509	-1.736658781	2.663222317
C	-1.930927472	-0.871622779	-1.542904009
H	-2.086896082	-0.382666165	-2.515361438
H	-2.402605542	-1.865067672	-1.578649051
C	-2.530449758	-0.047000868	-0.430583320
C	-2.513420501	1.356301189	-0.487224862
H	-2.104011068	1.845875219	-1.373805763
C	-3.011700502	2.119698707	0.569636576
H	-2.993709399	3.210432192	0.505269339
C	-3.537478174	1.494760118	1.704211018
H	-3.930008406	2.092555189	2.529505261
C	-3.568972035	0.100446441	1.769681015
H	-3.988799282	-0.397990106	2.646386658
C	-3.070673707	-0.661315962	0.709524137
H	-3.107265666	-1.753407173	0.763132006

———— 240\_GFA11: PBE+D3 ————

O	-5.237039322	0.644756241	-0.081933661
C	-4.068705281	0.965269453	-0.109548331
O	-3.611527743	2.061734610	0.518720065
H	-2.618462510	2.142394265	0.374401789
C	-2.992162253	0.168797404	-0.898575536
C	-3.595596773	-1.030492984	-1.614067591
H	-4.406342542	-0.703323654	-2.277137684
H	-2.828652297	-1.546637875	-2.210558514
H	-4.027449274	-1.738385164	-0.891775972
H	-2.564011573	0.875616408	-1.634093782
N	-1.891351187	-0.269278660	-0.034384967
H	-1.818767793	-1.268276874	0.224805256
C	-0.930724791	0.553757579	0.419564735
O	-0.969446427	1.792178177	0.270642829

C 0.201375399 -0.149419147 1.207992987  
H -0.300586490 -0.592825918 2.088316889  
N 0.815281929 -1.244826417 0.468504517  
H 1.760820441 -1.130920568 0.085377616  
C 0.274986771 -2.470838624 0.319526133  
O -0.866231141 -2.787544206 0.693871245  
C 1.191179141 -3.492534529 -0.360896099  
H 0.564337328 -4.049116425 -1.080015182  
H 1.471558301 -4.213754487 0.423503130  
N 2.397196195 -2.891114231 -0.933488350  
H 3.207525864 -3.501978461 -0.843629960  
H 2.279728500 -2.676430590 -1.924072559  
C 1.279300197 0.838305517 1.701754417  
H 0.762975708 1.760800052 2.003555470  
H 1.745541217 0.404952561 2.599227149  
C 2.362025868 1.147565035 0.689836181  
C 3.615265069 0.524350692 0.794197312  
H 3.807044775 -0.156409419 1.628816329  
C 4.624010424 0.769334812 -0.141540881  
H 5.593127096 0.277135342 -0.036763530  
C 4.392653628 1.647699730 -1.201010008  
H 5.178973378 1.847393299 -1.932276107  
C 3.150316606 2.279369550 -1.313048839  
H 2.964618173 2.975773458 -2.134071049  
C 2.143174291 2.032673790 -0.378656098  
H 1.173521099 2.524860261 -0.467769348

———— 241\_GFA09: PBE+D3 ————

O 1.833709939 3.752972894 0.432031655  
C 2.033928462 2.569813087 0.264803792  
O 2.494540830 1.777493667 1.249091306  
H 2.557895783 0.829295874 0.918974160  
C 1.802070478 1.854724532 -1.096304204  
C 1.361885569 2.834631476 -2.172238575  
H 1.253727489 2.321119111 -3.138720291  
H 0.404517746 3.303251966 -1.897753461  
H 2.100136405 3.639440105 -2.275457789  
H 2.757996545 1.376126246 -1.374621355  
N 0.808607194 0.781002540 -0.976527388  
H -0.145604137 1.004490549 -1.256680557  
C 1.015717068 -0.374743876 -0.312778536  
O 2.104325441 -0.655134048 0.227956313  
C -0.190613351 -1.300899227 -0.197236639  
H -0.790015486 -1.276481456 -1.122757426  
N 0.273440525 -2.650507602 -0.004631668  
H 1.204744212 -2.823853859 0.381488553  
C -0.473966960 -3.718055080 -0.386501937  
O -1.593690558 -3.628005288 -0.894341494  
C 0.201570834 -5.076083598 -0.164313475  
H 0.511734212 -5.424883047 -1.162900038  
H -0.589552884 -5.769002773 0.174327965  
N 1.380817895 -5.001451712 0.703275588  
H 2.053809152 -5.734309792 0.480216787  
H 1.124951808 -5.110524210 1.685808908  
C -1.114642723 -0.831377557 0.975331468  
H -1.895372608 -1.602071348 1.065131165

```
H -0.524139394 -0.829096352 1.904567218
C -1.724573166 0.521214411 0.720242780
C -1.236179334 1.670496418 1.358283917
H -0.441688703 1.576340052 2.103905427
C -1.725123915 2.936610525 1.028448000
H -1.311835139 3.818600201 1.520227533
C -2.718759309 3.070198179 0.055639828
H -3.099033996 4.058886473 -0.207630453
C -3.226839164 1.931304717 -0.576613239
H -4.012422830 2.027955736 -1.329463541
C -2.733363741 0.666852207 -0.246931762
H -3.132010191 -0.222210139 -0.743898536
```

## ——— 242\_GFA08: PBE+D3 ———

```
O -0.042341269 5.251405958 -0.626598917
C -0.093938990 4.085323501 -0.951776162
O 0.515388172 3.621414786 -2.056216474
H 0.356081466 2.630792492 -2.137498126
C -0.893033345 3.018507460 -0.151656730
C -1.592803875 3.629170333 1.052817824
H -2.198649508 2.870306618 1.570026842
H -0.861311349 4.048946897 1.758486176
H -2.245491566 4.450325605 0.730589275
H -1.638442476 2.601696498 -0.854731814
N -0.040675557 1.905534632 0.278125123
H 0.227482502 1.829424654 1.273861075
C 0.395383667 0.940083742 -0.549295877
O 0.236967100 0.980524728 -1.786299418
C 1.172431047 -0.201633443 0.151430117
H 2.046943059 0.293673595 0.612467227
N 0.418951834 -0.816325784 1.236047249
H -0.030323138 -1.727548079 1.093003682
C 0.281252269 -0.281057557 2.466366253
O 0.697970547 0.842853854 2.791849381
C -0.476111734 -1.157101261 3.466258369
H -1.446253811 -0.660754946 3.629573989
H 0.071744949 -1.082717892 4.422790394
N -0.705556320 -2.518272168 2.980219842
H 0.051494094 -3.146905432 3.251755314
H -1.573371050 -2.907216965 3.346346723
C 1.677524342 -1.271605470 -0.838715376
H 1.978488178 -0.748592640 -1.757995930
H 2.577772699 -1.732677614 -0.405647421
C 0.676584241 -2.360894572 -1.158796754
C -0.397655435 -2.140686836 -2.036480901
H -0.499580985 -1.164457876 -2.513112594
C -1.320387865 -3.155106709 -2.296967631
H -2.146311140 -2.967616592 -2.986947592
C -1.190565501 -4.406241964 -1.686933883
H -1.912740722 -5.198083907 -1.897055510
C -0.125504613 -4.638844835 -0.815688127
H -0.007220439 -5.614970550 -0.340663942
C 0.797994732 -3.622544264 -0.556355634
H 1.638295791 -3.815457996 0.117269960
```

## ——— 243\_GFA13: PBE+D3 ———



O 1.047937890 -0.520979431 -3.229237442  
C 0.022076839 -0.183260045 -3.785326343  
O -0.224225348 -0.432513689 -5.098875373  
H 0.563258242 -0.905291809 -5.441369041  
C -1.142937672 0.587498697 -3.145327760  
C -1.172562400 2.031890487 -3.658562173  
H -1.255905212 2.052757127 -4.753445983  
H -2.034969412 2.556907770 -3.224854466  
H -0.256816708 2.569355047 -3.365985515  
H -2.066419967 0.062324788 -3.435034994  
N -1.037300561 0.554836316 -1.704616097  
H -0.362136246 1.193218460 -1.259171890  
C -1.328861136 -0.593523516 -1.022107642  
O -1.965306522 -1.530954490 -1.498172922  
C -0.756612863 -0.647180554 0.413364593  
H -1.026722741 -1.645337555 0.785481414  
N 0.705778734 -0.617317761 0.364166716  
H 1.215903405 -1.506529940 0.367270873  
C 1.489204791 0.432845297 0.036772203  
O 1.096136162 1.598480233 -0.137811540  
C 2.969932983 0.072977320 -0.110580850  
H 3.462501857 0.325658026 0.843487442  
H 3.373357000 0.758871519 -0.876438838  
N 3.161473463 -1.353614009 -0.383847657  
H 2.992311263 -1.545578958 -1.374430899  
H 4.112695740 -1.649487533 -0.165285774  
C -1.379236606 0.403964019 1.361284106  
H -1.171667304 1.413498539 0.983082906  
H -2.470222543 0.250418149 1.329044519  
C -0.870375905 0.261957918 2.773123626  
C -1.444458889 -0.665983232 3.653732252  
H -2.300449114 -1.262201449 3.323456973  
C -0.943700946 -0.832384559 4.946222864  
H -1.408290958 -1.555671432 5.620182898  
C 0.145235037 -0.070846257 5.377999902  
H 0.537683819 -0.198060170 6.388859785  
C 0.723157886 0.858999547 4.510645481  
H 1.571640488 1.461782766 4.842587394  
C 0.218827252 1.023937025 3.218653623  
H 0.671566201 1.751637339 2.540263629

———— 244\_GFA12: PBE+D3 ————

O 5.232515402 -0.569072281 -0.058382828  
C 4.328729045 0.213990106 -0.256633315  
O 4.134013654 0.795050416 -1.452299583  
H 3.316420814 1.383838752 -1.411372992  
C 3.327559763 0.649380224 0.849503808  
C 3.660415768 0.010157488 2.188913005  
H 2.973799249 0.371794929 2.968375009  
H 3.589239918 -1.085399284 2.125380980  
H 4.690050853 0.257505599 2.475864076  
H 3.403474839 1.751073140 0.919584753  
N 1.942764331 0.334258048 0.482258311  
H 1.439397230 -0.410613474 0.996525938  
C 1.250784436 1.020283251 -0.442767256  
O 1.745717312 1.926695361 -1.143720645

C -0.242514383 0.676716473 -0.582318220  
H -0.549962928 1.162740288 -1.518060514  
N -0.516888862 -0.747293298 -0.762156933  
H -1.007584451 -1.061392017 -1.606948881  
C -0.427909514 -1.715730008 0.170861020  
O 0.095054872 -1.593731953 1.291443605  
C -1.055213292 -3.049074575 -0.250593742  
H -1.915423040 -3.193001771 0.422395321  
H -0.327140013 -3.837621374 0.004196174  
N -1.492661664 -3.070416789 -1.649877841  
H -0.850948497 -3.602682228 -2.236942918  
H -2.420071225 -3.479085020 -1.751807186  
C -1.053437517 1.307028851 0.582410714  
H -0.701087207 0.884737486 1.533556975  
H -0.824641365 2.384822411 0.585733765  
C -2.533173598 1.074384242 0.422072166  
C -3.287722226 1.843041090 -0.476193381  
H -2.805238946 2.656303010 -1.026291287  
C -4.646188749 1.587527484 -0.670678072  
H -5.219753105 2.200461451 -1.369406205  
C -5.272865281 0.554574879 0.032221018  
H -6.336062632 0.355250076 -0.117221953  
C -4.533534670 -0.212868294 0.935299127  
H -5.018454371 -1.014245042 1.497410460  
C -3.173854644 0.045743195 1.127051997  
H -2.597315306 -0.551950841 1.838445531

## ———— 245\_GFA06: PBE+D3 ————

O 0.829368887 5.359398909 0.903585145  
C 0.916968121 4.378639339 0.197245699  
O 2.096236630 3.938011588 -0.273009106  
H 1.951980854 3.105825539 -0.822306136  
C -0.318430892 3.555840074 -0.263884052  
C -1.615087519 4.150162575 0.264328127  
H -2.479372341 3.584793903 -0.113782213  
H -1.629426829 4.138791784 1.363556041  
H -1.703709979 5.196234234 -0.054557032  
H -0.307498088 3.580572553 -1.370414231  
N -0.214301220 2.148555008 0.137860826  
H -0.892318460 1.767614362 0.818813818  
C 0.588376092 1.262313226 -0.478155346  
O 1.436095339 1.581793042 -1.334320475  
C 0.395008070 -0.201728811 -0.023148864  
H 0.498572042 -0.208164219 1.077824480  
N -0.946755088 -0.686932914 -0.325048593  
H -1.096681655 -1.423342787 -1.023627621  
C -2.021853160 -0.436122012 0.450084202  
O -2.038621931 0.377054236 1.387654850  
C -3.266213042 -1.256727922 0.093979895  
H -4.087169376 -0.539073095 -0.064408722  
H -3.525381779 -1.815953266 1.007864522  
N -3.065512644 -2.147937470 -1.053538888  
H -3.232155115 -3.124258733 -0.815767628  
H -3.672667076 -1.906257027 -1.835159539  
C 1.451109844 -1.120585044 -0.648683584  
H 1.393846776 -1.038078841 -1.745171237

H 2.440762200 -0.730725211 -0.366341388  
 C 1.294803017 -2.558133446 -0.215543110  
 C 1.560433907 -2.943877058 1.107607634  
 H 1.913057503 -2.198552182 1.825823016  
 C 1.384692978 -4.266178517 1.516294919  
 H 1.601247142 -4.548263607 2.548636254  
 C 0.939523998 -5.230002812 0.606175241  
 H 0.805899314 -6.265461368 0.925386466  
 C 0.676725176 -4.861423664 -0.714351572  
 H 0.338782055 -5.608571872 -1.435744140  
 C 0.853250562 -3.534874870 -1.118366918  
 H 0.654025689 -3.253263624 -2.156340741

———— 246\_GFA16: PBE+D3 ————

O -5.154308564 0.365850535 -1.484322756  
 C -4.313451480 0.507756160 -0.619980830  
 O -4.111418680 1.676831312 0.000246621  
 H -3.374411342 1.579855642 0.689639130  
 C -3.467852332 -0.699481558 -0.137899487  
 C -4.039780466 -1.258538176 1.174377279  
 H -3.516138418 -2.186543530 1.446246924  
 H -3.928636939 -0.538076137 1.996469676  
 H -5.107929330 -1.482288160 1.043586131  
 H -3.588093637 -1.450188731 -0.930675950  
 N -2.021180539 -0.452371410 -0.050200365  
 H -1.388923672 -1.021476039 -0.644074582  
 C -1.418919101 0.406263932 0.785922127  
 O -2.015194722 1.233807885 1.508623525  
 C 0.117741244 0.408461513 0.786269663  
 H 0.384910590 0.902695477 1.730688718  
 N 0.758241058 -0.905510849 0.831966369  
 H 1.505102953 -1.041858042 1.522852723  
 C 0.848677636 -1.791016851 -0.184985149  
 O 0.118076052 -1.805727082 -1.189123527  
 C 1.951292841 -2.837393246 -0.001191540  
 H 2.337912299 -3.049836209 -1.013905779  
 H 1.465766810 -3.762458241 0.350177565  
 N 2.952915285 -2.416732045 0.979859307  
 H 3.646111654 -1.798012590 0.550893165  
 H 3.447185305 -3.214772274 1.377544460  
 C 0.653144524 1.282198650 -0.386374423  
 H 0.270000851 0.884563635 -1.336969380  
 H 0.239633284 2.294361865 -0.254289588  
 C 2.160046247 1.299259881 -0.400151614  
 C 2.871098560 0.527522110 -1.330421342  
 H 2.319680241 -0.027045019 -2.094483358  
 C 4.267234862 0.462180660 -1.290036665  
 H 4.804528572 -0.135576916 -2.030179892  
 C 4.973583188 1.167492358 -0.312055694  
 H 6.064437693 1.119917236 -0.278891181  
 C 4.275736846 1.950974350 0.612292200  
 H 4.820779455 2.517307218 1.370497793  
 C 2.881976113 2.015462580 0.566192557  
 H 2.345555063 2.632770106 1.292837172

———— 247\_GFA03: PBE+D3 ————

O -3.112152165 0.648535489 -1.454868625  
C -3.044472475 1.452338776 -0.546450973  
O -4.132975165 2.003906459 0.045513057  
H -4.913303948 1.630174574 -0.415449052  
C -1.753405905 1.993782195 0.046334226  
C -1.542529162 3.464822772 -0.355998605  
H -2.366301615 4.089514205 0.016763697  
H -0.600508794 3.816416896 0.085003444  
H -1.483723375 3.558564805 -1.450388324  
H -1.818942742 1.937577570 1.146740750  
N -0.672202364 1.133072428 -0.398523131  
H -0.919214374 0.439011338 -1.104237034  
C 0.461468150 0.987019878 0.336041678  
O 0.739923157 1.704856700 1.299994020  
C 1.356043606 -0.183921517 -0.075513205  
H 1.204940341 -0.452015560 -1.133608820  
N 2.734745345 0.209073134 0.088703577  
H 2.979890482 0.893447448 0.808776946  
C 3.738968866 -0.363095456 -0.621294059  
O 3.573662675 -1.234496730 -1.478372904  
C 5.139923162 0.149329713 -0.266405525  
H 5.688760383 0.242233165 -1.221229859  
H 5.627185492 -0.666024822 0.292881895  
N 5.126327370 1.353723608 0.568369022  
H 5.976184369 1.428636121 1.127181325  
H 5.062141485 2.197815072 -0.002617957  
C 1.010149328 -1.427331529 0.799062977  
H 1.714458376 -2.220295272 0.503188791  
H 1.209036320 -1.163820549 1.849663318  
C -0.414455163 -1.881237633 0.624536733  
C -0.797147210 -2.598983984 -0.519347097  
H -0.036449876 -2.881790713 -1.252631207  
C -2.130530288 -2.956409587 -0.726689365  
H -2.410338287 -3.512798913 -1.623694801  
C -3.105283646 -2.604801266 0.210303037  
H -4.148021422 -2.884260871 0.047819112  
C -2.736521899 -1.897465721 1.357159504  
H -3.490354616 -1.625115220 2.099666781  
C -1.402030857 -1.538193923 1.559722569  
H -1.118413559 -0.977413080 2.454504082

———— 248\_GFA01: PBE+D3 ————

O -1.425255380 -0.620007411 -3.149666453  
C -0.519899393 -1.426984361 -3.078304749  
O 0.087493826 -1.966145309 -4.164495635  
H -0.360989849 -1.581959520 -4.947010780  
C 0.050889007 -1.987062078 -1.785341459  
C -0.361238294 -3.458746310 -1.599685634  
H 0.060946875 -3.823852185 -0.654240901  
H -1.456893069 -3.548764281 -1.561703303  
H 0.023867632 -4.074717917 -2.424307163  
H 1.152400251 -1.935180306 -1.833191632  
N -0.406961666 -1.138040949 -0.700372101  
H -1.108881604 -0.440390777 -0.947922060  
C 0.308494491 -1.012018866 0.447397080  
O 1.265363664 -1.737390827 0.731018722

```

C -0.114009161  0.146420256  1.353217187
H -1.168681793  0.420547003  1.187403455
N  0.033817007 -0.268911174  2.727305082
H  0.694603231 -1.015319151  2.958312099
C -0.662928066  0.307351507  3.737741680
O -1.480925371  1.217950126  3.585691468
C -0.381621695 -0.290559571  5.122424078
H -1.261133835 -0.906836364  5.370097940
H -0.382631515  0.555276039  5.833431925
N  0.815854624 -1.135087891  5.158201890
H  1.651417673 -0.583156180  5.357501672
H  0.745850604 -1.853512967  5.878264666
C  0.769037950  1.392119485  1.037511599
H  0.468933727  2.173834134  1.752327728
H  1.816245560  1.119898708  1.242382117
C  0.610974711  1.871290905 -0.380596509
C  1.557290919  1.545194023 -1.363228293
H  2.448492496  0.978840375 -1.079379062
C  1.370462640  1.928072055 -2.693469590
H  2.121566642  1.668498416 -3.443320756
C  0.228179381  2.642370086 -3.063041401
H  0.077727232  2.939863793 -4.102552268
C -0.719766597  2.977448676 -2.093048335
H -1.613312942  3.539171645 -2.373327874
C -0.527901486  2.596818777 -0.763761719
H -1.269708427  2.866968386 -0.006702709

```

————— 249\_GFA14: PBE+D3 —————

```

O  0.533614278 -3.139802437 -0.788621013
C  0.183761257 -2.674465438 -1.856826645
O  0.717777270 -3.070216123 -3.038182064
H  1.401877787 -3.735818768 -2.813741241
C -0.962275868 -1.662554046 -2.036565616
C -0.935299123 -0.884108574 -3.354367679
H -0.979210065 -1.567204921 -4.212828432
H -1.805119923 -0.212764275 -3.390807941
H -0.020963994 -0.281743805 -3.423707643
H -1.875970903 -2.283184424 -2.011374329
N -1.033002489 -0.794631417 -0.869034546
H -1.710710495 -1.026294734 -0.134109455
C  0.084466246 -0.128093971 -0.452592636
O  1.107301205 -0.030366116 -1.129980930
C -0.014033828  0.371179530  1.007711593
H -1.045807681  0.695604844  1.215494955
N  0.240913066 -0.797057265  1.845306080
H  1.199048868 -1.147214755  1.952627238
C -0.714116110 -1.734238907  2.077245176
O -1.913550122 -1.585195106  1.807768099
C -0.182175258 -3.024286399  2.704434459
H -0.851060111 -3.829313861  2.350859012
H -0.319293314 -2.944520809  3.796081644
N  1.240628797 -3.215492870  2.411225257
H  1.352724991 -3.560371945  1.454084086
H  1.663213727 -3.892052057  3.046527395
C  0.972176697  1.503602651  1.304096356
H  1.033780611  1.617191258  2.398105559

```

H	1.966125180	1.208074958	0.932835073
C	0.548815040	2.809287930	0.672866783
C	-0.365275791	3.646578853	1.329625133
H	-0.745749107	3.359062360	2.313682953
C	-0.786845226	4.843406438	0.748103052
H	-1.494890436	5.485305596	1.277171604
C	-0.298504653	5.222130604	-0.505015174
H	-0.624171702	6.159589398	-0.959913916
C	0.611400987	4.396109246	-1.168820085
H	0.998223636	4.684393281	-2.148318211
C	1.030652193	3.198548344	-0.584983134
H	1.728844363	2.542967730	-1.109890815

## ——— 250\_GFA05: PBE+D3 ———

O	-2.157052363	1.493784789	-1.791837897
C	-2.327940726	0.445389935	-2.376893560
O	-2.862883039	0.363279097	-3.623437882
H	-3.047403523	1.284467799	-3.903350682
C	-2.040843045	-0.955398908	-1.818233929
C	-3.330199144	-1.558179635	-1.248391810
H	-3.135989371	-2.576281374	-0.882360554
H	-3.704598155	-0.947505071	-0.411821150
H	-4.107544524	-1.605646974	-2.022909267
H	-1.672989837	-1.566412141	-2.656745222
N	-1.018329679	-0.909814446	-0.794083156
H	-1.325045397	-0.824707323	0.174774580
C	0.244657662	-0.493679189	-1.101749962
O	0.620460628	-0.325803043	-2.261884405
C	1.157025217	-0.242364617	0.105119938
H	1.154340220	-1.129165857	0.762773895
N	2.496400792	-0.041626543	-0.387404539
H	2.636896814	0.101387619	-1.391774483
C	3.578572300	-0.220338656	0.407769631
O	3.513227527	-0.497502237	1.609615838
C	4.929583348	-0.071922914	-0.302004048
H	5.338283627	-1.092102027	-0.383530006
H	5.592385472	0.472828053	0.395373842
N	4.822730220	0.505955501	-1.644224488
H	4.848579485	1.526115229	-1.611661289
H	5.586595355	0.197975163	-2.245582672
C	0.662311467	0.971751648	0.955311284
H	1.531569216	1.290879562	1.549152900
H	0.383622594	1.795867840	0.281204988
C	-0.476209283	0.629716192	1.883451079
C	-1.773568787	1.120863499	1.667958577
H	-1.961408820	1.773205547	0.810799907
C	-2.822990086	0.762193515	2.520144877
H	-3.825319905	1.156744921	2.339103323
C	-2.589999111	-0.091821213	3.600252892
H	-3.408372975	-0.372411940	4.266637042
C	-1.299596609	-0.581421322	3.827600182
H	-1.107057178	-1.242792480	4.675382246
C	-0.252311462	-0.223598067	2.977788691
H	0.757741078	-0.601419934	3.159785288

## ——— 251\_GFA04: PBE+D3 ———

```

O 1.806459480 1.496439744 -2.150551025
C 2.403247309 0.450758960 -2.294920076
O 3.661306477 0.371261291 -2.802843678
H 3.937643666 1.292032443 -2.994834866
C 1.848656781 -0.950129563 -2.000169406
C 1.297972965 -1.568869232 -3.290214600
H 0.463965900 -0.965718521 -3.681926017
H 2.082921147 -1.621434124 -4.056795370
H 0.933703390 -2.586452916 -3.089919843
H 2.685276033 -1.553347957 -1.615815898
N 0.810783262 -0.898208619 -0.991486584
H -0.153733512 -0.818462091 -1.313571412
C 1.098614915 -0.459803696 0.268879406
O 2.252560494 -0.280666350 0.658244527
C -0.122365515 -0.199392157 1.159785827
H -0.771196580 -1.092420421 1.168402178
N 0.347676044 0.029400788 2.501801907
H 1.336615294 0.246523449 2.653145817
C -0.458777284 -0.139898668 3.576659957
O -1.650492769 -0.455616883 3.501564406
C 0.215423626 0.116655189 4.929165818
H -0.203866783 -0.628472281 5.630190483
H -0.146572226 1.100642723 5.269661461
N 1.677438930 0.153519844 4.849248268
H 2.075032909 -0.785586875 4.905021432
H 2.078794448 0.700779450 5.610486226
C -0.979687852 0.995301389 0.630139859
H -1.588658716 1.323315665 1.485534007
H -0.311671780 1.822279483 0.345199116
C -1.888493205 0.620946671 -0.513471426
C -1.661437559 1.089496613 -1.817411204
H -0.809588142 1.748456388 -2.006680254
C -2.495571220 0.700921626 -2.870660907
H -2.305845255 1.078267084 -3.878015294
C -3.569592296 -0.160074926 -2.635119111
H -4.222226844 -0.463446246 -3.456360494
C -3.808633351 -0.626950310 -1.338413192
H -4.651828621 -1.293583753 -1.143818310
C -2.976526470 -0.239802529 -0.287477290
H -3.167787093 -0.600190685 0.727305564

```

**11.2.13 GGF: PBE+D3**

———— 221\_GGF14: PBE+D3 ————

```

O -4.239749377 -0.675176831 -1.299108126
C -3.482640910 -0.186847877 -0.486341372
O -3.913652998 0.489603650 0.586769318
H -3.126610456 0.785585213 1.151994923
C -1.951883768 -0.384751519 -0.610756931
H -1.789851480 -0.690486685 -1.652497477
N -1.151347963 0.827507145 -0.427912119
H -0.516992056 1.108379108 -1.193239336
C -0.993386230 1.496616930 0.728855895
O -1.688735345 1.313499273 1.748473610
C 0.115198444 2.557466587 0.708531476
H 0.143110568 3.018937658 1.702284016
H -0.153884278 3.328871306 -0.033558029

```

N	1.429699734	2.030672529	0.388357838
H	2.135425749	1.864604694	1.111692325
C	1.817586886	1.692718681	-0.860385190
O	1.086354939	1.765161456	-1.860753194
C	3.262589286	1.204285716	-0.964488069
H	3.822688199	2.002637361	-1.477999078
H	3.247082932	0.337722888	-1.648620549
N	3.863354067	0.936251260	0.344326813
H	4.864911370	1.125799433	0.343153912
H	3.726450334	-0.043737607	0.602435085
C	-1.517290747	-1.541641159	0.325927399
H	-1.820046731	-1.312569977	1.357463289
H	-2.087258462	-2.431402173	0.010768304
C	-0.036172650	-1.828360316	0.290234045
C	0.591778046	-2.275984876	-0.882901655
H	0.002370124	-2.412407996	-1.793590205
C	1.955823659	-2.568586993	-0.898991812
H	2.422244241	-2.928577935	-1.818486259
C	2.718610732	-2.428126267	0.265730166
H	3.778726439	-2.691667750	0.261487597
C	2.107512014	-1.974830921	1.438255675
H	2.689692195	-1.871205151	2.357399673
C	0.744024072	-1.665720873	1.443151742
H	0.269489421	-1.308837983	2.360896298

## ——— 222\_GGF13: PBE+D3 ———

O	-4.249200955	-1.231908024	0.766523870
C	-3.493642567	-0.449400233	0.228632153
O	-3.927494207	0.579905827	-0.510588584
H	-3.142119043	1.126158984	-0.842902715
C	-1.963119093	-0.561064973	0.434814642
H	-1.799380560	-1.583223129	0.801053390
N	-1.159086979	-0.445207159	-0.783945751
H	-0.519166942	-1.221585825	-1.016203213
C	-1.007508845	0.669149886	-1.523163683
O	-1.709341653	1.693980083	-1.405269976
C	0.106217595	0.594385451	-2.576614723
H	0.122312946	1.555985300	-3.102943206
H	-0.148140332	-0.200892416	-3.298150503
N	1.422489639	0.325316227	-2.027217421
H	2.099052450	1.073847761	-1.853972135
C	1.815603209	-0.894402824	-1.601510324
O	1.099770844	-1.907972515	-1.636063157
C	3.226753502	-0.943505727	-1.020826415
H	3.715275087	-1.838602480	-1.442266395
H	3.091424986	-1.135820455	0.055419647
N	3.973881647	0.304842404	-1.209000296
H	4.623166365	0.239923789	-1.993385213
H	4.513067250	0.542079764	-0.377422967
C	-1.526959578	0.436695212	1.540983920
H	-1.795147936	1.458638638	1.237245257
H	-2.122277751	0.193439185	2.435926534
C	-0.052737813	0.367610900	1.851000951
C	0.811493143	1.391314903	1.438292956
H	0.402034218	2.246161394	0.893442870
C	2.176564336	1.341582118	1.732054703



H	2.828247541	2.158479823	1.413994358
C	2.701439946	0.256655495	2.438368188
H	3.764419538	0.222054770	2.688364331
C	1.852619916	-0.779456949	2.842197599
H	2.252823754	-1.629321666	3.399531229
C	0.488956210	-0.721727271	2.550695734
H	-0.168939864	-1.527896270	2.887104343

———— 223\_GGF07: PBE+D3 ————

O	4.127425271	1.447558312	0.558405855
C	3.453222239	0.449829288	0.397558319
O	3.910562987	-0.803180588	0.647750993
H	4.837617248	-0.687411643	0.946456424
C	2.014465159	0.475344616	-0.121480588
H	2.107706028	0.719329782	-1.195333730
N	1.333870034	-0.795251240	-0.064591245
H	0.943758395	-1.125223015	0.828634044
C	0.902777102	-1.428937037	-1.191793665
O	1.192484296	-1.088886887	-2.338510081
C	-0.034235528	-2.611664761	-0.889889119
H	0.442948015	-3.290753067	-0.164097829
H	-0.209994909	-3.148631267	-1.829185151
N	-1.306748705	-2.167516988	-0.345859115
H	-2.118885942	-2.004193800	-0.947134911
C	-1.476929928	-1.795794748	0.941894663
O	-0.584848164	-1.828098425	1.803338646
C	-2.894483061	-1.329673267	1.278722615
H	-2.781137151	-0.485316744	1.981725918
H	-3.369727940	-2.151103899	1.840057282
N	-3.686283536	-1.029318509	0.083538810
H	-3.550204948	-0.053495440	-0.195147717
H	-4.682223038	-1.167676482	0.253698650
C	1.230895384	1.584065714	0.611048890
H	1.218980212	1.357714901	1.690409888
H	1.802425753	2.520699534	0.501415692
C	-0.190961476	1.780316898	0.135363003
C	-1.184250669	2.126284192	1.064154120
H	-0.922184441	2.198510164	2.122936344
C	-2.495611767	2.385682717	0.658995584
H	-3.246965871	2.667097878	1.400338022
C	-2.842196123	2.288050670	-0.692266231
H	-3.862320907	2.503951297	-1.017732141
C	-1.867948983	1.918993788	-1.624452167
H	-2.128175276	1.827576164	-2.681247374
C	-0.555936636	1.669148725	-1.215433198
H	0.182026877	1.369053166	-1.962589500

———— 224\_GGF12: PBE+D3 ————

O	1.501248830	-3.111447058	-0.117603541
C	1.005605183	-1.900134915	0.250765300
O	1.709241561	-0.934092127	0.461613526
H	2.475590419	-3.009252710	-0.155386098
C	-0.527348618	-1.940894396	0.331396236
H	-0.788439707	-2.857446769	0.883408028
N	-1.030335178	-0.805062669	1.066485321
H	-1.222919045	0.059945224	0.554800482

```
C -0.780416433 -0.700396946 2.411270801
O -0.398200678 -1.642313459 3.100041915
C -0.958956454 0.721923547 2.968743758
H -0.818835890 0.679007501 4.055730389
H -1.963711557 1.107994840 2.737582628
N 0.016867612 1.617674406 2.371189211
H 1.004842162 1.551344131 2.634105986
C -0.195900652 2.188941815 1.158630114
O -1.295332710 2.200195582 0.588473126
C 1.050280731 2.801170834 0.518189026
H 1.018633184 3.888467649 0.701893907
H 0.927526285 2.653049250 -0.570997717
N 2.280839795 2.248905017 1.090403240
H 3.083651548 2.842818407 0.883951428
H 2.463340626 1.318894501 0.703137400
C -1.143961442 -2.025125375 -1.089505300
H -0.825937825 -2.980706041 -1.531799590
H -2.237185510 -2.062676760 -0.963612002
C -0.753780315 -0.877914770 -1.991529681
C 0.402710188 -0.955686784 -2.783804431
H 0.991063760 -1.877047573 -2.784288627
C 0.806785584 0.125188983 -3.568425801
H 1.708448873 0.045177932 -4.179494867
C 0.058791468 1.306665044 -3.572229165
H 0.375542036 2.154893797 -4.182767238
C -1.099734243 1.392580392 -2.798288603
H -1.688851434 2.311112279 -2.785471420
C -1.504572179 0.305481747 -2.021020629
H -2.414809971 0.386295472 -1.422007114
```

———— 225\_GGF10: PBE+D3 ————

```
O -1.237211215 4.249923940 0.144009140
C -0.169221299 3.452829160 0.437107954
O 0.784454386 3.829945389 1.080650940
H -1.046523256 5.118393772 0.556675666
C -0.374681668 2.048078614 -0.128682274
H -0.661170256 2.159737778 -1.186904733
N 0.852328772 1.294373731 -0.111556318
H 1.211324583 0.923203591 0.777249626
C 1.426768083 0.830952916 -1.256849853
O 1.052873491 1.119272723 -2.393471002
C 2.587049823 -0.143778219 -0.990398052
H 3.300790773 0.308269666 -0.282114310
H 3.091156281 -0.332425972 -1.945257751
N 2.117672972 -1.403672581 -0.438949202
H 1.916071862 -2.208250573 -1.038062124
C 1.781886075 -1.567039764 0.860055581
O 1.869566807 -0.680770315 1.722289998
C 1.285441117 -2.971835030 1.208166051
H 0.467748966 -2.837362130 1.938308020
H 2.110774416 -3.471995291 1.741188716
N 0.925131571 -3.753110898 0.021680647
H 1.034996490 -4.753159974 0.189493475
H -0.053568640 -3.585530352 -0.227512107
C -1.497660619 1.333767143 0.661185125
H -1.231983234 1.332129773 1.731456107
```

```

H -2.417321994  1.935434725  0.565845857
C -1.767839379 -0.088890522  0.221533581
C -2.075930995 -1.061527019  1.183872503
H -2.065745412 -0.788006103  2.242187520
C -2.398780433 -2.368647417  0.811871129
H -2.649459263 -3.104795036  1.579082765
C -2.403158575 -2.730387881 -0.538629870
H -2.670182003 -3.746781692 -0.836913703
C -2.070489511 -1.776601628 -1.505319108
H -2.057059412 -2.049949882 -2.562645457
C -1.757975106 -0.468588387 -1.129166245
H -1.485074196  0.254043745 -1.901068294

```

———— 226\_GGF15: PBE+D3 ————

```

O  3.866933431 -1.534051939 -0.945009691
C  3.367086424 -0.698397395 -0.223030867
O  4.083030832  0.280033850  0.352767654
H  3.474961822  0.860366458  0.910175294
C  1.858503666 -0.684985668  0.141622150
H  1.813229046 -0.760683410  1.244318395
N  1.217371784  0.579809330 -0.215110064
H  0.563505731  0.617886500 -1.008654357
C  1.336700723  1.688408536  0.542196996
O  2.167801693  1.795587543  1.464219138
C  0.371381247  2.824983084  0.194626193
H  0.637992876  3.217753404 -0.801309665
H  0.517710024  3.618038269  0.937847320
N -1.023268228  2.425048464  0.176414374
H -1.618683815  2.514548902  1.003503347
C -1.591442760  1.785653333 -0.873534942
O -0.974130622  1.472569501 -1.901284542
C -3.080701545  1.491074914 -0.697231609
H -3.289650851  0.578938504 -1.281532041
H -3.625848935  2.318439798 -1.181802866
N -3.461517710  1.424040881  0.715706885
H -4.455166581  1.618339861  0.839101032
H -3.286534369  0.481803460  1.077341510
C  1.110515804 -1.858717494 -0.492352231
H  1.189822022 -1.786833641 -1.588439220
H  1.650769805 -2.778080667 -0.215622893
C -0.341052391 -1.950244167 -0.077727905
C -0.708334660 -2.054873422  1.274031418
H  0.064372007 -2.069606187  2.047462145
C -2.048418781 -2.157958391  1.649348676
H -2.310167743 -2.248276956  2.705993504
C -3.052540027 -2.169018683  0.674686261
H -4.100152326 -2.275016948  0.965188947
C -2.701193731 -2.066529023 -0.673739820
H -3.474281070 -2.084506279 -1.445137435
C -1.357774035 -1.949451471 -1.041927228
H -1.092018757 -1.854212849 -2.097843862

```

———— 227\_GGF04: PBE+D3 ————

```

O -0.452557151  1.238956883  3.803591798
C  0.365374062  0.433610031  3.418391777
O  1.396729834 -0.013958178  4.191470218

```

```
H 1.309313339 0.447935896 5.051618511
C 0.423149363 -0.194749184 2.027224665
H 0.521594249 -1.283876612 2.161774659
N -0.806263086 0.021802534 1.309423371
H -1.040983942 0.962212921 0.966580915
C -1.567582587 -1.014544284 0.858783038
O -1.366914359 -2.199237932 1.126743926
C -2.704375967 -0.560623597 -0.074018452
H -3.290560632 0.237884074 0.409584147
H -3.350701232 -1.426418166 -0.259615243
N -2.195757728 -0.060381916 -1.340206712
H -2.086236304 -0.671349733 -2.153641555
C -1.679648643 1.179808268 -1.491069499
O -1.627138429 2.029146224 -0.589593109
C -1.162916541 1.478929824 -2.899974715
H -0.247220228 2.082635783 -2.770068712
H -1.911973741 2.134266114 -3.374928407
N -0.990220784 0.267947591 -3.706618146
H -0.053400819 -0.120933655 -3.566439651
H -1.096357999 0.467507886 -4.701043485
C 1.648390926 0.362951807 1.261049158
H 1.591320751 1.464367755 1.255229448
H 2.555030565 0.100002844 1.832686991
C 1.780988326 -0.128505644 -0.163443812
C 2.230143332 0.755522460 -1.155738115
H 2.426846651 1.797991557 -0.892431944
C 2.435193384 0.324518695 -2.468717656
H 2.798751937 1.028545999 -3.220702563
C 2.176233752 -1.005117490 -2.815992836
H 2.346223846 -1.351851126 -3.837814991
C 1.701807227 -1.888767624 -1.841902005
H 1.482430487 -2.925896285 -2.103842287
C 1.509432263 -1.456331382 -0.528160434
H 1.121375878 -2.161842334 0.209661706
```

———— 228\_GGF08: PBE+D3 ————

```
O -3.978402697 -0.758211028 -0.607939815
C -2.806104589 -0.960588678 0.056932552
O -2.348749285 -2.063081136 0.270430788
H -4.313844711 -1.650317723 -0.835716138
C -2.180947054 0.358955387 0.479316413
H -2.935883589 0.891691170 1.086230987
N -1.024106581 0.074073415 1.297603833
H -0.641994759 -0.881379889 1.304348964
C -0.393650961 1.050192080 2.000669151
O -0.788091306 2.217039689 2.059949188
C 0.878830086 0.575518364 2.727045384
H 0.615619083 -0.237786948 3.423763354
H 1.264054563 1.430210042 3.295755213
N 1.908152330 0.091246719 1.826136992
H 2.650530626 0.702239898 1.479712220
C 1.895821740 -1.157225452 1.303847686
O 1.029205900 -2.003642712 1.556202535
C 3.059881258 -1.465576126 0.360344097
H 2.632447143 -2.043885088 -0.477804969
H 3.730728971 -2.148452969 0.906983360
```

N 3.801508187 -0.265627801 -0.041166512  
H 3.382374044 0.140059609 -0.881218043  
H 4.774583795 -0.484405001 -0.253468457  
C -1.868895159 1.290025941 -0.732727272  
H -2.754105317 1.299245344 -1.387723060  
H -1.744663019 2.300690804 -0.322538126  
C -0.630429302 0.914897248 -1.507938129  
C 0.490936886 1.755603638 -1.477640108  
H 0.454122038 2.666981387 -0.875682376  
C 1.640036462 1.450243288 -2.211881078  
H 2.490148544 2.137511820 -2.196660588  
C 1.695956901 0.277461054 -2.970435881  
H 2.588462089 0.038109382 -3.553280964  
C 0.591437560 -0.579991341 -2.992982357  
H 0.623096603 -1.497594849 -3.584250976  
C -0.561937817 -0.257412291 -2.276715192  
H -1.423308664 -0.927987248 -2.325092677

———— 229\_GGF11: PBE+D3 ————

O -0.578071810 3.625050759 -0.928331614  
C 0.466653019 3.057781194 -0.314414280  
O 1.613350028 3.361698507 -0.574149364  
H -1.444600432 3.260102642 -0.552234627  
C 0.084110516 2.030927703 0.789374493  
H -0.496342994 2.610183034 1.532135266  
N -0.791499723 0.977456548 0.285350685  
H -0.396836175 0.041166111 0.194939897  
C -2.093016261 1.144926401 -0.010620614  
O -2.654379593 2.256905028 -0.005239227  
C -2.874416108 -0.123392609 -0.347308838  
H -3.556099371 0.121582600 -1.175006149  
H -3.485176284 -0.370929292 0.537887537  
N -2.065584151 -1.275833386 -0.661667062  
H -1.663857692 -1.424272550 -1.591426811  
C -1.862597194 -2.301359209 0.219696730  
O -2.288106356 -2.317503171 1.371933086  
C -1.057148520 -3.464640206 -0.370569776  
H -1.785478189 -4.267887407 -0.568236525  
H -0.396645441 -3.828697888 0.435820265  
N -0.372184325 -3.112891791 -1.618343032  
H 0.561514476 -2.740244463 -1.424563178  
H -0.256535830 -3.928338809 -2.219913262  
C 1.308514561 1.411133064 1.492798236  
H 2.069991427 2.201551631 1.564695030  
H 1.011637779 1.133143571 2.515365417  
C 1.886315915 0.192386903 0.806032279  
C 2.648747560 0.302857770 -0.369581215  
H 2.834350913 1.293640351 -0.788101505  
C 3.165345960 -0.834866834 -0.990385112  
H 3.759572943 -0.728993796 -1.900451077  
C 2.941751130 -2.103688230 -0.444228278  
H 3.369569928 -2.989673233 -0.918452312  
C 2.185585276 -2.226288429 0.724147730  
H 2.018698411 -3.208476506 1.171536003  
C 1.653985425 -1.086977455 1.336116083  
H 1.063541181 -1.191928552 2.250105124

## ———— 230\_GGF09: PBE+D3 ————

O -0.301793600 -2.067843786 -2.266702336  
C -0.206299986 -0.969830187 -2.771213738  
O 0.341340526 -0.761875743 -4.002043293  
H 0.604085802 -1.647407139 -4.329352758  
C -0.663186548 0.337666686 -2.145415470  
H -1.355966970 0.822044986 -2.856896075  
N -1.370667645 0.032809070 -0.922395843  
H -1.270540546 -0.905283454 -0.512827078  
C -2.100415030 0.973403841 -0.268304261  
O -2.281017594 2.117908505 -0.690238166  
C -2.689194918 0.491919523 1.070888701  
H -3.327962707 -0.388612373 0.890928374  
H -3.301160324 1.311198755 1.467780765  
N -1.679519212 0.122275696 2.046379878  
H -1.289428992 0.803835190 2.699559323  
C -1.068713995 -1.086995526 2.033518808  
O -1.339757480 -1.987448039 1.230291125  
C 0.034189894 -1.259179567 3.075857203  
H 0.977777668 -1.242451293 2.506854383  
H -0.070001353 -2.278814232 3.487251445  
N 0.062147561 -0.185013563 4.075910029  
H 1.010436777 -0.027577696 4.416446384  
H -0.515539452 -0.419617565 4.884628380  
C 0.521141335 1.334045710 -1.942403843  
H 1.056550753 1.417533541 -2.900002337  
H 0.066777676 2.309314149 -1.721551129  
C 1.460642869 0.943567780 -0.831371786  
C 2.459039295 -0.023576203 -1.022376031  
H 2.575864088 -0.489964013 -2.003773099  
C 3.311723048 -0.389290662 0.020614343  
H 4.083258768 -1.143560136 -0.148743059  
C 3.186092802 0.215600399 1.274633022  
H 3.864022305 -0.060031581 2.085764514  
C 2.198805137 1.183353139 1.477040758  
H 2.092669639 1.668076987 2.450042508  
C 1.340213563 1.536331613 0.433691675  
H 0.568386844 2.294007190 0.594058685

## ———— 231\_GGF01: PBE+D3 ————

O 2.080789061 -2.910517326 1.071639094  
C 1.079749842 -2.269677925 0.821185446  
O 0.238301860 -1.888985451 1.790503266  
H -0.520447313 -1.324597817 1.486322297  
C 0.770299571 -1.880549582 -0.650915508  
H 0.658437979 -2.842319452 -1.175455801  
N -0.448340364 -1.128107005 -0.834683691  
H -0.392691282 -0.116935979 -0.731556651  
C -1.686255749 -1.687347317 -0.947299083  
O -1.898075404 -2.885135719 -1.093487625  
C -2.853279138 -0.686215052 -0.860593291  
H -3.583918351 -1.148576981 -0.178276807  
H -3.320122479 -0.610360161 -1.852483673  
N -2.499333762 0.644236467 -0.402977522  
H -2.629557517 1.481693844 -0.977022667  
C -2.042963590 0.883490739 0.850401261

O -1.828199625 -0.005080859 1.685007610  
C -1.785295419 2.356660469 1.168650461  
H -0.838550294 2.390022456 1.736409948  
H -2.580921972 2.666121857 1.865866557  
N -1.807966323 3.207501901 -0.025566288  
H -0.862133092 3.314363926 -0.400262167  
H -2.162003687 4.139371173 0.188817141  
C 1.967865938 -1.103183367 -1.249668799  
H 2.881542749 -1.636221055 -0.948080538  
H 1.895197552 -1.141393521 -2.347172995  
C 2.004274669 0.337426689 -0.792410458  
C 2.393762769 0.675568726 0.515565761  
H 2.725423844 -0.109904560 1.198594244  
C 2.364265030 2.001871003 0.948756693  
H 2.672700966 2.243832085 1.967621876  
C 1.957741329 3.020485961 0.080234492  
H 1.955720006 4.059917990 0.416100119  
C 1.576909833 2.700774677 -1.225709563  
H 1.285171829 3.489624193 -1.923797181  
C 1.593429389 1.368521464 -1.651921169  
H 1.297951146 1.122833511 -2.675774788

———— 232\_GGF06: PBE+D3 ————

O -0.549991552 1.539286467 4.093483169  
C -0.396683382 0.513974962 3.470209084  
O -0.641905920 -0.700262300 4.013983445  
H -0.461961155 -1.361346249 3.304424860  
C 0.117931847 0.487806830 2.015792190  
H 1.199030770 0.697183708 2.093591887  
N 0.002433868 -0.829426555 1.402566003  
H -0.873566590 -1.060587059 0.901224401  
C 1.119519835 -1.498255224 0.946252094  
O 2.269299536 -1.210652001 1.257209922  
C 0.778941638 -2.650283856 -0.014565297  
H 0.016289493 -3.304585894 0.440578259  
H 1.695986885 -3.225980321 -0.185017341  
N 0.275142009 -2.161193162 -1.286415486  
H 0.884435101 -2.046052657 -2.101591132  
C -0.990216368 -1.724117468 -1.465823343  
O -1.849573826 -1.694661850 -0.570112003  
C -1.302337158 -1.266270722 -2.890177998  
H -1.947871523 -0.376005453 -2.792991151  
H -1.918608558 -2.059880749 -3.344460105  
N -0.092854206 -1.059503391 -3.689114702  
H 0.231044561 -0.092398214 -3.599627516  
H -0.263051949 -1.242152332 -4.677560389  
C -0.587480798 1.575161322 1.191726459  
H -1.669155560 1.360465690 1.167347738  
H -0.480512901 2.519471545 1.751576396  
C -0.087466423 1.749870115 -0.224855136  
C -0.991398760 2.139921043 -1.225482461  
H -2.047620487 2.260428778 -0.971199141  
C -0.564091174 2.384704039 -2.532315887  
H -1.285547101 2.702491767 -3.288467825  
C 0.784714995 2.228558878 -2.868414836  
H 1.128090933 2.434794527 -3.884635251

C 1.691441935 1.816956783 -1.887546238  
H 2.746046972 1.683491356 -2.138231072  
C 1.260149449 1.581239925 -0.579638878  
H 1.989955565 1.255847719 0.164907282

———— 233\_GGF03: PBE+D3 ————

O -1.476768660 -2.224313921 0.697262519  
C -2.090948028 -1.294039560 1.178710016  
O -3.426783208 -1.332094888 1.425424394  
H -3.732177827 -2.214475668 1.127094688  
C -1.495747088 0.054095813 1.551231528  
H -1.772037094 0.298941995 2.589646906  
N -0.059571457 -0.047438461 1.484405643  
H 0.340851404 -0.644083354 0.764301818  
C 0.762266203 0.691696203 2.274119395  
O 0.367044848 1.447334046 3.159840251  
C 2.264803678 0.530775827 1.990050981  
H 2.743112412 0.210813855 2.927859243  
H 2.644485246 1.534543551 1.744559820  
N 2.613844135 -0.362609615 0.910686462  
H 2.700284524 -1.374765453 1.036541440  
C 2.849775287 0.073696093 -0.359454958  
O 2.824824803 1.253575316 -0.707794688  
C 3.104986568 -1.055026836 -1.366220420  
H 3.923451172 -0.718222584 -2.025434768  
H 2.198664907 -1.096856351 -1.992955674  
N 3.326329911 -2.360806558 -0.734408181  
H 4.320527947 -2.572960931 -0.648563157  
H 2.892007337 -3.116198467 -1.262386974  
C -2.055042157 1.187377277 0.632889135  
H -3.143250511 1.245642967 0.783802876  
H -1.611610855 2.123908921 1.002943008  
C -1.725031881 0.972259046 -0.822121154  
C -0.481881550 1.366711295 -1.340109234  
H 0.239448085 1.884986938 -0.705042308  
C -0.143979210 1.099211027 -2.668996197  
H 0.833366509 1.412691964 -3.041045648  
C -1.050040711 0.441625413 -3.505166364  
H -0.790458585 0.238506775 -4.546303481  
C -2.297323473 0.057543154 -3.005402828  
H -3.017569854 -0.444515734 -3.655287012  
C -2.628764260 0.319267701 -1.674543036  
H -3.605938567 0.016883207 -1.288714040

———— 234\_GGF02: PBE+D3 ————

O 1.841533909 -2.757748624 0.821359669  
C 0.822689534 -2.941041499 -0.056867564  
O 0.912261029 -3.660504308 -1.031491970  
H 2.590819825 -3.290679712 0.481471918  
C -0.443127242 -2.191254049 0.346784668  
H -1.037698491 -2.925992371 0.925429048  
N -0.148380561 -1.075496133 1.223188338  
H 0.791850755 -0.657589992 1.241276582  
C -1.120818175 -0.475241823 1.956206403  
O -2.287201111 -0.868196512 2.012317104  
C -0.627365274 0.762514756 2.731984948



H	0.173431321	0.455125956	3.425775176
H	-1.477698601	1.143329430	3.309493451
N	-0.118994579	1.820131263	1.875536438
H	-0.695529640	2.625247543	1.621109843
C	1.108158764	1.796926262	1.311509534
O	1.925195150	0.875428495	1.459788466
C	1.442331988	3.018635242	0.455525718
H	1.950859001	2.633908435	-0.445738627
H	2.191401890	3.597244423	1.020388153
N	0.273600458	3.860147908	0.181045817
H	-0.180286743	3.556433091	-0.683428707
H	0.538158783	4.838105300	0.066278222
C	-1.303945738	-1.808699638	-0.884947311
H	-1.282097307	-2.666313400	-1.575282123
H	-2.334743862	-1.681533832	-0.528806173
C	-0.862021622	-0.547719663	-1.586513978
C	-1.649286649	0.609858438	-1.507127906
H	-2.575097291	0.583656500	-0.927011966
C	-1.277988933	1.780787264	-2.174110467
H	-1.930789775	2.657171250	-2.131898722
C	-0.089056488	1.822903096	-2.908087048
H	0.201159691	2.732657324	-3.438695255
C	0.714618628	0.680849609	-2.978661462
H	1.640619160	0.699688439	-3.557463355
C	0.325459418	-0.494826457	-2.334480254
H	0.943178780	-1.391002013	-2.428146607

———— 235\_GGF05: PBE+D3 ————

O	-1.872738683	0.479740220	1.820296671
C	-2.346515954	0.968295250	0.812660020
O	-3.680103159	1.121188304	0.617292132
H	-4.116388879	0.754009931	1.414742460
C	-1.545324467	1.446125384	-0.387548747
H	-1.859107954	2.468740925	-0.653251080
N	-0.155964593	1.475919453	-0.005490021
H	0.146376452	0.805376329	0.696853668
C	0.763230403	2.275743191	-0.605872344
O	0.492058099	3.102193490	-1.474761398
C	2.210393524	2.077797415	-0.122607880
H	2.577763695	3.053465391	0.228832152
H	2.801621489	1.794235897	-1.006966771
N	2.398338045	1.065141501	0.890334718
H	2.211040724	1.240253518	1.881082118
C	2.774179337	-0.213455396	0.595185781
O	3.065715811	-0.609650207	-0.531876501
C	2.805096656	-1.147334337	1.811211555
H	3.867127584	-1.313460146	2.052078917
H	2.404040917	-2.115555786	1.464183284
N	2.124785726	-0.584032653	2.983238850
H	1.130103612	-0.820079171	2.979756411
H	2.517914584	-0.946239296	3.851325350
C	-1.805820125	0.531603598	-1.628069722
H	-2.867001913	0.619642934	-1.903186812
H	-1.208160403	0.957406980	-2.448010399
C	-1.431927583	-0.906339109	-1.374560572
C	-0.096114978	-1.324527322	-1.474553978

H 0.674636568 -0.622158473 -1.796818445  
C 0.268603801 -2.635230122 -1.158660204  
H 1.317957851 -2.927142780 -1.235133306  
C -0.701798859 -3.554261792 -0.750635670  
H -0.419319145 -4.581416985 -0.510414820  
C -2.038343296 -3.155108423 -0.663289023  
H -2.805142223 -3.870043332 -0.356908907  
C -2.397410358 -1.840585919 -0.969243525  
H -3.444322305 -1.532588462 -0.896943962

**11.2.14 WGG: PBE+D3**

———— 206\_WGG06: PBE+D3 ————

O -1.693795275 -3.448295407 -0.039035166  
C -0.569528968 -3.203860778 0.365677676  
O 0.492866358 -3.225033792 -0.442379637  
H 1.309010760 -2.893745793 0.066021591  
C -0.280222647 -2.849073048 1.835273025  
H 0.409122613 -3.607164038 2.248365832  
H -1.226920244 -2.893192809 2.383553619  
N 0.295798913 -1.522392078 2.019671853  
H -0.249753109 -0.768933146 2.473097547  
C 1.543870982 -1.208812231 1.626693874  
O 2.290092479 -1.995248337 1.009621919  
C 2.023972649 0.192620973 2.026838915  
H 3.048421688 0.298183628 1.651956623  
H 2.038031303 0.250283408 3.129015293  
N 1.222377934 1.289858112 1.513313463  
H 1.550031531 1.854397888 0.725546411  
C 0.013313900 1.635233239 2.007677383  
O -0.578973514 0.994759151 2.892918242  
C -0.611557761 2.880305192 1.372944753  
H -1.109505626 3.411175510 2.206805839  
N 0.407935875 3.692991856 0.698569604  
H 0.944116834 4.238300544 1.377528837  
H -0.038827873 4.359740108 0.066052147  
C -1.726334686 2.442017371 0.379764532  
H -2.023462244 3.340847125 -0.192826555  
H -2.600484992 2.161629013 0.985741421  
C -1.402442640 1.297532839 -0.532290146  
C -1.978620752 0.044757529 -0.426342506  
H -2.720308557 -0.314094620 0.283576789  
N -1.490302028 -0.790016469 -1.404672406  
H -1.691196382 -1.787211876 -1.456721804  
C -0.560036221 -0.109505484 -2.158336958  
C 0.219859643 -0.549390238 -3.232721899  
H 0.157897812 -1.579730952 -3.587762409  
C 1.080292536 0.371047157 -3.822187999  
H 1.703125662 0.061639567 -4.663770968  
C 1.161330418 1.697743234 -3.349524892  
H 1.844034710 2.396483529 -3.837828023  
C 0.393482337 2.129146181 -2.272816343  
H 0.489803733 3.152301188 -1.908685171  
C -0.486167147 1.224706754 -1.646474305

———— 207\_WGG08: PBE+D3 ————

O 0.479519273 3.259040618 1.986179834

C	0.742381930	3.093861388	0.808105153
O	-0.150447398	3.342540321	-0.155888691
H	0.226951820	3.037827714	-1.050420541
C	2.112598918	2.583612930	0.325933501
H	2.752402564	2.454263777	1.205329352
H	2.560009830	3.350026396	-0.332344561
N	2.046318915	1.312091870	-0.385993789
H	2.456205153	0.460970384	0.026369366
C	1.483042550	1.184584759	-1.602223702
O	0.918451540	2.122211155	-2.200130791
C	1.590849343	-0.208678091	-2.231334698
H	2.655795876	-0.452227413	-2.377679703
H	1.097082229	-0.160190786	-3.208390935
N	0.985184099	-1.277595009	-1.451050771
H	0.017570189	-1.529786562	-1.643576849
C	1.590154302	-1.830980570	-0.371002776
O	2.681582801	-1.424730171	0.061607141
C	0.851206860	-2.988568023	0.299736989
H	0.070761680	-3.351338058	-0.389756934
N	1.820627106	-4.064177155	0.497740947
H	2.655714377	-3.667344203	0.939213856
H	1.438045044	-4.765431927	1.136692882
C	0.161842031	-2.478289324	1.600272190
H	0.954798333	-2.269402774	2.336634177
H	-0.437565130	-3.318165528	1.997941568
C	-0.673227045	-1.252122125	1.404206068
C	-0.472529040	-0.030846874	2.017776851
H	0.258436944	0.253918555	2.770543313
N	-1.372004015	0.896733857	1.538685955
H	-1.340160366	1.887221728	1.768867689
C	-2.154949157	0.311189773	0.569379147
C	-3.155346293	0.858128968	-0.240121124
H	-3.430067349	1.911636534	-0.161535121
C	-3.776367323	0.015067321	-1.157796279
H	-4.558811634	0.413190513	-1.806566780
C	-3.417562787	-1.345267126	-1.260116690
H	-3.938985325	-1.982218445	-1.977568843
C	-2.419643142	-1.889113874	-0.454675734
H	-2.178092396	-2.952915948	-0.528466181
C	-1.756505305	-1.060098578	0.472655512

———— 208\_WGG04: PBE+D3 ————

O	-1.552316112	2.325037665	-1.903684547
C	-0.916454900	2.611407763	-0.907234214
O	-1.477099553	3.249386886	0.130277461
H	-0.775068636	3.404610387	0.840641778
C	0.586704714	2.300731246	-0.754673707
H	1.126951612	3.261882123	-0.702489860
H	0.914411942	1.750403270	-1.642260876
N	0.921237411	1.504778069	0.423518418
H	1.197843642	0.531395148	0.283565632
C	0.858739689	2.002181631	1.677182306
O	0.471566544	3.162503117	1.917950270
C	1.232521348	1.036990849	2.806691651
H	1.198073530	1.603756601	3.745838033
H	2.244781619	0.631859515	2.651204731

N 0.315423522 -0.082660814 2.851954447  
H -0.647872015 0.025080735 3.179203602  
C 0.581187696 -1.254564196 2.216922302  
O 1.672304631 -1.515380465 1.702483036  
C -0.601848990 -2.240254273 2.186392525  
H -0.389689232 -2.991942438 2.967125101  
N -1.845908726 -1.555105917 2.560318901  
H -2.235643625 -1.087603150 1.734797999  
H -2.542672470 -2.224213234 2.889906943  
C -0.641694393 -2.971219417 0.818124749  
H -1.455700131 -3.714440223 0.866871218  
H 0.297749523 -3.529875569 0.696665071  
C -0.829718415 -2.054438164 -0.354978576  
C -2.008240777 -1.468555234 -0.786606136  
H -3.021642713 -1.579930286 -0.407446464  
N -1.777162593 -0.712456412 -1.920197183  
H -2.407866406 -0.006071314 -2.285847092  
C -0.437312695 -0.768047199 -2.235967111  
C 0.267262453 -0.166600342 -3.285847863  
H -0.236837181 0.487674501 -3.998835166  
C 1.633592925 -0.419125372 -3.366737484  
H 2.215067192 0.033690463 -4.172287535  
C 2.280707217 -1.251020504 -2.425880385  
H 3.354022536 -1.427933869 -2.520350691  
C 1.577621150 -1.849480129 -1.385746074  
H 2.089957804 -2.470202667 -0.649526340  
C 0.193650862 -1.611258783 -1.273658870

———— 209\_WGG03: PBE+D3 ————

O -1.980554489 3.262767933 0.485877214  
C -0.799601003 3.094047884 0.733583063  
O 0.153705711 3.337825744 -0.171642235  
H 1.052503154 3.034733900 0.196549735  
C -0.302365663 2.584785256 2.098772520  
H -1.175178265 2.454884448 2.747433561  
H 0.359613308 3.352235301 2.538965532  
N 0.410351950 1.314028317 2.026570740  
H 0.002293723 0.461742467 2.439374511  
C 1.621663455 1.187717676 1.452807936  
O 2.212920224 2.125051997 0.880472205  
C 2.255352226 -0.203821189 1.559232295  
H 2.409495282 -0.443005327 2.624014977  
H 3.228947590 -0.153302359 1.058482643  
N 1.472881298 -1.278049557 0.963697617  
H 1.638827773 -1.507224289 -0.015430914  
C 0.387717549 -1.824638338 1.571887697  
O -0.031648641 -1.418211119 2.669508533  
C -0.282982669 -2.999634653 0.843724991  
H 0.404020586 -3.370666903 0.066159405  
N -0.585655896 -4.111816516 1.741983914  
H 0.281204308 -4.522976056 2.098302121  
H -1.079245054 -3.737821733 2.559385499  
C -1.586127353 -2.515204239 0.164688072  
H -2.328106502 -2.326252796 0.957809669  
H -1.965721918 -3.359498710 -0.434995237  
C -1.407626889 -1.273503841 -0.651435271

C -2.039547149 -0.064055923 -0.438699930  
H -2.793099990 0.202346252 0.298457257  
N -1.580372770 0.878201085 -1.333497435  
H -1.824309914 1.865168168 -1.292031333  
C -0.604742548 0.314458015 -2.124521913  
C 0.192676178 0.882519179 -3.122643387  
H 0.096857075 1.937084825 -3.387737898  
C 1.121875441 0.059355207 -3.753490847  
H 1.761683166 0.474325662 -4.534531595  
C 1.246096515 -1.302348382 -3.407177546  
H 1.970314250 -1.924013806 -3.937710265  
C 0.452185297 -1.867581861 -2.411606736  
H 0.538741910 -2.933402876 -2.183656972  
C -0.485241255 -1.058298843 -1.737882192

———— 210\_WGG05: PBE+D3 ————

O -0.923438115 -1.854001721 0.233556850  
C -1.871089127 -1.319360697 -0.304098333  
O -2.655974670 -1.951396229 -1.220148805  
H -2.296401316 -2.859331731 -1.299347254  
C -2.357269634 0.108888889 -0.078345016  
H -3.435125575 0.067180309 0.139483382  
H -2.220438800 0.669363943 -1.016200623  
N -1.657561719 0.767510904 0.991639672  
H -0.788681052 1.254612085 0.769888540  
C -1.886411438 0.394001949 2.288700037  
O -2.854428146 -0.278154394 2.634900886  
C -0.788171374 0.834718273 3.270534966  
H -1.108813218 0.553093585 4.280774992  
H -0.628170232 1.922801361 3.219453273  
N 0.467019426 0.183105144 2.940676655  
H 0.576742310 -0.824312991 3.082957397  
C 1.334109372 0.720548998 2.046578601  
O 1.244504292 1.881122789 1.625878202  
C 2.465705108 -0.231185046 1.610582736  
H 3.299039225 -0.029332253 2.308944057  
N 2.051277712 -1.619351033 1.817754140  
H 2.852090609 -2.251129754 1.779916422  
H 1.387918580 -1.898792074 1.085375379  
C 2.976530074 0.127281376 0.186395556  
H 3.942750733 -0.385841564 0.050302053  
H 3.178187453 1.208645616 0.163011722  
C 2.053472103 -0.247280497 -0.933438126  
C 1.999074359 -1.478732429 -1.557386367  
H 2.602544384 -2.367348195 -1.388012714  
N 1.028377194 -1.472296440 -2.541372709  
H 0.815599580 -2.247693093 -3.155890242  
C 0.431902668 -0.230500244 -2.586254593  
C -0.582021573 0.257190146 -3.417884053  
H -1.051224908 -0.374871810 -4.175102378  
C -0.976427277 1.580938974 -3.240699451  
H -1.766458168 1.994096934 -3.870924533  
C -0.369661056 2.396862346 -2.260983124  
H -0.700460539 3.431527489 -2.151336156  
C 0.639533443 1.909773461 -1.435018558  
H 1.092312819 2.540398625 -0.668765643

C 1.055286497 0.571828998 -1.580636841

———— 211\_WGG02: PBE+D3 ————

O 2.035266767 -1.112227551 -2.850538417  
C 2.569112232 -0.346167003 -2.065000312  
O 3.807857321 -0.544419829 -1.609647007  
H 4.009508718 0.142631721 -0.894788230  
C 1.870072211 0.914294208 -1.520368429  
H 0.912900742 1.044499692 -2.036314232  
H 2.510630693 1.789490092 -1.721048784  
N 1.619784839 0.836860599 -0.087667537  
H 0.692404787 0.561437591 0.235283885  
C 2.612749623 0.938172343 0.820380340  
O 3.805973491 1.088949643 0.497858137  
C 2.209550262 0.842968351 2.290344716  
H 2.685185111 1.684399055 2.817156335  
H 2.648376068 -0.089271776 2.682938276  
N 0.789637592 0.803879755 2.526758962  
H 0.201502453 1.642237304 2.524314160  
C 0.113242140 -0.362815565 2.746458005  
O 0.656332702 -1.461833783 2.842895864  
C -1.418480480 -0.189042893 2.825360199  
H -1.691382843 -0.405967944 3.871933185  
N -1.808091476 1.198384564 2.529357092  
H -2.648972264 1.461106009 3.043281340  
H -2.019648122 1.299146587 1.531624400  
C -2.076133087 -1.258796079 1.914622492  
H -3.169648076 -1.194919060 2.041955828  
H -1.759551191 -2.247944698 2.274977026  
C -1.706366278 -1.097678651 0.469230604  
C -0.640820574 -1.706785454 -0.173372205  
H 0.092355466 -2.401440925 0.229017800  
N -0.594131674 -1.312684613 -1.495354053  
H 0.174258822 -1.511186407 -2.141929632  
C -1.611325191 -0.415678290 -1.737621073  
C -1.948777329 0.273331723 -2.908569113  
H -1.369419897 0.143969684 -3.825342230  
C -3.057970491 1.113680346 -2.864359003  
H -3.350776609 1.662558876 -3.761064762  
C -3.820419882 1.254861689 -1.685533016  
H -4.698146960 1.904101324 -1.693596673  
C -3.481270211 0.573224685 -0.520739822  
H -4.098687777 0.679842742 0.375021034  
C -2.349651626 -0.266998061 -0.520695149

———— 212\_WGG14: PBE+D3 ————

O -1.324270849 -3.574629658 -0.187640527  
C -0.719712228 -2.920418987 -1.017295625  
O -1.349337348 -2.247495577 -1.986737994  
H -0.660357445 -1.763538878 -2.553278239  
C 0.819781231 -2.815147135 -1.038051743  
H 1.185186542 -3.254748304 -1.982012768  
H 1.213939027 -3.394206503 -0.197245241  
N 1.325916355 -1.449160241 -0.934516507  
H 1.647786460 -1.131128711 -0.017936413  
C 1.201633578 -0.564556143 -1.943663963

O 0.622336008 -0.852078868 -3.013189022  
C 1.731920956 0.842390388 -1.720082137  
H 2.291776307 1.134576253 -2.625860965  
H 2.405862332 0.923121414 -0.853732594  
N 0.589813421 1.704639355 -1.487594207  
H -0.329220389 1.465722306 -1.869493998  
C 0.603796492 2.723354287 -0.591552882  
O 1.612102194 3.136479488 -0.016925523  
C -0.793084107 3.288390453 -0.282602607  
H -0.661844841 4.381432901 -0.177596830  
N -1.763693174 2.913816970 -1.319981661  
H -2.719480383 2.998178812 -0.968534479  
H -1.684100764 3.529861164 -2.131937181  
C -1.240265670 2.748908401 1.102925735  
H -2.248540184 3.151729942 1.304270829  
H -0.571055514 3.197967872 1.852731520  
C -1.232923315 1.257369926 1.259839309  
C -2.260855868 0.372693749 0.997868310  
H -3.260247579 0.563991478 0.615610254  
N -1.870727043 -0.916435856 1.304631211  
H -2.376306386 -1.762405436 1.057396212  
C -0.567167920 -0.901748668 1.749691926  
C 0.263031653 -1.952308592 2.157646637  
H -0.099592586 -2.981139815 2.168285477  
C 1.571403422 -1.633304215 2.518092305  
H 2.248322042 -2.428374140 2.837412563  
C 2.032871644 -0.296885648 2.490110081  
H 3.063004225 -0.081739368 2.780265311  
C 1.193755453 0.749605013 2.114348461  
H 1.564923796 1.775216039 2.080159772  
C -0.128909545 0.457664531 1.731227195

———— 213\_WGG15: PBE+D3 ————

O -1.522871582 -3.325979463 0.695107661  
C -2.266530451 -2.430359729 0.332066719  
O -3.246184971 -1.966010743 1.109306690  
H -3.731356264 -1.213042044 0.626442744  
C -2.159847358 -1.789718866 -1.065229749  
H -3.069031211 -2.068363770 -1.629089842  
H -1.290374995 -2.227228781 -1.567972880  
N -2.007184918 -0.340134087 -1.076978387  
H -1.121296694 0.084021065 -1.402084148  
C -2.973318338 0.510500492 -0.689005823  
O -4.066532019 0.142374888 -0.210528243  
C -2.656052958 1.999529477 -0.886646519  
H -3.535303484 2.561653490 -0.552342561  
H -2.495836988 2.185123901 -1.963044749  
N -1.490660591 2.457699614 -0.147469097  
H -1.584508829 3.117693243 0.626209475  
C -0.220916503 2.202455527 -0.547990325  
O 0.050611695 1.490606587 -1.525676512  
C 0.865543288 2.806964721 0.343270901  
H 1.756954598 2.895949301 -0.303510856  
N 0.407420921 4.076759162 0.924880518  
H 0.494624636 4.842586860 0.253038230  
H 0.977802773 4.321136759 1.737611740

C 1.191111405 1.833424124 1.510958873  
H 0.361136445 1.903827836 2.235295868  
H 2.091512293 2.232124907 2.014716859  
C 1.388560823 0.406171390 1.121998130  
C 0.511436980 -0.626567840 1.389361761  
H -0.425230265 -0.613889442 1.941790983  
N 0.985576218 -1.802396701 0.848243136  
H 0.446608582 -2.667937129 0.831721167  
C 2.178242177 -1.555069478 0.202183532  
C 3.023721545 -2.418325747 -0.502967723  
H 2.784331467 -3.477995793 -0.616808494  
C 4.183660882 -1.877504237 -1.050921291  
H 4.865962472 -2.524251205 -1.606142715  
C 4.496076395 -0.510038799 -0.898713804  
H 5.416299262 -0.121920354 -1.339409694  
C 3.652051631 0.347395040 -0.200774980  
H 3.907143237 1.404926621 -0.095794449  
C 2.470798695 -0.165570794 0.364037852

———— 214\_WGG01: PBE+D3 ————

O -3.076140621 -1.150150005 -1.371119228  
C -2.452688181 -0.336444687 -2.031743085  
O -2.550025745 0.977391046 -1.814825111  
H -1.911494385 1.466361124 -2.431988736  
C -1.502119907 -0.752233368 -3.169572345  
H -1.874808722 -0.318313834 -4.113331226  
H -1.525744438 -1.844931610 -3.248376147  
N -0.121433284 -0.331153298 -2.962528402  
H 0.591875651 -1.002948985 -2.632853407  
C 0.261156626 0.959657193 -3.027243547  
O -0.528601837 1.900084819 -3.243493682  
C 1.758887303 1.197859675 -2.794636667  
H 1.962579954 2.250311789 -3.021886443  
H 2.343737598 0.557849837 -3.476063431  
N 2.154198040 0.920971537 -1.425550955  
H 2.352013201 1.664262112 -0.747230820  
C 2.328906206 -0.328085678 -0.943261382  
O 2.121638668 -1.356464109 -1.610786727  
C 2.832183946 -0.379657638 0.512612512  
H 3.891122478 -0.684904353 0.434712776  
N 2.787836612 0.960402502 1.113847540  
H 3.521373982 1.071117310 1.814141995  
H 1.890221077 1.094619365 1.591799745  
C 2.065717901 -1.476852925 1.295824042  
H 2.577084785 -1.628801639 2.260584708  
H 2.148062403 -2.416706347 0.729989592  
C 0.626571125 -1.123379608 1.513702153  
C -0.426922209 -1.432150982 0.672366856  
H -0.430169611 -2.026795811 -0.236440047  
N -1.595838139 -0.884467174 1.150818368  
H -2.475807544 -0.909663066 0.635514561  
C -1.332882578 -0.189650878 2.309096858  
C -2.185280652 0.539086469 3.145358029  
H -3.248320098 0.642118583 2.917002874  
C -1.630494520 1.126802272 4.278663490  
H -2.269708245 1.701183583 4.951969563



C	-0.258598380	0.986511238	4.578377486
H	0.138686158	1.447075947	5.484910427
C	0.590388001	0.266044494	3.744418961
H	1.648451448	0.157942728	3.998085189
C	0.065755931	-0.330007629	2.579993665

———— 215\_WGG07: PBE+D3 ————

O	1.321026313	0.187744654	3.575009672
C	0.715406164	1.014173029	2.917638954
O	1.344300507	1.980888596	2.240207704
H	0.654826668	2.547614234	1.757204727
C	-0.824073654	1.033289799	2.812643076
H	-1.189517765	1.976731549	3.253304971
H	-1.216935006	0.192110121	3.391948574
N	-1.330806921	0.929534530	1.447096326
H	-1.653740928	0.013023751	1.129921982
C	-1.207816424	1.938233324	0.562191360
O	-0.628523290	3.008119027	0.848751806
C	-1.739624933	1.714884863	-0.844292797
H	-2.303560770	2.618789460	-1.134221313
H	-2.410287536	0.846123265	-0.925684118
N	-0.597254899	1.487944584	-1.707655919
H	0.319755451	1.874886446	-1.469010783
C	-0.605789385	0.589669607	-2.724334820
O	-1.610675676	0.009234955	-3.137748281
C	0.793356343	0.286544692	-3.287251885
H	0.664594830	0.181504910	-4.380476410
N	1.759097199	1.327841888	-2.910899875
H	1.682106880	2.136846212	-3.530994540
H	2.716272495	0.978283691	-2.986003148
C	1.244920456	-1.097516218	-2.747643948
H	2.254187319	-1.295103836	-3.149726449
H	0.578597089	-1.849444949	-3.197305230
C	1.237571569	-1.255312894	-1.256189457
C	2.265813295	-0.994439453	-0.371592055
H	3.265195514	-0.612227580	-0.563000400
N	1.876844670	-1.303520709	0.917227761
H	2.381481401	-1.054088574	1.763150792
C	0.573147504	-1.748246061	0.902570531
C	-0.256051492	-2.158280141	1.953086333
H	0.107265232	-2.170276443	2.981594790
C	-1.564490941	-2.518848805	1.634394816
H	-2.240824718	-2.839747526	2.429260989
C	-2.026764192	-2.489237477	0.298296062
H	-3.056764898	-2.779909059	0.083421840
C	-1.188437496	-2.111710350	-0.748292955
H	-1.560301258	-2.076242854	-1.773572428
C	0.134075286	-1.728064260	-0.456526255

———— 216\_WGG11: PBE+D3 ————

O	-4.652441475	0.014260391	0.070813297
C	-3.351850567	0.343843121	0.247600825
O	-2.956503351	1.495239979	0.230578043
H	-5.137606002	0.856163680	-0.063010664
C	-2.497727867	-0.910966094	0.400968580
H	-2.300109806	-1.289672536	-0.615616082

H -3.093460006 -1.662992798 0.938758314  
N -1.250948283 -0.711190706 1.089765859  
H -0.405810834 -0.484821457 0.570902295  
C -1.201330418 -0.750261581 2.456544769  
O -2.198397242 -0.916340973 3.153601850  
C 0.189410241 -0.588089108 3.081360979  
H 0.219058557 -1.259173871 3.954289020  
H 0.285660864 0.444604868 3.455279130  
N 1.289561238 -0.818248995 2.177469164  
H 1.459295735 -1.731328082 1.747261175  
C 2.232416579 0.121091054 1.886815122  
O 2.284125824 1.237515120 2.402789242  
C 3.215970968 -0.307844293 0.776606019  
H 4.216015267 -0.326130651 1.240947895  
N 2.910423679 -1.660790750 0.284563434  
H 2.287351512 -1.609982631 -0.527386980  
H 3.758640187 -2.143298352 -0.011734670  
C 3.195302476 0.796633662 -0.318035506  
H 3.916779088 0.521650698 -1.104542664  
H 3.542714337 1.733610730 0.140156401  
C 1.820120449 0.985509245 -0.886126041  
C 0.849872200 1.827848286 -0.374060015  
H 0.916683835 2.509496466 0.469315274  
N -0.328306971 1.684689553 -1.078248193  
H -1.234415579 2.000131124 -0.730053360  
C -0.164702718 0.709755134 -2.038496582  
C -1.077771374 0.181453338 -2.958005070  
H -2.106943194 0.545051524 -3.005133949  
C -0.623060675 -0.810252144 -3.824254143  
H -1.310494316 -1.243072341 -4.553441267  
C 0.716797351 -1.251301237 -3.788154300  
H 1.044595928 -2.015545070 -4.495928816  
C 1.625758045 -0.723080656 -2.876264895  
H 2.664184258 -1.063721021 -2.875212311  
C 1.192322059 0.259077374 -1.963341177

———— 217\_WGG09: PBE+D3 ————

O -1.402832432 -0.704924581 -3.814524758  
C -0.166826392 -0.587095527 -3.319128738  
O 0.671578408 -1.462585966 -3.449973570  
H -1.952391153 0.086755528 -3.514776718  
C 0.109258139 0.730556153 -2.572699843  
H -0.131203400 1.574451299 -3.240625060  
H 1.169178136 0.776757370 -2.302232397  
N -0.683619310 0.859302578 -1.358046727  
H -0.257782645 0.616518624 -0.463112607  
C -2.003081482 1.136787067 -1.400788502  
O -2.627229032 1.269093649 -2.469425207  
C -2.722745520 1.292880048 -0.064731232  
H -3.501591751 0.514768640 -0.019867668  
H -3.227812970 2.271713219 -0.076462967  
N -1.894616327 1.131594164 1.109630345  
H -1.261937608 1.876552577 1.385203223  
C -1.937424798 -0.011396092 1.876061848  
O -2.714621361 -0.933514873 1.640541140  
C -0.946568068 -0.067740787 3.047033380

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H -0.381642361  0.879574390  3.106761555
N -1.610047069 -0.279563000  4.334506288
H -2.227914020  0.507335669  4.550437853
H -2.214070795 -1.104551662  4.253962422
C  0.042527783 -1.225212804  2.789584588
H -0.539670437 -2.160973840  2.792489364
H  0.727396248 -1.261506573  3.652772118
C  0.801153041 -1.112457191  1.503915406
C  0.651745336 -1.907058035  0.382484674
H -0.042051022 -2.725806843  0.208935517
N  1.555779834 -1.532641905 -0.593474142
H  1.519417140 -1.833543381 -1.569623772
C  2.288650387 -0.456631000 -0.138215693
C  3.297789719  0.284158017 -0.766064001
H  3.635399882  0.039078828 -1.775367714
C  3.866524792  1.334042413 -0.048715998
H  4.657311954  1.929563633 -0.508522805
C  3.451476808  1.631670167  1.266826545
H  3.931727576  2.452227681  1.803226511
C  2.453062448  0.891582453  1.892566418
H  2.157062983  1.120068515  2.919047589
C  1.843129339 -0.165678622  1.189323337

```

———— 218\_WGG13: PBE+D3 ————

```

O -1.641000071  2.423489550  1.672752441
C -0.787642037  3.065732604  0.866221870
O  0.154030829  3.703141433  1.298551534
H -2.339982694  1.956547788  1.106102654
C -1.096175123  2.949942970 -0.642680812
H -0.325519889  3.500135993 -1.191157185
H -2.078071309  3.416331593 -0.832318517
N -1.124934446  1.577954791 -1.144909407
H -0.290263139  1.235054907 -1.626844402
C -2.108253724  0.718676034 -0.818713231
O -3.044991805  1.032928537 -0.052031177
C -2.015236365 -0.702855357 -1.348003996
H -1.247140617 -0.834600362 -2.124001902
H -2.996611768 -0.974263087 -1.773666904
N -1.660338921 -1.545715470 -0.217682605
H -1.957578039 -1.243071193  0.705477349
C -0.840521574 -2.625099085 -0.329934577
O -0.488693970 -3.095967613 -1.412662736
C -0.306659068 -3.173221336  0.994260471
H -0.890711736 -2.752553511  1.833326044
N -0.473865198 -4.621196472  0.978926814
H  0.111854999 -5.059201811  1.693628482
H -0.165009532 -4.970592896  0.066036062
C  1.172684745 -2.692684083  1.151349069
H  1.755633536 -3.192319364  0.360193870
H  1.538467451 -3.084076953  2.115615328
C  1.388370009 -1.211536778  1.078096157
C  1.361881556 -0.304859917  2.121040908
H  1.185562795 -0.474434666  3.180840228
N  1.630818679  0.968369131  1.654568926
H  1.521971848  1.828480090  2.184452491
C  1.814453594  0.921404236  0.290558902

```

C 2.098110626 1.945495767 -0.620755061  
H 2.217925304 2.976512901 -0.285569250  
C 2.188946533 1.599002439 -1.968458764  
H 2.404997524 2.373172809 -2.707749977  
C 2.018765529 0.260513806 -2.392132339  
H 2.099823737 0.023052622 -3.454838441  
C 1.771585650 -0.761215253 -1.477899297  
H 1.635748380 -1.788382520 -1.819980297  
C 1.661347699 -0.441402275 -0.111308721

———— 219\_WGG10: PBE+D3 ————

O 1.504587467 -0.694606224 3.335366620  
C 2.252394526 -0.332109883 2.442961920  
O 3.233494257 -1.110294357 1.983135528  
H 3.723239052 -0.627467612 1.233304761  
C 2.149813428 1.065049278 1.801774987  
H 3.058116897 1.627908121 2.085324914  
H 1.278565363 1.568540906 2.234844741  
N 2.004871466 1.077563185 0.351426329  
H 1.120923559 1.401894994 -0.077198890  
C 2.975605850 0.689289838 -0.493941305  
O 4.066630835 0.210754418 -0.119634023  
C 2.666393163 0.887024608 -1.984631031  
H 3.548885855 0.553892449 -2.542304346  
H 2.505621747 1.963277657 -2.170475920  
N 1.504224013 0.146894683 -2.449396592  
H 1.602453739 -0.627959739 -3.107316332  
C 0.232878070 0.547017011 -2.201675571  
O -0.042967415 1.525542527 -1.492642598  
C -0.849809670 -0.345344603 -2.811309206  
H -1.741163480 0.300843299 -2.905007933  
N -0.384579409 -0.927415123 -4.078270766  
H -0.953880032 -1.739994456 -4.325728356  
H -0.467348923 -0.255690592 -4.844702388  
C -1.179558281 -1.512637433 -1.838779022  
H -0.348402789 -2.236100925 -1.903892196  
H -2.077069096 -2.017773014 -2.242212457  
C -1.385330124 -1.122830210 -0.412914793  
C -0.513867543 -1.389530184 0.624841567  
H 0.422752243 -1.942082083 0.617530111  
N -0.994651869 -0.847923675 1.797671103  
H -0.460840886 -0.830447767 2.666361357  
C -2.185860537 -0.201903419 1.543334274  
C -3.036022505 0.503683333 2.401597256  
H -2.802579406 0.618006114 3.462541297  
C -4.192914040 1.051454777 1.854100477  
H -4.878759126 1.607020865 2.496778991  
C -4.497721163 0.898595001 0.484998153  
H -5.415759475 1.339162447 0.091590854  
C -3.649028213 0.200249802 -0.367444770  
H -3.898394542 0.094808067 -1.426287978  
C -2.470603004 -0.364352082 0.152281232

———— 220\_WGG12: PBE+D3 ————

O -1.400611134 -3.483908624 -0.111497482  
C -0.826878324 -2.846360588 -0.973641702

```

O -1.492743177 -2.145610185 -1.901151560
H -0.823667763 -1.705924875 -2.522558760
C 0.711161528 -2.794298326 -1.092395685
H 1.000626374 -3.256211754 -2.051902549
H 1.136844579 -3.377971456 -0.270624782
N 1.268978867 -1.445321920 -1.035773714
H 1.659068674 -1.130548086 -0.143810719
C 1.113358384 -0.567462344 -2.044678906
O 0.462195075 -0.844759285 -3.076240006
C 1.672452005 0.834982312 -1.863606766
H 2.198929962 1.114823004 -2.792184861
H 2.372095025 0.927776231 -1.019703392
N 0.534307165 1.697024992 -1.598086197
H -0.363008980 1.432696050 -1.996177328
C 0.551602600 2.691041933 -0.667262397
O 1.584598444 3.105253360 -0.140597072
C -0.837624491 3.222675954 -0.252515851
H -0.748264353 4.321676321 -0.251304887
N -1.991193801 2.859161764 -1.065754448
H -1.897740308 3.125961223 -2.045690753
H -2.216465381 1.864379033 -0.994062997
C -1.085635304 2.778085959 1.216031095
H -2.045347872 3.219564207 1.525423229
H -0.295418330 3.220564132 1.839824719
C -1.104331428 1.289584857 1.406415513
C -2.191540753 0.441295907 1.297248408
H -3.231426397 0.675473870 1.080646849
N -1.808867604 -0.861060965 1.561372945
H -2.371514102 -1.688453257 1.386887964
C -0.458158237 -0.891499164 1.826282771
C 0.378346186 -1.969317101 2.139527618
H -0.016268461 -2.983988915 2.206583904
C 1.731214975 -1.697040402 2.333138080
H 2.412926821 -2.514522665 2.576859048
C 2.234192228 -0.378940593 2.231379392
H 3.298954399 -0.199983088 2.394213682
C 1.393512843 0.695520276 1.948484830
H 1.793218886 1.706846752 1.860990846
C 0.023401180 0.450315456 1.734541922

```

**11.2.15 WG: PBE+D3**

———— 191\_WG03: PBE+D3 ————

```

O 2.727205063 -3.259697377 -1.111816088
C 2.915288019 -2.153880524 -0.652948774
O 2.925294156 -1.910426983 0.669313838
H 3.078429293 -0.918927926 0.823469524
C 3.195461245 -0.922406373 -1.541626283
H 3.148539868 -1.246955355 -2.586861274
H 4.219127627 -0.567111401 -1.324451807
N 2.254318479 0.171262660 -1.348202707
H 1.606942644 0.468206842 -2.085081795
C 2.196603839 0.918759778 -0.235501553
O 2.910766774 0.712300176 0.769550529
C 1.160287675 2.052297649 -0.257743806
H 1.749641839 2.985199964 -0.226788759
N 0.387329814 2.025279136 -1.506814465

```

H -0.498497442 1.531101017 -1.357306980  
H 0.161588995 2.968381896 -1.820312078  
C 0.303927767 1.968662817 1.034867757  
H -0.283988026 2.896333058 1.120381260  
H 0.990034352 1.932839979 1.893798863  
C -0.606616612 0.778354346 1.026521566  
C -0.277505760 -0.516103262 1.382654781  
H 0.652502919 -0.914682483 1.778782487  
N -1.352484000 -1.350703309 1.152989815  
H -1.354370301 -2.348750202 1.325079509  
C -2.405199877 -0.623217438 0.640843331  
C -3.688822464 -1.022702954 0.254792285  
H -4.006688573 -2.064830797 0.330254102  
C -4.550565811 -0.041393396 -0.228241077  
H -5.558795116 -0.320547911 -0.538600164  
C -4.145256261 1.307072065 -0.319627148  
H -4.851216024 2.051260161 -0.693220275  
C -2.867882146 1.702422650 0.064344333  
H -2.574870811 2.753567009 -0.002141646  
C -1.966791143 0.734106487 0.549112700

———— 192\_WG10: PBE+D3 ————

O 2.173020640 -2.688901581 0.701793700  
C 1.048941253 -2.014805658 1.051518086  
O 0.991409860 -1.248575611 1.992199385  
H 2.870517048 -2.394967592 1.324184934  
C -0.103452417 -2.374154367 0.138383208  
H -0.332413187 -3.446604216 0.288484641  
H 0.204214235 -2.265926446 -0.914362640  
N -1.237020883 -1.523924034 0.396060050  
H -1.258759377 -0.993468301 1.271066435  
C -2.001056436 -1.044752982 -0.622244348  
O -1.951325888 -1.462400598 -1.780331762  
C -2.907747965 0.131960710 -0.235503418  
H -3.820682291 0.020144823 -0.850398924  
N -3.162345206 0.162873518 1.208947548  
H -3.606554959 1.045224832 1.472583810  
H -3.802363737 -0.588080250 1.476843379  
C -2.215224116 1.448968060 -0.684265860  
H -2.892937571 2.283348990 -0.430968663  
H -2.146922717 1.419652025 -1.782770746  
C -0.857471645 1.680539071 -0.096032197  
C -0.561729276 2.303896208 1.098452896  
H -1.227607827 2.764684815 1.823142530  
N 0.802822039 2.284223733 1.316085341  
H 1.261712248 2.612084652 2.156289206  
C 1.423696855 1.625968747 0.276309873  
C 2.773814296 1.329103474 0.065002027  
H 3.541168481 1.630585193 0.781573071  
C 3.103128951 0.626226960 -1.091569223  
H 4.147518769 0.374839983 -1.287279287  
C 2.111215418 0.235437194 -2.016133214  
H 2.405894776 -0.316045289 -2.911023429  
C 0.768919012 0.535569376 -1.805749306  
H 0.007542446 0.204874318 -2.515173091  
C 0.402299172 1.238210244 -0.642444010

## ———— 193\_WG06: PBE+D3 ————

O -2.201880821 2.278819905 -0.595598208  
C -1.242062664 2.504469432 0.319022371  
O -0.374746305 3.337335684 0.153728582  
H -2.749863123 1.483309823 -0.306300712  
C -1.334312942 1.630245528 1.587102760  
H -2.328165115 1.761371348 2.046330676  
H -0.567166677 1.972075986 2.290419399  
N -1.122909279 0.210531242 1.325335705  
H -0.182702454 -0.160726086 1.450715853  
C -2.001108516 -0.541041924 0.625124077  
O -3.093327325 -0.090640768 0.225413922  
C -1.550934987 -1.954371156 0.272988166  
H -0.793653969 -2.276555908 1.008573526  
N -2.703203748 -2.840635754 0.362104796  
H -2.514714921 -3.718956679 -0.125427130  
H -3.500400885 -2.390140945 -0.097595241  
C -0.860423151 -1.895894427 -1.135169746  
H -1.633691118 -1.640555029 -1.876949732  
H -0.510986680 -2.918658218 -1.363168840  
C 0.258965985 -0.906558591 -1.190439947  
C 0.228094169 0.327120897 -1.808658660  
H -0.545864017 0.768688090 -2.431069359  
N 1.365207194 1.044327983 -1.493503044  
H 1.488621193 2.030496508 -1.694381709  
C 2.146286311 0.306202465 -0.630144013  
C 3.360036862 0.616137904 -0.008357619  
H 3.850931478 1.578219581 -0.169968793  
C 3.919045106 -0.345037967 0.829866658  
H 4.865350234 -0.133136109 1.330217665  
C 3.287922889 -1.588943110 1.040930023  
H 3.758889295 -2.321479284 1.699376744  
C 2.080667592 -1.896863274 0.421342237  
H 1.609525151 -2.868943158 0.586509009  
C 1.483615239 -0.945263991 -0.428729416

## ———— 194\_WG02: PBE+D3 ————

O -2.120555762 2.338216691 -0.564680732  
C -1.138067089 2.533904519 0.332324074  
O -0.253855282 3.346590500 0.155833578  
H -2.684928521 1.556604749 -0.267640919  
C -1.226685342 1.652713618 1.595701151  
H -2.205363571 1.810575046 2.078441987  
H -0.433313817 1.966082655 2.283210667  
N -1.066651190 0.228124975 1.318760625  
H -0.124692158 -0.158598643 1.380136340  
C -1.985590317 -0.490171716 0.631750683  
O -3.075273096 -0.001849441 0.269868807  
C -1.600526725 -1.931759147 0.271128792  
H -0.872420261 -2.299815320 1.012517411  
N -2.733372129 -2.847957698 0.246360683  
H -3.103309027 -2.971076066 1.192486939  
H -3.489317535 -2.411677101 -0.292762321  
C -0.908426299 -1.915816038 -1.124762783  
H -1.672303664 -1.662681619 -1.877685618  
H -0.583702648 -2.949336869 -1.327516423

C 0.220825566 -0.938092267 -1.195223964  
C 0.210608378 0.279764427 -1.843550010  
H -0.553812087 0.715875585 -2.481437923  
N 1.355757797 0.989558920 -1.539492887  
H 1.494019726 1.968955602 -1.762280844  
C 2.120827328 0.262900110 -0.652471922  
C 3.332106481 0.573643862 -0.026484817  
H 3.836530316 1.525231836 -0.207223819  
C 3.869905814 -0.372229384 0.842543538  
H 4.813386597 -0.158919994 1.347634161  
C 3.221172166 -1.602419953 1.078893641  
H 3.676851019 -2.323684482 1.760199756  
C 2.016794868 -1.912069531 0.454295233  
H 1.533165954 -2.875016201 0.635744986  
C 1.440594514 -0.974851628 -0.425968070

———— 195\_WG01: PBE+D3 ————

O -3.160449207 -0.930538148 1.223031204  
C -3.359028291 0.388576165 1.388373791  
O -3.517508962 0.893852239 2.478538903  
H -3.035095601 -1.126461743 0.234973238  
C -3.407692570 1.208288085 0.080320532  
H -3.548776842 2.259900810 0.351755335  
H -4.283016242 0.870063645 -0.503236771  
N -2.209741097 1.094542243 -0.738967253  
H -1.593697611 1.895052323 -0.914612967  
C -1.853283657 -0.020934047 -1.393649824  
O -2.482125332 -1.098323391 -1.309712702  
C -0.588635547 0.100275458 -2.258233078  
H -0.938403034 -0.008120775 -3.299852381  
N 0.018901608 1.428599216 -2.102668884  
H 0.416642406 1.760354412 -2.980714694  
H 0.778635245 1.386616887 -1.415111103  
C 0.356643479 -1.086764992 -1.930478996  
H 1.155982257 -1.113347123 -2.688338328  
H -0.222771491 -2.016557454 -2.028090624  
C 0.948260781 -0.969314817 -0.557968876  
C 0.357489896 -1.352108658 0.631912786  
H -0.594652993 -1.843686328 0.809436681  
N 1.172329735 -1.005225811 1.690351407  
H 0.948975097 -1.162606466 2.665617165  
C 2.309463580 -0.385362517 1.218446273  
C 3.414504400 0.135963746 1.898790168  
H 3.480286631 0.099425709 2.988691316  
C 4.431320177 0.703614056 1.135653449  
H 5.307569756 1.120053041 1.635893969  
C 4.352072225 0.746199958 -0.272413206  
H 5.173174664 1.190082515 -0.838781063  
C 3.252443634 0.226326816 -0.947440934  
H 3.210762923 0.256639160 -2.039616421  
C 2.201239984 -0.347844216 -0.206278112

———— 196\_WG14: PBE+D3 ————

O 0.543339727 2.308018908 2.761312506  
C 1.020471923 1.290799168 2.005551373  
O 1.919296979 1.416790149 1.196780820



H	1.040541841	3.107719982	2.489857734
C	0.310526158	-0.006798224	2.320477361
H	-0.780175057	0.137254822	2.256121744
H	0.529903127	-0.275137401	3.370652204
N	0.733588996	-1.029805035	1.394566437
H	1.507166624	-0.775801910	0.780373292
C	-0.106913481	-2.032233502	1.021140481
O	-1.172798707	-2.263021752	1.596319177
C	0.334678897	-2.836936541	-0.205560752
H	1.431298871	-2.751687281	-0.317980807
N	-0.022700779	-4.229956825	0.026606109
H	-0.929646323	-4.246048964	0.505252527
H	-0.122185538	-4.730187777	-0.859058894
C	-0.319777935	-2.209160524	-1.480299723
H	-1.413528542	-2.303581970	-1.371724261
H	-0.024509737	-2.840838694	-2.335795617
C	0.057059191	-0.783403132	-1.733764755
C	1.171630955	-0.324378225	-2.408703902
H	1.944624739	-0.883436745	-2.930708331
N	1.208771665	1.057954056	-2.371340057
H	1.949652833	1.631169518	-2.754391079
C	0.127466968	1.527097934	-1.657081984
C	-0.246068769	2.832909603	-1.323212783
H	0.346421535	3.693105662	-1.641747969
C	-1.397693152	2.994879823	-0.557702938
H	-1.718546474	4.000276362	-0.278572052
C	-2.160573916	1.883645817	-0.138979129
H	-3.058500352	2.049590250	0.459115554
C	-1.788673233	0.585764306	-0.475011034
H	-2.377828078	-0.267396228	-0.131589093
C	-0.625950956	0.388154369	-1.242732157

———— 197\_WG07: PBE+D3 ————

O	2.232476821	0.497362055	2.911577315
C	1.136075105	0.935520546	2.238647266
O	1.171452754	1.801654553	1.390261910
H	2.991676767	0.994116019	2.540455903
C	-0.120002391	0.233155518	2.726769159
H	-0.310508941	0.568218851	3.763806195
H	0.040446298	-0.855475625	2.768699289
N	-1.226183383	0.493734277	1.848738693
H	-1.364685428	1.427392346	1.457130535
C	-1.911171205	-0.505128282	1.235957444
O	-1.833029126	-1.696128073	1.548292917
C	-2.789129925	-0.045179361	0.055989019
H	-3.807857358	-0.390524414	0.295134613
N	-2.797255755	1.413920782	-0.088733693
H	-2.142001471	1.696262375	-0.825634626
H	-3.722868950	1.761659686	-0.334959333
C	-2.322680448	-0.802532093	-1.227406364
H	-3.104426630	-0.678175421	-1.994789381
H	-2.263548299	-1.873935622	-0.981828790
C	-1.013247824	-0.300570368	-1.751307115
C	-0.846600670	0.665608335	-2.726809159
H	-1.593034904	1.160008473	-3.344152196
N	0.498423837	0.939479701	-2.896219416

```
H 0.881394843 1.603129243 -3.557391281
C 1.236467023 0.158334176 -2.031863581
C 2.619214794 0.088542041 -1.832248379
H 3.308380284 0.716174212 -2.401690497
C 3.084395063 -0.811774428 -0.878410227
H 4.158738635 -0.894346028 -0.698892846
C 2.193188771 -1.625844997 -0.148060698
H 2.593107096 -2.326169450 0.588342024
C 0.818255269 -1.553660408 -0.347082303
H 0.136816465 -2.179875580 0.231685278
C 0.313992883 -0.643273038 -1.295077675
```

———— 198\_WG09: PBE+D3 ————

```
O 0.518537620 2.331530001 2.745586584
C 1.005242916 1.306563691 2.006636759
O 1.902986556 1.427578282 1.195855056
H 1.006263561 3.131831656 2.459071484
C 0.307912584 0.007233498 2.342127607
H -0.784443285 0.139971526 2.282438799
H 0.536464608 -0.244765676 3.394394653
N 0.732722324 -1.025432080 1.425554870
H 1.495686852 -0.762168052 0.800966259
C -0.122655392 -2.013842428 1.035745087
O -1.196140024 -2.230277360 1.602509092
C 0.324454756 -2.837900932 -0.184247926
H 1.422752665 -2.789444263 -0.279540935
N -0.070553047 -4.242706706 -0.088773744
H -1.049040726 -4.261962232 0.222845765
H 0.457024438 -4.691925822 0.665132384
C -0.296408448 -2.224601369 -1.468130562
H -1.393013724 -2.318981212 -1.386115579
H 0.016552329 -2.867956214 -2.304823526
C 0.076311561 -0.795483233 -1.716287644
C 1.186486085 -0.337503613 -2.398325184
H 1.960479932 -0.898818789 -2.916383535
N 1.217244424 1.045206587 -2.374692181
H 1.951994299 1.618342835 -2.769401034
C 0.133778181 1.516267561 -1.665110314
C -0.246599627 2.823724973 -1.345765225
H 0.341631304 3.683378788 -1.673540194
C -1.399881749 2.988296294 -0.583282325
H -1.726476384 3.995070043 -0.315983568
C -2.157751311 1.877662024 -0.154004834
H -3.057992351 2.045356729 0.440110137
C -1.778891444 0.578089323 -0.475227239
H -2.365461421 -0.273905547 -0.124866963
C -0.613598062 0.377431715 -1.238732027
```

———— 199\_WG15: PBE+D3 ————

```
O -2.883793553 0.757221457 0.389904362
C -2.310208801 0.230968614 -0.541599287
O -1.617050608 0.913007153 -1.488194754
H -1.509985509 1.841344796 -1.178540057
C -2.251849081 -1.268917192 -0.813822820
H -2.880227254 -1.489852731 -1.695390652
H -2.656617261 -1.804423523 0.053875466
```

N -0.886517382 -1.709405816 -1.022204459  
H -0.276531887 -1.168646714 -1.640271667  
C -0.235769859 -2.493843140 -0.115868276  
O -0.778612500 -3.105763218 0.802936582  
C 1.291233813 -2.511321783 -0.292405708  
H 1.608734343 -3.554012794 -0.102532135  
N 1.691623837 -2.015639761 -1.616431845  
H 2.693655413 -1.816178560 -1.629823361  
H 1.518164077 -2.724923829 -2.332590116  
C 1.903420318 -1.629347581 0.837006444  
H 2.967485249 -1.457255600 0.593684716  
H 1.887998422 -2.233398174 1.755904242  
C 1.191443443 -0.337226242 1.105788747  
C 0.281176573 -0.154048145 2.127851316  
H -0.055107471 -0.865445526 2.877412799  
N -0.233816525 1.125254401 2.084016825  
H -1.049330889 1.431905932 2.601164369  
C 0.295343018 1.789342800 0.999164622  
C 0.016565445 3.066934897 0.499953835  
H -0.702568125 3.723824364 0.994412200  
C 0.687572153 3.467389379 -0.655606574  
H 0.494895008 4.457896586 -1.071782992  
C 1.618746630 2.615966275 -1.287391114  
H 2.127149215 2.960593685 -2.189606877  
C 1.890146818 1.346246784 -0.787650398  
H 2.590098473 0.690689206 -1.307928361  
C 1.219804457 0.900684001 0.365564926

———— 200\_WG13: PBE+D3 ————

O -2.698129206 -0.591642829 -2.377423872  
C -2.044259632 -0.981415847 -1.256871640  
O -1.192509450 -1.848122286 -1.240908729  
H -2.312283239 -1.111582367 -3.113355276  
C -2.539691069 -0.231459865 -0.037755732  
H -3.596593946 -0.511172429 0.130778113  
H -2.528420047 0.854611558 -0.222179959  
N -1.697735970 -0.533617150 1.093864346  
H -1.117051148 -1.365476216 0.993622733  
C -1.269336662 0.452570204 1.936515624  
O -1.763559361 1.580986269 1.954217517  
C -0.091418004 0.084717927 2.861950638  
H -0.346819413 0.538120916 3.834571766  
N 0.211102958 -1.325349871 3.072826710  
H -0.615960365 -1.867652001 3.324826785  
H 0.646277247 -1.737626263 2.243037761  
C 1.184017232 0.807664375 2.343378287  
H 1.959417514 0.688967661 3.116065467  
H 0.952454581 1.880285037 2.260391913  
C 1.676050308 0.276198652 1.031631341  
C 2.604436318 -0.730667016 0.843999750  
H 3.186324460 -1.278354361 1.581395744  
N 2.761252816 -0.980992133 -0.507490743  
H 3.381093579 -1.675787374 -0.904250998  
C 1.935319974 -0.144357986 -1.228017321  
C 1.735060329 -0.032182106 -2.607725033  
H 2.274600234 -0.666655083 -3.314347544

C 0.818271106 0.918541651 -3.047745382  
H 0.639775132 1.035271229 -4.118983775  
C 0.123294293 1.740618416 -2.135363718  
H -0.584621585 2.479464949 -2.516825596  
C 0.324976295 1.627782788 -0.763192088  
H -0.224710012 2.262377976 -0.064493080  
C 1.237594735 0.668813571 -0.285814012

———— 201\_WG12: PBE+D3 ————

O 2.241100862 -2.835795521 -0.506139994  
C 2.640283985 -1.695446233 -0.395810599  
O 3.174291091 -1.225145588 0.744721800  
H 3.319222391 -0.227534540 0.650960642  
C 2.579950166 -0.671384080 -1.549451877  
H 2.231410681 -1.192278532 -2.448158572  
H 3.592120765 -0.274957529 -1.734265415  
N 1.679522533 0.442566275 -1.277269512  
H 0.742244061 0.418802085 -1.671454537  
C 1.919011224 1.375130599 -0.328676702  
O 2.966506496 1.379341650 0.349682342  
C 0.806685876 2.401339118 -0.072602187  
H 1.3344446602 3.343776416 0.154037127  
N -0.146681763 2.642426276 -1.144938491  
H -0.837102909 1.895010163 -1.241777905  
H 0.295918461 2.830544157 -2.044098408  
C 0.055283281 1.963224629 1.219518647  
H -0.683321961 2.748524265 1.444219295  
H 0.786653386 1.946469235 2.041059564  
C -0.604417101 0.623077083 1.090919220  
C -0.042166736 -0.589825248 1.440325929  
H 0.913402971 -0.802814173 1.912221745  
N -0.885494622 -1.621172375 1.083335645  
H -0.647339165 -2.603883648 1.153234081  
C -2.015198778 -1.106705328 0.483291560  
C -3.138988926 -1.750311539 -0.045163819  
H -3.223799710 -2.839416447 -0.040575807  
C -4.149274632 -0.951799490 -0.574529052  
H -5.039623594 -1.423077024 -0.994985445  
C -4.046876511 0.455223226 -0.569102819  
H -4.865446054 1.050624461 -0.978288400  
C -2.928458357 1.095351151 -0.044358018  
H -2.868023254 2.186696132 -0.038553970  
C -1.878730758 0.317170374 0.484583933

———— 202\_WG08: PBE+D3 ————

O 0.301285085 -1.248404232 3.980349709  
C 0.892055292 -0.052903124 3.836789022  
O 1.421555026 0.531441188 4.758145537  
H -0.054220238 -1.561488390 3.086781757  
C 0.901539992 0.513696703 2.400871779  
H 1.573012310 -0.117433114 1.790179696  
H 1.323573515 1.522948538 2.449298890  
N -0.397868059 0.585941445 1.748863563  
H -0.831345321 1.482601553 1.509073194  
C -1.093236679 -0.481715194 1.332052783  
O -0.775250085 -1.662627755 1.592430860

C -2.340998186 -0.169965871 0.495228676  
H -3.177289102 -0.613887700 1.060608070  
N -2.549500279 1.276251315 0.367808833  
H -2.294104997 1.581817611 -0.577282400  
H -3.522348489 1.530511650 0.532345152  
C -2.254118763 -0.918576104 -0.869945701  
H -3.267608094 -0.946155185 -1.301195334  
H -1.954922953 -1.957841027 -0.665287822  
C -1.314415483 -0.268872682 -1.836562540  
C -1.669333979 0.605370032 -2.847717756  
H -2.658208659 0.914805930 -3.177699474  
N -0.536880384 1.062873654 -3.494870360  
H -0.532630564 1.668088138 -4.306298074  
C 0.580405401 0.487890252 -2.923391553  
C 1.935360664 0.634180451 -3.239334362  
H 2.264107162 1.288379069 -4.050106730  
C 2.851519608 -0.090754254 -2.483597920  
H 3.917128818 -0.001433239 -2.703990749  
C 2.426905972 -0.945444516 -1.444723235  
H 3.172331073 -1.510105243 -0.881486435  
C 1.079228140 -1.089593411 -1.131696853  
H 0.763842645 -1.761839836 -0.331023202  
C 0.126919613 -0.359946649 -1.868817022

———— 203\_WG11: PBE+D3 ————

O 1.638839337 -0.367450281 -1.580603447  
C 2.655272190 0.151472379 -0.844683498  
O 3.663496260 -0.460242362 -0.562285590  
H 1.844457283 -1.318970065 -1.701387146  
C 2.408818884 1.602823136 -0.442763329  
H 3.084427967 2.226801372 -1.052793614  
H 2.721390312 1.706541074 0.606886730  
N 1.045231954 2.050560189 -0.540985901  
H 0.552381769 2.108293306 -1.434139959  
C 0.262143382 2.223844633 0.555097823  
O 0.671429373 2.187250336 1.717951034  
C -1.228312509 2.464834061 0.241025318  
H -1.453198098 3.457303437 0.665293686  
N -1.490212131 2.493850114 -1.202747003  
H -2.172863363 3.211616425 -1.442936691  
H -1.865611154 1.587518278 -1.502865244  
C -2.085496760 1.418344306 1.016739366  
H -3.129590285 1.772218212 1.021066277  
H -1.734549310 1.405065290 2.059489011  
C -2.017597153 0.049517074 0.413309804  
C -2.907181955 -0.475966177 -0.505904142  
H -3.840099517 -0.060841416 -0.879232087  
N -2.480007967 -1.726091996 -0.916581034  
H -2.979764771 -2.335055242 -1.552112517  
C -1.303364124 -2.041825873 -0.268112543  
C -0.492215902 -3.178421475 -0.365062746  
H -0.751370652 -4.008840851 -1.026243407  
C 0.654698039 -3.216604530 0.425219297  
H 1.309234924 -4.089470211 0.377825349  
C 0.978743959 -2.152540502 1.294113004  
H 1.887394552 -2.214606829 1.895197887

C 0.173768621 -1.021753402 1.383870505  
H 0.446239451 -0.194363315 2.041611838  
C -0.984052604 -0.944389095 0.586562969

———— 204\_WG04: PBE+D3 ————

O 0.887854203 -0.283999262 -4.027472163  
C -0.321564847 -0.826509765 -3.824830537  
O -0.985314142 -1.303721543 -4.720520418  
H 1.270655462 0.031728665 -3.145356367  
C -0.797500548 -0.852537667 -2.356503055  
H -0.163289317 -1.571664180 -1.806294349  
H -1.827470155 -1.224863927 -2.352105218  
N -0.764767200 0.427157426 -1.663741562  
H -1.622533851 0.897236379 -1.359779968  
C 0.359383399 1.059696640 -1.298140918  
O 1.504592929 0.696293522 -1.644995966  
C 0.162973503 2.293599267 -0.407884134  
H 0.590497168 3.129201457 -0.986899007  
N -1.259701294 2.552369814 -0.163727312  
H -1.507957553 2.246066466 0.783323633  
H -1.478392393 3.544334518 -0.243255149  
C 1.014104299 2.141731252 0.890413446  
H 1.121467748 3.141689573 1.339497058  
H 2.018991149 1.802740078 0.596159991  
C 0.401173057 1.206566471 1.885025467  
C -0.373014889 1.572961935 2.970923024  
H -0.610654067 2.565712062 3.345759481  
N -0.830981459 0.445344447 3.626022420  
H -1.369496927 0.446527692 4.483093039  
C -0.356244763 -0.680927616 2.984427272  
C -0.541751743 -2.036076295 3.278249055  
H -1.145297442 -2.357351240 4.130183452  
C 0.077287039 -2.962700974 2.444852327  
H -0.046508116 -4.028863859 2.645106241  
C 0.868226872 -2.549136134 1.352150387  
H 1.350506630 -3.304019685 0.728334422  
C 1.051447011 -1.201293163 1.061343439  
H 1.673127875 -0.892847038 0.218495603  
C 0.426612363 -0.237855318 1.876386368

———— 205\_WG05: PBE+D3 ————

O -4.604288540 -0.729888699 0.037278130  
C -4.472333840 0.452280964 0.658741758  
O -5.420773638 1.143610669 0.961765914  
H -3.692239588 -1.143881820 -0.098809878  
C -3.023276749 0.854667408 1.010236037  
H -2.663946182 0.158734275 1.790285588  
H -3.055660789 1.865135800 1.431387558  
N -2.085760122 0.844490531 -0.102539496  
H -1.662012256 1.706843942 -0.457777407  
C -1.645512498 -0.271507225 -0.705093884  
O -2.083367765 -1.411888976 -0.443472203  
C -0.573160917 -0.051761120 -1.784093834  
H -1.101207276 -0.200722150 -2.742943908  
N -0.084527654 1.332162255 -1.748874202  
H 0.197113132 1.645259208 -2.677747389

```

H 0.737914999 1.399311895 -1.140342749
C 0.515394638 -1.147190462 -1.657867575
H 1.169913314 -1.086610365 -2.542476034
H 0.014775996 -2.126143274 -1.684427969
C 1.325663596 -1.008076614 -0.405333437
C 1.020302364 -1.541855093 0.831724564
H 0.184963232 -2.175883152 1.117455783
N 1.967204859 -1.147733508 1.757765696
H 1.988146378 -1.438898385 2.727118299
C 2.913515637 -0.354729838 1.143634722
C 4.056648697 0.264917202 1.658561361
H 4.330827317 0.168898989 2.711509681
C 4.837289243 1.008564232 0.777796512
H 5.737592892 1.502387657 1.147326116
C 4.489336044 1.129624198 -0.584159224
H 5.130218693 1.713491550 -1.247709307
C 3.351967372 0.512327502 -1.093964515
H 3.102641149 0.605847362 -2.154190588
C 2.535178262 -0.242834957 -0.229844120

```

### 11.3 C<sub>60</sub>@C<sub>60</sub>H<sub>28</sub> buckyball catcher host-guest complex

#### 11.3.1 C<sub>60</sub>H<sub>28</sub> buckyball catcher host

———— C<sub>60</sub>H<sub>28</sub> conformer a: PBE+MBD@rsSCS ————

$R_p = 12.992 \text{ \AA}$  and  $R_t = 6.303 \text{ \AA}$

```

C 6.442203709 -1.375292472 2.449638882
C 5.550213509 -0.695137101 1.604193912
C 5.549137257 0.712722788 1.604357219
C 6.439800675 1.394075739 2.450226332
C 7.328773126 0.707940535 3.274185042
C 7.330038541 -0.688069718 3.273839433
C 4.597349486 1.522357527 0.809250766
C 3.768985094 2.414738367 1.488750102
C 2.963176191 3.360765973 0.840905903
C 2.989949335 3.395601016 -0.608940325
C 3.797467454 2.459916820 -1.271200486
C 4.602208339 1.534196339 -0.605927155
C 2.110394142 4.282074478 1.594517412
C 1.596646108 5.328798982 0.855281054
C 1.636426328 5.374444498 -0.570938756
C 2.183457967 4.370839623 -1.346566142
C 0.561512739 6.181529743 -1.007375481
C -0.143486905 6.631462259 0.135096873
C 0.494511833 6.102535394 1.282865202
C -1.492027695 6.960230550 0.107048518
C -2.065392135 7.022047440 -1.217239082
C -1.374165292 6.579880113 -2.340551338
C -0.040929662 6.032453342 -2.251693443
C 0.642416008 5.126791105 -3.136326384
C 1.701686679 4.330747004 -2.701159883
C -2.144937351 6.921565002 1.394836144
C -1.520077172 6.398354551 2.522515506
C -0.179005351 5.864847842 2.476172786
C 0.459270902 4.903780203 3.336097640
C 1.551977027 4.147355525 2.912842107
C 5.537866314 0.714386699 -1.411736750

```

```
C 5.538094664 -0.696409026 -1.411860684
C 6.415063262 -1.374155592 -2.275862162
C 7.284713076 -0.688843265 -3.120124796
C 7.284857628 0.706871765 -3.119797099
C 6.415166438 1.392244195 -2.275360587
C 4.599693532 -1.506236043 0.809143113
C 3.773926219 -2.401140851 1.488311821
C 2.971273131 -3.349482156 0.840072262
C 2.997710191 -3.383652899 -0.609714572
C 3.801665119 -2.444981287 -1.271641348
C 4.603920861 -1.517374220 -0.606019002
C 2.195008281 -4.361626367 -1.347505892
C 1.652516047 -5.368051771 -0.572300082
C 1.613103213 -5.323106660 0.854121138
C 2.122237123 -4.274340667 1.593244376
C 0.513768347 -6.101016179 1.281737370
C -0.122526611 -6.631666435 0.133828167
C 0.580392527 -6.178746995 -1.008791793
C 1.712532607 -4.321925240 -2.701808925
C 0.655967432 -5.121360054 -3.136951863
C -0.023407041 -6.030205305 -2.252546589
C -1.355232015 -6.580802017 -2.341359729
C -2.044370211 -7.026027796 -1.218060888
C -1.470114419 -6.964267722 0.105745753
C 1.563032119 -4.140763218 2.911254482
C 0.472943785 -4.901031838 3.334416376
C -0.161006199 -5.864963615 2.474734585
C -1.500385330 -6.402499312 2.521017240
C -2.123097645 -6.927853524 1.393304059
H 0.265711504 4.976797725 -4.150181085
H 2.102035279 3.591659835 -3.397535210
H 1.917627396 3.363171951 3.578458253
H 0.023168801 4.680119418 4.311843946
H -2.102778996 6.305964240 3.441472588
H -3.192368720 7.220014354 1.474255697
H -3.104644803 7.334762941 -1.337919418
H -1.898532126 6.562852558 -3.298310282
H -1.880296079 -6.563339025 -3.298702346
H -3.083209378 -7.340375502 -1.338052371
H -3.169957063 -7.228588697 1.472122866
H -2.083904591 -6.310827149 3.439512862
H 0.035079026 -4.677971821 4.309488735
H 1.925196042 -3.354409433 3.576098144
H 2.109754605 -3.580520335 -3.397492437
H 0.277730911 -4.971591146 -4.150248212
H 3.785616678 2.400503201 2.580078004
H 3.832814052 2.478456937 -2.362028141
H 3.790617142 -2.387441826 2.579679276
H 3.837033090 -2.462990296 -2.362469760
H 6.408680297 2.483175278 -2.270365628
H 7.959251474 1.260321090 -3.773443962
H 7.958948607 -1.242244481 -3.774038179
H 6.408540960 -2.465102849 -2.270796170
H 6.429497052 2.485060424 2.447314279
H 8.017208181 1.260976551 3.913456092
H 8.019504233 -1.240191148 3.912782969
```



H 6.433753126 -2.466278911 2.446219187

———— C<sub>60</sub>H<sub>28</sub> conformer **b**: PBE+MBD@rsSCS ————  
R<sub>p</sub> = 11.970 Å and R<sub>t</sub> = 6.190 Å

C -3.807093653 -2.745724025 2.302958563  
C -2.748921546 -2.314673488 1.489694283  
C -1.541513101 -3.042384724 1.489641746  
C -1.428607271 -4.179520453 2.302629615  
C -2.492976227 -4.607681651 3.094789655  
C -3.688874920 -3.886895570 3.095064303  
C -0.363917868 -2.594991313 0.707574529  
C 0.795211577 -2.222420940 1.383248728  
C 1.965575877 -1.812123883 0.725769004  
C 1.965575877 -1.812123883 -0.725769004  
C 0.795211577 -2.222420940 -1.383248728  
C -0.363917868 -2.594991313 -0.707574529  
C 3.175223881 -1.458391807 1.472754625  
C 4.186144602 -0.902479794 0.713757325  
C 4.186144602 -0.902479794 -0.713757325  
C 3.175223881 -1.458391807 -1.472754625  
C 5.531404343 -0.854062673 -1.146363854  
C 6.361601083 -0.825415191 0.000000000  
C 5.531404343 -0.854062673 1.146363854  
C 7.663924933 -1.307725560 0.000000000  
C 8.179493012 -1.641009424 -1.307638179  
C 7.364957572 -1.669164193 -2.435354853  
C 5.954166558 -1.367301353 -2.367560724  
C 4.884760170 -1.767167504 -3.243764548  
C 3.559138888 -1.813466839 -2.813907682  
C 8.179493012 -1.641009424 1.307638179  
C 7.364957572 -1.669164193 2.435354853  
C 5.954166558 -1.367301353 2.367560724  
C 4.884760170 -1.767167504 3.243764548  
C 3.559138888 -1.813466839 2.813907682  
C -1.541513101 -3.042384724 -1.489641746  
C -2.748921546 -2.314673488 -1.489694283  
C -3.807093653 -2.745724025 -2.302958563  
C -3.688874920 -3.886895570 -3.095064303  
C -2.492976227 -4.607681651 -3.094789655  
C -1.428607271 -4.179520453 -2.302629615  
C -2.902272857 -1.064375304 0.707654940  
C -3.117317989 0.133959792 1.383421833  
C -3.324410286 1.356541141 0.725711641  
C -3.324410286 1.356541141 -0.725711641  
C -3.117317989 0.133959792 -1.383421833  
C -2.902272857 -1.064375304 -0.707654940  
C -3.472363970 2.607889493 -1.472548493  
C -3.854932131 3.696884037 -0.713923126  
C -3.854932131 3.696884037 0.713923126  
C -3.472363970 2.607889493 1.472548493  
C -3.679623493 5.031590059 1.146573580  
C -3.570668669 5.855060886 0.000000000  
C -3.679623493 5.031590059 -1.146573580  
C -3.055401595 2.927102203 -2.812683690  
C -2.882059402 4.241993018 -3.242726302  
C -3.101770912 5.362969261 -2.367360565

```

C -2.569430034  6.704021399 -2.435013060
C -2.463323349  7.512070569 -1.307361013
C -2.878874266  7.059252240  0.000000000
C -3.055401595  2.927102203  2.812683690
C -2.882059402  4.241993018  3.242726302
C -3.101770912  5.362969261  2.367360565
C -2.569430034  6.704021399  2.435013060
C -2.463323349  7.512070569  1.307361013
H  5.118339144 -2.140991783 -4.242660922
H  2.816756643 -2.225752190 -3.499652193
H  2.816756643 -2.225752190  3.499652193
H  5.118339144 -2.140991783  4.242660922
H  7.793045204 -2.023511993  3.375438362
H  9.215013904 -1.973568460  1.406683147
H  9.215013904 -1.973568460 -1.406683147
H  7.793045204 -2.023511993 -3.375438362
H -2.146996653  7.066604219 -3.374520740
H -1.962121750  8.477426915 -1.405731472
H -1.962121750  8.477426915  1.405731472
H -2.146996653  7.066604219  3.374520740
H -2.470256171  4.410484796  4.239763621
H -2.765705864  2.126623111  3.495751197
H -2.765705864  2.126623111 -3.495751197
H -2.470256171  4.410484796 -4.239763621
H  0.779796555 -2.231872971  2.474975895
H  0.779796555 -2.231872971 -2.474975895
H -3.125370912  0.115016071  2.475111266
H -3.125370912  0.115016071 -2.475111266
H -0.489125254 -4.734838094 -2.300281284
H -2.388553346 -5.501666872 -3.710088907
H -4.527644138 -4.211966009 -3.711052082
H -4.736434759 -2.173758943 -2.301492941
H -0.489125254 -4.734838094  2.300281284
H -2.388553346 -5.501666872  3.710088907
H -4.527644138 -4.211966009  3.711052082
H -4.736434759 -2.173758943  2.301492941

```

———— C<sub>60</sub>H<sub>28</sub> conformer a: PBE+TS ————  
 $R_p = 12.969 \text{ \AA}$  and  $R_t = 6.080 \text{ \AA}$

```

C  6.593396679 -1.382650976  2.372190418
C  5.649396907 -0.701496459  1.586672342
C  5.647398258  0.708986559  1.588643292
C  6.589368411  1.390253809  2.376564650
C  7.527805778  0.701536272  3.143496457
C  7.530048420 -0.694084628  3.141209813
C  4.662739314  1.506961474  0.810385378
C  3.798533370  2.367082840  1.488183964
C  2.945515887  3.271154760  0.834499074
C  2.957463902  3.286832180 -0.617357635
C  3.812167942  2.388848435 -1.277524200
C  4.665829045  1.512927719 -0.606355208
C  2.071436348  4.184104710  1.585987735
C  1.528402569  5.205255464  0.831968844
C  1.544391317  5.224547299 -0.595888739
C  2.101285281  4.220830144 -1.363215306
C  0.456658306  6.014850496 -1.029589912

```

C	-0.228624700	6.488214047	0.115599320
C	0.430302385	5.983063154	1.262788933
C	-1.573457896	6.829393291	0.105013606
C	-2.166804265	6.869558846	-1.213145146
C	-1.496691843	6.399073883	-2.338566031
C	-0.163608289	5.844634182	-2.262014726
C	0.512141212	4.923622680	-3.138327493
C	1.589691005	4.147236693	-2.707643570
C	-2.196824212	6.832665276	1.409749518
C	-1.551989377	6.332284466	2.537177913
C	-0.216707902	5.780755202	2.476298694
C	0.441728323	4.838948561	3.344077768
C	1.531010532	4.076435863	2.917020225
C	5.647661262	0.712793552	-1.387251418
C	5.649430596	-0.698905519	-1.388549322
C	6.595294464	-1.377248095	-2.174712551
C	7.535976349	-0.687258852	-2.937481954
C	7.534270220	0.708225891	-2.936499855
C	6.591670730	1.394609416	-2.172824802
C	4.666264339	-1.499778597	0.807144603
C	3.803494964	-2.362400592	1.483557685
C	2.951296942	-3.265637164	0.827938007
C	2.963871053	-3.278728605	-0.623992001
C	3.817345868	-2.378559778	-1.282522395
C	4.669298017	-1.502621810	-0.609553880
C	2.109182552	-4.211867455	-1.372139067
C	1.551269367	-5.216453157	-0.606550257
C	1.533896891	-5.199268694	0.821175503
C	2.076736672	-4.179755992	1.577461658
C	0.435303201	-5.977783580	1.249760073
C	-0.222178732	-6.481129153	0.101018087
C	0.464400178	-6.006731001	-1.042965202
C	1.600358081	-4.137626265	-2.717464192
C	0.523574044	-4.913637700	-3.150495050
C	-0.153927203	-5.835561001	-2.276092653
C	-1.487307240	-6.389689670	-2.355398824
C	-2.158639964	-6.861823294	-1.231213034
C	-1.566997740	-6.822940103	0.087843613
C	1.534938770	-4.073995867	2.908168011
C	0.444836105	-4.836851660	3.332921887
C	-0.212860232	-5.777549763	2.463120866
C	-1.548155770	-6.329922032	2.521312408
C	-2.191320704	-6.828762093	1.392054798
H	0.119708663	4.749634702	-4.141996337
H	1.982615173	3.399830685	-3.398378227
H	1.910901247	3.313009449	3.597416021
H	0.026954989	4.637773438	4.333776344
H	-2.112571324	6.278320326	3.472209139
H	-3.236156303	7.152425111	1.506421525
H	-3.203863741	7.191427201	-1.325533614
H	-2.034356776	6.371603348	-3.288136496
H	-2.023158406	-6.363093239	-3.306014629
H	-3.195462054	-7.184282894	-1.345269353
H	-3.230566454	-7.149502017	1.487534105
H	-2.109506969	-6.278812850	3.456182648
H	0.028827128	-4.636840647	4.322374298

H 1.914409605 -3.311890143 3.590291008  
H 1.994547041 -3.389784415 -3.407106681  
H 0.133272006 -4.739005788 -4.154742871  
H 3.820301376 2.361349120 2.578605363  
H 3.841666343 2.400053757 -2.367722863  
H 3.825673733 -2.359196012 2.574091996  
H 3.846526995 -2.387134860 -2.372752371  
H 6.588716311 2.484845094 -2.164242317  
H 8.266422379 1.261774122 -3.524614364  
H 8.269295356 -1.238437611 -3.526064655  
H 6.594272803 -2.467534412 -2.167652627  
H 6.586196910 2.480536244 2.369544382  
H 8.256160943 1.253614829 3.737304433  
H 8.260077148 -1.246307318 3.733026752  
H 6.593080122 -2.472852872 2.361168710

———— C<sub>60</sub>H<sub>28</sub> conformer **b**: PBE+TS —————

$R_p = 11.977 \text{ \AA}$  and  $R_t = 6.206 \text{ \AA}$

C -3.818217154 -2.758142091 2.308043593  
C -2.760076869 -2.324071876 1.494692934  
C -1.550127342 -3.051542959 1.494926507  
C -1.439012305 -4.190125846 2.308126601  
C -2.502358929 -4.617287796 3.102980501  
C -3.698260667 -3.897487972 3.103045604  
C -0.369586109 -2.601837651 0.708343407  
C 0.790004040 -2.220606924 1.381859247  
C 1.964769222 -1.814451312 0.725873487  
C 1.964769222 -1.814451312 -0.725873487  
C 0.790004040 -2.220606924 -1.381859247  
C -0.369586109 -2.601837651 -0.708343407  
C 3.179004415 -1.463069307 1.475329465  
C 4.192006447 -0.912962630 0.714058031  
C 4.192006447 -0.912962630 -0.714058031  
C 3.179004415 -1.463069307 -1.475329465  
C 5.537953959 -0.864268745 -1.146786892  
C 6.368358896 -0.835199204 0.000000000  
C 5.537953959 -0.864268745 1.146786892  
C 7.672615506 -1.312376266 0.000000000  
C 8.188998047 -1.642442809 -1.308628668  
C 7.374995969 -1.669939799 -2.436770898  
C 5.962600701 -1.371480094 -2.369768545  
C 4.892436590 -1.766647152 -3.248100398  
C 3.566061278 -1.812971749 -2.818646991  
C 8.188998047 -1.642442809 1.308628668  
C 7.374995969 -1.669939799 2.436770898  
C 5.962600701 -1.371480094 2.369768545  
C 4.892436590 -1.766647152 3.248100398  
C 3.566061278 -1.812971749 2.818646991  
C -1.550127342 -3.051542959 -1.494926507  
C -2.760076869 -2.324071876 -1.494692934  
C -3.818217154 -2.758142091 -2.308043593  
C -3.698260667 -3.897487972 -3.103045604  
C -2.502358929 -4.617287796 -3.102980501  
C -1.439012305 -4.190125846 -2.308126601  
C -2.913909952 -1.070711679 0.708276915  
C -3.120064951 0.131860292 1.382139305

```

C -3.320287815  1.358053860  0.725810265
C -3.320287815  1.358053860 -0.725810265
C -3.120064951  0.131860292 -1.382139305
C -2.913909952 -1.070711679 -0.708276915
C -3.464406470  2.613191360 -1.475204699
C -3.842178997  3.702591417 -0.714189604
C -3.842178997  3.702591417  0.714189604
C -3.464406470  2.613191360  1.475204699
C -3.668867570  5.038121706  1.146935808
C -3.561196411  5.862113318  0.000000000
C -3.668867570  5.038121706 -1.146935808
C -3.053634732  2.936363282 -2.817957003
C -2.882044962  4.252185492 -3.247628969
C -3.097360063  5.372728965 -2.369680868
C -2.568901351  6.716000914 -2.436483660
C -2.462450561  7.523553944 -1.308419628
C -2.874977192  7.069644699  0.000000000
C -3.053634732  2.936363282  2.817957003
C -2.882044962  4.252185492  3.247628969
C -3.097360063  5.372728965  2.369680868
C -2.568901351  6.716000914  2.436483660
C -2.462450561  7.523553944  1.308419628
H  5.125257937 -2.133919239 -4.249316394
H  2.824777494 -2.218001242 -3.508753572
H  2.824777494 -2.218001242  3.508753572
H  5.125257937 -2.133919239  4.249316394
H  7.804771524 -2.018523480  3.377706209
H  9.225309269 -1.971329195  1.407686111
H  9.225309269 -1.971329195 -1.407686111
H  7.804771524 -2.018523480 -3.377706209
H -2.150938202  7.080663423 -3.376659185
H -1.963661463  8.489678129 -1.406790316
H -1.963661463  8.489678129  1.406790316
H -2.150938202  7.080663423  3.376659185
H -2.478525839  4.421641590  4.247555359
H -2.770485072  2.138430988  3.505672554
H -2.770485072  2.138430988 -3.505672554
H -2.478525839  4.421641590 -4.247555359
H  0.770466407 -2.222526735  2.472245097
H  0.770466407 -2.222526735 -2.472245097
H -3.125425815  0.111601443  2.472475745
H -3.125425815  0.111601443 -2.472475745
H -0.500751908 -4.746115089 -2.305144056
H -2.396043908 -5.509389669 -3.720203819
H -4.536148214 -4.220555683 -3.720799638
H -4.748086477 -2.188349275 -2.305404351
H -0.500751908 -4.746115089  2.305144056
H -2.396043908 -5.509389669  3.720203819
H -4.536148214 -4.220555683  3.720799638
H -4.748086477 -2.188349275  2.305404351

```

———— C<sub>60</sub>H<sub>28</sub> conformer a: PBE+D3 —————  
 $R_p = 12.987 \text{ \AA}$  and  $R_t = 6.286 \text{ \AA}$

```

C  4.635513544 -1.378297450  2.337650289
C  3.724319969 -0.697354156  1.514887461
C  3.721135234  0.713858884  1.515587434

```

```
C 4.629212863 1.398087790 2.339082786
C 5.539857517 0.709597409 3.140530912
C 5.543028253 -0.686515661 3.139801717
C 2.735128179 1.495666575 0.724395468
C 1.824569375 2.312557172 1.394447304
C 0.904856549 3.143061814 0.732463573
C 0.913196285 3.143942974 -0.719108750
C 1.840542052 2.314291380 -1.371445405
C 2.743256587 1.496482491 -0.691913847
C -0.072834010 3.947735407 1.476533974
C -0.769993994 4.866240815 0.713702508
C -0.761792867 4.867170533 -0.717465800
C -0.055945191 3.949580385 -1.473372019
C -1.973976757 5.453065785 -1.157674228
C -2.730646868 5.813313385 -0.012514946
C -1.987076971 5.451555767 1.140740014
C -4.117630002 5.894790129 -0.020346714
C -4.715408585 5.797774458 -1.332807922
C -3.975233087 5.442686562 -2.456249808
C -2.561855453 5.151416030 -2.382231431
C -1.739937891 4.352081477 -3.253180511
C -0.546473303 3.776863737 -2.816916885
C -4.730308655 5.796304780 1.285137091
C -4.002966279 5.439868435 2.416519115
C -2.588840365 5.148577296 2.358166456
C -1.777015273 4.348076985 3.237455021
C -0.578702816 3.773358410 2.814123058
C 3.738400751 0.715452265 -1.472284704
C 3.741660706 -0.695792829 -1.472893117
C 4.662905231 -1.375820412 -2.285120792
C 5.580257609 -0.683289323 -3.075337536
C 5.576988299 0.712810429 -3.074803527
C 4.656424424 1.400427935 -2.284019426
C 2.741868015 -1.482871656 0.722935487
C 1.835151373 -2.304719226 1.392131170
C 0.919520342 -3.138999094 0.729225367
C 0.927941322 -3.138360716 -0.722363052
C 1.851262400 -2.303548987 -1.373824057
C 2.750057349 -1.482185052 -0.693372117
C -0.037193025 -3.947982091 -1.477537322
C -0.738621416 -4.869714811 -0.722574685
C -0.746906240 -4.870270108 0.708588901
C -0.054258672 -3.949211506 1.472436810
C -1.961084677 -5.462049507 1.134947398
C -2.702806582 -5.826265015 -0.018709992
C -1.947859437 -5.461158137 -1.163449146
C -0.528423111 -3.776493671 -2.820994744
C -1.718997717 -4.357168689 -3.257915911
C -2.537109171 -5.161277580 -2.387775950
C -3.949019958 -5.459471495 -2.462175752
C -4.687519720 -5.819228533 -1.339112580
C -4.089367659 -5.914605759 -0.026705925
C -0.561004756 -3.778860352 2.810227203
C -1.756478220 -4.359933952 3.232887542
C -2.564367163 -5.163397329 2.352684037
C -3.977031309 -5.461751215 2.410657887
```

```

C -4.702570520 -5.820496318 1.278844130
H -2.100877268 4.100801836 -4.253788950
H -0.031461410 3.095565404 -3.498479866
H -0.071590869 3.091149086 3.500678961
H -2.149433364 4.095551096 4.233546742
H -4.543292295 5.286334304 3.354849271
H -5.813844570 5.910581189 1.378573585
H -5.797784738 5.912227905 -1.438447460
H -4.504891771 5.290229784 -3.400810894
H -4.479378538 -5.308801003 -3.406636724
H -5.769298725 -5.938902346 -1.444982228
H -5.785523264 -5.940191601 1.372139397
H -4.518163114 -5.311973739 3.349138069
H -2.130122777 -4.110369727 4.229274295
H -0.057294797 -3.094954547 3.497597993
H -0.016702423 -3.092078979 -3.501914922
H -2.081014796 -4.106789132 -4.258363027
H 1.839333203 2.308951141 2.487279137
H 1.867884075 2.312025139 -2.464038622
H 1.849868694 -2.302172277 2.484957920
H 1.878683503 -2.300065170 -2.466405257
H 4.643720818 2.493346404 -2.280805574
H 6.289911855 1.267532093 -3.688329330
H 6.295783089 -1.234201881 -3.689268105
H 4.655259685 -2.468786044 -2.282819858
H 4.616625861 2.490995070 2.336710762
H 6.245132086 1.263629734 3.763449206
H 6.250821757 -1.237992558 3.762131430
H 4.627853580 -2.471248046 2.334172535

```

———— C<sub>60</sub>H<sub>28</sub> conformer b: PBE+D3 —————

R<sub>p</sub> = 12.080 Å and R<sub>t</sub> = 6.190 Å

```

C -3.798715442 -2.740101182 2.302098265
C -2.738483913 -2.305538758 1.491297580
C -1.529424798 -3.033802927 1.492810840
C -1.418851641 -4.171650588 2.307216192
C -2.485426477 -4.602266221 3.096381782
C -3.682176506 -3.882837660 3.093183771
C -0.348662885 -2.588091625 0.708201799
C 0.814918481 -2.220949981 1.382948270
C 1.990116012 -1.819376247 0.725958694
C 1.990115959 -1.819376106 -0.725957982
C 0.814918402 -2.220949615 -1.382947510
C -0.348662862 -2.588091453 -0.708201040
C 3.204845049 -1.473126092 1.475086426
C 4.219817629 -0.922053503 0.715369980
C 4.219817524 -0.922053308 -0.715369524
C 3.204844849 -1.473125729 -1.475085926
C 5.568197816 -0.883004907 -1.148936648
C 6.400480875 -0.860359737 0.000000031
C 5.568197998 -0.883005255 1.148936846
C 7.699038933 -1.355247199 -0.000000141
C 8.211096899 -1.694194064 -1.308778271
C 7.396463450 -1.715939506 -2.436585540
C 5.987420563 -1.401895877 -2.370007942
C 4.914664692 -1.794219261 -3.246893315

```

```
C 3.588224438 -1.830692619 -2.817329376
C 8.211097143 -1.694194369 1.308777818
C 7.396463887 -1.715940141 2.436585237
C 5.987420968 -1.401896531 2.370007942
C 4.914665258 -1.794220235 3.246893344
C 3.588224915 -1.830693406 2.817329662
C -1.529424523 -3.033802873 -1.492810320
C -2.738483719 -2.305538913 -1.491297191
C -3.798715044 -2.740101429 -2.302098072
C -3.682175756 -3.882837687 -3.093183800
C -2.485425488 -4.602265834 -3.096381966
C -1.418850880 -4.171650204 -2.307216069
C -2.893671085 -1.052082103 0.707975530
C -3.113374673 0.147894896 1.383045345
C -3.327879388 1.370966973 0.725992245
C -3.327879446 1.370966930 -0.725992410
C -3.113374677 0.147894761 -1.383045332
C -2.893671100 -1.052082152 -0.707975324
C -3.488469885 2.623867715 -1.474914495
C -3.886880384 3.708416972 -0.715672935
C -3.886880362 3.708417024 0.715672837
C -3.488469746 2.623867793 1.474914346
C -3.727327525 5.047759359 1.149061542
C -3.627677669 5.874223867 -0.000000109
C -3.727327505 5.047759255 -1.149061687
C -3.072661490 2.949807822 -2.815011466
C -2.914693006 4.267306505 -3.244501458
C -3.150354579 5.385870813 -2.369211628
C -2.632285542 6.733321038 -2.435879672
C -2.535079819 7.542309114 -1.308303748
C -2.946461736 7.085628183 -0.000000173
C -3.072661301 2.949807905 2.815011316
C -2.914692850 4.267306621 3.244501267
C -3.150354482 5.385870946 2.369211420
C -2.632285385 6.733321139 2.435879305
C -2.535079754 7.542309185 1.308303337
H 5.146532748 -2.169304039 -4.247204559
H 2.843277248 -2.238549916 -3.504452962
H 2.843277850 -2.238551019 3.504453200
H 5.146533484 -2.169305240 4.247204462
H 7.820609954 -2.075894125 3.377780555
H 9.244422707 -2.036994331 1.406697513
H 9.244422391 -2.036994075 -1.406698215
H 7.820609380 -2.075893254 -3.377781001
H -2.212749690 7.099401610 -3.376722950
H -2.044209393 8.514074531 -1.406090825
H -2.044209342 8.514074603 1.406090344
H -2.212749465 7.099401767 3.376722535
H -2.501884486 4.441892832 4.241562944
H -2.769249359 2.153270403 3.498327089
H -2.769249515 2.153270303 -3.498327203
H -2.501884652 4.441892655 -4.241563145
H 0.798015984 -2.228069701 2.475585186
H 0.798015825 -2.228069163 -2.475584407
H -3.124006200 0.126939870 2.475651930
H -3.124006210 0.126939518 -2.475651912
```



```

H -0.477897341 -4.726726394 -2.306077565
H -2.382039010 -5.499290810 -3.710086428
H -4.525096341 -4.210037880 -3.705215623
H -4.729764358 -2.168530828 -2.297684308
H -0.477898325 -4.726727123 2.306077607
H -2.382040385 -5.499291515 3.710085853
H -4.525097213 -4.210037753 3.705215476
H -4.729764659 -2.168530413 2.297684512

```

### 11.3.2 C<sub>60</sub> buckyball

The C<sub>60</sub> buckyball has icosahedral symmetry. Experimental gas-phase electron diffraction indicates that the C-C bond lengths for bonds within five-membered rings (fusing pentagons and hexagons) are of length  $d_{(5/6)} = 1.458(6)$  Å while bonds fusing hexagonal rings are of length  $d_{(6/6)} = 1.401(10)$  Å.<sup>40</sup> For each of the DFT-vdW optimized structures below we report these two bond lengths and their standard deviations.

————— C<sub>60</sub>: PBE+MBD@rsSCS —————  
 $d_{(5/6)} = 1.45192(5)$  Å and  $d_{(6/6)} = 1.39804(3)$  Å

```

C 1.235039200 0.000000000 -3.328049500
C 0.381720360 1.174635850 -3.328062410
C -0.999173400 0.725953290 -3.327998740
C -0.999173400 -0.725953290 -3.327998740
C -1.961280580 1.424973050 -2.593019090
C 0.749180830 2.305670960 -2.593036450
C 0.381720360 -1.174635850 -3.328062410
C 2.424309060 0.000000000 -2.593112650
C 0.749180830 -2.305670960 -2.593036450
C -1.961280580 -1.424973050 -2.593019090
C -2.960502730 0.699010950 -1.829681940
C -1.579640820 2.599604780 -1.829684760
C -2.960502730 -0.699010950 -1.829681940
C -1.579640820 -2.599604780 -1.829684760
C -0.250070520 -3.031623110 -1.829683690
C 1.984252110 -2.305673080 -1.829658650
C 2.806095680 -1.174625400 -1.829630330
C 2.806095680 1.174625400 -1.829630330
C 1.984252110 2.305673080 -1.829658650
C -0.250070520 3.031623110 -1.829683690
C -3.196370790 1.424992360 -0.594615820
C -2.342928880 2.599641490 -0.594619140
C 1.748289970 3.031668120 -0.594639390
C 0.367473730 3.480360060 -0.594643240
C 3.423457800 -0.725934750 -0.594612620
C 3.423457800 0.725934750 -0.594612620
C 1.748289970 -3.031668120 -0.594639390
C 0.367473730 -3.480360060 -0.594643240
C -2.342928880 -2.599641490 -0.594619140
C -3.196370790 -1.424992360 -0.594615820
C -3.423457800 -0.725934750 0.594612620
C -3.423457800 0.725934750 0.594612620
C -1.748289970 3.031668120 0.594639390
C -0.367473730 3.480360060 0.594643240
C 3.196370790 1.424992360 0.594615820
C 2.342928880 2.599641490 0.594619140
C 2.342928880 -2.599641490 0.594619140
C 3.196370790 -1.424992360 0.594615820
C -0.367473730 -3.480360060 0.594643240

```

```

C -1.748289970 -3.031668120 0.594639390
C -2.806095680 1.174625400 1.829630330
C -1.984252110 2.305673080 1.829658650
C 0.250070520 3.031623110 1.829683690
C 1.579640820 2.599604780 1.829684760
C 2.960502730 0.699010950 1.829681940
C 2.960502730 -0.699010950 1.829681940
C 1.579640820 -2.599604780 1.829684760
C 0.250070520 -3.031623110 1.829683690
C -1.984252110 -2.305673080 1.829658650
C -2.806095680 -1.174625400 1.829630330
C -0.749180830 -2.305670960 2.593036450
C -2.424309060 0.000000000 2.593112650
C -0.749180830 2.305670960 2.593036450
C 1.961280580 1.424973050 2.593019090
C 1.961280580 -1.424973050 2.593019090
C 0.999173400 -0.725953290 3.327998740
C -0.381720360 -1.174635850 3.328062410
C -1.235039200 0.000000000 3.328049500
C -0.381720360 1.174635850 3.328062410
C 0.999173400 0.725953290 3.327998740

```

———— C<sub>60</sub>: PBE+TS ————

$d_{(5/6)} = 1.45154(5)$  Å and  $d_{(6/6)} = 1.39787(3)$  Å

```

C 1.234717798 0.000000000 -3.327366084
C 0.381626194 1.174329066 -3.327380309
C -0.998904919 0.725762062 -3.327306897
C -0.998904919 -0.725762062 -3.327306897
C -1.960893306 1.424693070 -2.592419422
C 0.749040410 2.305223054 -2.592438375
C 0.381626194 -1.174329066 -3.327380309
C 2.423840919 0.000000000 -2.592521182
C 0.749040410 -2.305223054 -2.592438375
C -1.960893306 -1.424693070 -2.592419422
C -2.959854115 0.698924266 -1.829281419
C -1.579356124 2.599018222 -1.829285313
C -2.959854115 -0.698924266 -1.829281419
C -1.579356124 -2.599018222 -1.829285313
C -0.249954109 -3.030983127 -1.829285394
C 1.983783739 -2.305224907 -1.829255005
C 2.805531341 -1.174315234 -1.829229362
C 2.805531341 1.174315234 -1.829229362
C 1.983783739 2.305224907 -1.829255005
C -0.249954109 3.030983127 -1.829285394
C -3.195658501 1.424717613 -0.594541133
C -2.342438784 2.599059755 -0.594543034
C 1.747873934 3.031033997 -0.594565624
C 0.367423589 3.479615852 -0.594572353
C 3.422718412 -0.725742269 -0.594533330
C 3.422718412 0.725742269 -0.594533330
C 1.747873934 -3.031033997 -0.594565624
C 0.367423589 -3.479615852 -0.594572353
C -2.342438784 -2.599059755 -0.594543034
C -3.195658501 -1.424717613 -0.594541133
C -3.422718412 -0.725742269 0.594533330
C -3.422718412 0.725742269 0.594533330

```

```

C -1.747873934  3.031033997  0.594565624
C -0.367423589  3.479615852  0.594572353
C  3.195658501  1.424717613  0.594541133
C  2.342438784  2.599059755  0.594543034
C  2.342438784 -2.599059755  0.594543034
C  3.195658501 -1.424717613  0.594541133
C -0.367423589 -3.479615852  0.594572353
C -1.747873934 -3.031033997  0.594565624
C -2.805531341  1.174315234  1.829229362
C -1.983783739  2.305224907  1.829255005
C  0.249954109  3.030983127  1.829285394
C  1.579356124  2.599018222  1.829285313
C  2.959854115  0.698924266  1.829281419
C  2.959854115 -0.698924266  1.829281419
C  1.579356124 -2.599018222  1.829285313
C  0.249954109 -3.030983127  1.829285394
C -1.983783739 -2.305224907  1.829255005
C -2.805531341 -1.174315234  1.829229362
C -0.749040410 -2.305223054  2.592438375
C -2.423840919  0.000000000  2.592521182
C -0.749040410  2.305223054  2.592438375
C  1.960893306  1.424693070  2.592419422
C  1.960893306 -1.424693070  2.592419422
C  0.998904919 -0.725762062  3.327306897
C -0.381626194 -1.174329066  3.327380309
C -1.234717798  0.000000000  3.327366084
C -0.381626194  1.174329066  3.327380309
C  0.998904919  0.725762062  3.327306897

```

———— C<sub>60</sub>: PBE+D3 —————

$d_{(5/6)} = 1.45370(18) \text{ \AA}$  and  $d_{(6/6)} = 1.39866(15) \text{ \AA}$

```

C  1.237215971  0.000000012 -3.332816805
C  0.382467861  1.176112514 -3.331723385
C -0.999984683  0.726806323 -3.331486131
C -0.999984674 -0.726806240 -3.331486046
C -1.962324574  1.425714055 -2.595146142
C  0.749902109  2.307384382 -2.595870510
C  0.382467830 -1.176112452 -3.331723305
C  2.426571489  0.000000029 -2.596151550
C  0.749902054 -2.307384333 -2.595870442
C -1.962324646 -1.425714042 -2.595146175
C -2.963513180  0.699252481 -1.831500063
C -1.580063488  2.601205672 -1.830664749
C -2.963513248 -0.699252523 -1.831500067
C -1.580063523 -2.601205609 -1.830664699
C -0.250181343 -3.033920742 -1.831290662
C  1.986150970 -2.307782371 -1.831557983
C  2.808254042 -1.176285191 -1.831435429
C  2.808254138  1.176285302 -1.831435529
C  1.986151044  2.307782464 -1.831558055
C -0.250181293  3.033920787 -1.831290729
C -3.199664251  1.426194389 -0.594647038
C -2.345470691  2.602430448 -0.594583944
C  1.750731946  3.035095249 -0.595202218
C  0.367788604  3.483547707 -0.594739085

```

```

C  3.426501728 -0.726877536 -0.595031243
C  3.426501738  0.726877608 -0.595031284
C  1.750731916 -3.035095207 -0.595202174
C  0.367788574 -3.483547707 -0.594739052
C -2.345470766 -2.602430494 -0.594583922
C -3.199664426 -1.426194474 -0.594647050
C -3.426501857 -0.726877591  0.595031206
C -3.426501781  0.726877548  0.595031193
C -1.750731843  3.035095042  0.595202205
C -0.367788566  3.483547736  0.594739131
C  3.199664232  1.426194474  0.594646920
C  2.345470731  2.602430593  0.594583939
C  2.345470684 -2.602430497  0.594583986
C  3.199664245 -1.426194428  0.594647000
C -0.367788585 -3.483547747  0.594739175
C -1.750731887 -3.035095127  0.595202240
C -2.808254120  1.176285236  1.831435438
C -1.986150915  2.307782311  1.831558019
C  0.250181351  3.033920881  1.831290799
C  1.580063496  2.601205656  1.830664733
C  2.963513118  0.699252491  1.831499906
C  2.963513165 -0.699252472  1.831499967
C  1.580063465 -2.601205648  1.830664788
C  0.250181307 -3.033920939  1.831290885
C -1.986150978 -2.307782399  1.831558051
C -2.808254107 -1.176285263  1.831435433
C -0.749902105 -2.307384485  2.595870644
C -2.426571406 -0.000000021  2.596151414
C -0.749902035  2.307384398  2.595870571
C  1.962324579  1.425714002  2.595146080
C  1.962324633 -1.425714036  2.595146154
C  0.999984710 -0.726806313  3.331486145
C -0.382467806 -1.176112540  3.331723396
C -1.237215871 -0.000000032  3.332816620
C -0.382467783  1.176112448  3.331723344
C  0.999984698  0.726806220  3.331486087

```

### 11.3.3 C<sub>60</sub>@C<sub>60</sub>H<sub>28</sub> *host-guest complex*

———— C<sub>60</sub>@C<sub>60</sub>H<sub>28</sub>: PBE+MBD@rsSCS ————  
 $R_p = 12.992 \text{ \AA}$  and  $R_t = 6.303 \text{ \AA}$  and  $R_c = 8.312 \text{ \AA}$

```

C  2.338383408 -1.383389254 -6.288730846
C  1.501591343 -0.704799575 -5.386818344
C  1.501591343  0.704799575 -5.386818344
C  2.338383408  1.383389254 -6.288730846
C  3.151468141  0.697826925 -7.187705785
C  3.151468141 -0.697826925 -7.187705785
C  0.707506472  1.527672493 -4.444879922
C  1.379574425  2.450629969 -3.643869106
C  0.725969703  3.401383740 -2.847342484
C -0.725969703  3.401383740 -2.847342484
C -1.379574425  2.450629969 -3.643869106
C -0.707506472  1.527672493 -4.444879922
C  1.476001750  4.329677454 -1.998985985
C  0.713591639  5.319733952 -1.410584580
C -0.713591639  5.319733952 -1.410584580
C -1.476001750  4.329677454 -1.998985985

```

```
C -1.146746736 6.051265997 -0.280615553
C 0.000000000 6.496219649 0.419898924
C 1.146746736 6.051265997 -0.280615553
C 0.000000000 6.742233697 1.786504257
C -1.308411323 6.716412589 2.398219929
C -2.438111737 6.287656961 1.708485828
C -2.372833304 5.835668507 0.338332754
C -3.254992680 4.959161346 -0.387390759
C -2.824323261 4.238227191 -1.499770383
C 1.308411323 6.716412589 2.398219929
C 2.438111737 6.287656961 1.708485828
C 2.372833304 5.835668507 0.338332754
C 3.254992680 4.959161346 -0.387390759
C 2.824323261 4.238227191 -1.499770383
C -1.501591343 0.704799575 -5.386818344
C -1.501591343 -0.704799575 -5.386818344
C -2.338383408 -1.383389254 -6.288730846
C -3.151468141 -0.697826925 -7.187705785
C -3.151468141 0.697826925 -7.187705785
C -2.338383408 1.383389254 -6.288730846
C 0.707506472 -1.527672493 -4.444879922
C 1.379574425 -2.450629969 -3.643869106
C 0.725969703 -3.401383740 -2.847342484
C -0.725969703 -3.401383740 -2.847342484
C -1.379574425 -2.450629969 -3.643869106
C -0.707506472 -1.527672493 -4.444879922
C -1.476001750 -4.329677454 -1.998985985
C -0.713591639 -5.319733952 -1.410584580
C 0.713591639 -5.319733952 -1.410584580
C 1.476001750 -4.329677454 -1.998985985
C 1.146746736 -6.051265997 -0.280615553
C 0.000000000 -6.496219649 0.419898924
C -1.146746736 -6.051265997 -0.280615553
C -2.824323261 -4.238227191 -1.499770383
C -3.254992680 -4.959161346 -0.387390759
C -2.372833304 -5.835668507 0.338332754
C -2.438111737 -6.287656961 1.708485828
C -1.308411323 -6.716412589 2.398219929
C 0.000000000 -6.742233697 1.786504257
C 2.824323261 -4.238227191 -1.499770383
C 3.254992680 -4.959161346 -0.387390759
C 2.372833304 -5.835668507 0.338332754
C 2.438111737 -6.287656961 1.708485828
C 1.308411323 -6.716412589 2.398219929
H -4.258049340 4.764752792 -0.001747702
H -3.514509548 3.510224182 -1.930114323
H 3.514509548 3.510224182 -1.930114323
H 4.258049340 4.764752792 -0.001747702
H 3.377313210 6.197768824 2.258535072
H 1.406163322 6.944636565 3.461754345
H -1.406163322 6.944636565 3.461754345
H -3.377313210 6.197768824 2.258535072
H -3.377313210 -6.197768824 2.258535072
H -1.406163322 -6.944636565 3.461754345
H 1.406163322 -6.944636565 3.461754345
H 3.377313210 -6.197768824 2.258535072
```

```
H 4.258049340 -4.764752792 -0.001747702
H 3.514509548 -3.510224182 -1.930114323
H -3.514509548 -3.510224182 -1.930114323
H -4.258049340 -4.764752792 -0.001747702
H 2.470863741 2.449708953 -3.668384654
H -2.470863741 2.449708953 -3.668384654
H 2.470863741 -2.449708953 -3.668384654
H -2.470863741 -2.449708953 -3.668384654
H -2.332778622 2.474347134 -6.282514030
H -3.779786094 1.251037095 -7.885976941
H -3.779786094 -1.251037095 -7.885976941
H -2.332778622 -2.474347134 -6.282514030
H 2.332778622 2.474347134 -6.282514030
H 3.779786094 1.251037095 -7.885976941
H 3.779786094 -1.251037095 -7.885976941
H 2.332778622 -2.474347134 -6.282514030
C -3.481309121 0.699185052 2.923857466
C -3.033088463 1.425621730 1.749002883
C -2.305925899 2.598243914 2.199335999
C -2.306682102 2.600068780 3.650879184
C -1.172408747 3.023548407 1.503284193
C -2.600230152 0.726057521 0.616890507
C -3.032295246 1.425139389 4.099412087
C -3.481309121 -0.699185052 2.923857466
C -2.600402166 0.726057240 5.230953919
C -1.175124375 3.032565327 4.350794535
C 0.000000000 3.471726208 2.228248935
C -0.725076276 2.300011840 0.329871587
C 0.000000000 3.478558087 3.624793622
C -0.726347768 2.305961555 5.524970209
C -1.425517852 1.174690324 5.957047505
C -2.600402166 -0.726057240 5.230953919
C -3.032295246 -1.425139389 4.099412087
C -3.033088463 -1.425621730 1.749002883
C -2.600230152 -0.726057521 0.616890507
C -1.424246941 1.172755520 -0.107992779
C 1.172408747 3.023548407 1.503284193
C 0.725076276 2.300011840 0.329871587
C -1.424246941 -1.172755520 -0.107992779
C -0.699680148 0.000000000 -0.561542523
C -2.306682102 -2.600068780 3.650879184
C -2.305925899 -2.598243914 2.199335999
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C -0.699135257 0.000000000 6.405689101
C 0.726347768 2.305961555 5.524970209
C 1.175124375 3.032565327 4.350794535
C 2.306682102 2.600068780 3.650879184
C 2.305925899 2.598243914 2.199335999
C 1.424246941 1.172755520 -0.107992779
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C -0.726347768 -2.305961555 5.524970209
C -1.175124375 -3.032565327 4.350794535
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C 2.600230152 0.726057521 0.616890507
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C 0.725076276 -2.300011840 0.329871587
C 0.000000000 -3.471726208 2.228248935
C 0.000000000 -3.478558087 3.624793622
C 0.726347768 -2.305961555 5.524970209
C 1.425517852 -1.174690324 5.957047505
C 2.600402166 0.726057240 5.230953919
C 3.032295246 1.425139389 4.099412087
C 2.600402166 -0.726057240 5.230953919
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C 2.600230152 -0.726057521 0.616890507
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C 1.175124375 -3.032565327 4.350794535
C 2.306682102 -2.600068780 3.650879184
C 3.032295246 -1.425139389 4.099412087
C 3.481309121 -0.699185052 2.923857466
C 3.033088463 -1.425621730 1.749002883
C 2.305925899 -2.598243914 2.199335999

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———— C<sub>60</sub>@C<sub>60</sub>H<sub>28</sub>: PBE+TS ————  
 $R_p = 12.974 \text{ \AA}$  and  $R_f = 6.337 \text{ \AA}$  and  $R_c = 8.361 \text{ \AA}$

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C 1.508562066 0.706284635 -5.422405593
C 2.347980203 1.383260939 -6.325067826
C 3.168401660 0.697475927 -7.217746051
C 3.168401660 -0.697475927 -7.217746051
C 0.708422819 1.531157546 -4.477051549
C 1.378883358 2.442635236 -3.658080437
C 0.725728980 3.391290791 -2.854828369
C -0.725728980 3.391290791 -2.854828369
C -1.378883358 2.442635236 -3.658080437
C -0.708422819 1.531157546 -4.477051549
C 1.476835474 4.319146771 -1.997765675
C 0.713463824 5.306420554 -1.405849847
C -0.713463824 5.306420554 -1.405849847
C -1.476835474 4.319146771 -1.997765675
C -1.146251715 6.040241693 -0.276514385
C 0.000000000 6.486996477 0.423680202
C 1.146251715 6.040241693 -0.276514385
C 0.000000000 6.741281668 1.788543974
C -1.309376600 6.718842601 2.399753528
C -2.438535872 6.288924843 1.710575494
C -2.373002646 5.831705321 0.341232660
C -3.255547941 4.955884689 -0.385280410
C -2.826149849 4.232692933 -1.497078277
C 1.309376600 6.718842601 2.399753528
C 2.438535872 6.288924843 1.710575494
C 2.373002646 5.831705321 0.341232660
C 3.255547941 4.955884689 -0.385280410
C 2.826149849 4.232692933 -1.497078277
C -1.508562066 0.706284635 -5.422405593
C -1.508562066 -0.706284635 -5.422405593
C -2.347980203 -1.383260939 -6.325067826

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C -3.168401660 0.697475927 -7.217746051
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C 1.378883358 -2.442635236 -3.658080437
C 0.725728980 -3.391290791 -2.854828369
C -0.725728980 -3.391290791 -2.854828369
C -1.378883358 -2.442635236 -3.658080437
C -0.708422819 -1.531157546 -4.477051549
C -1.476835474 -4.319146771 -1.997765675
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C 0.713463824 -5.306420554 -1.405849847
C 1.476835474 -4.319146771 -1.997765675
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C -2.373002646 -5.831705321 0.341232660
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C 2.373002646 -5.831705321 0.341232660
C 2.438535872 -6.288924843 1.710575494
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H 3.519610833 3.509292945 -1.926842174
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H 2.342391263 2.473533528 -6.324312790
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H 3.801153795 -1.250517839 -7.911715517
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C -1.171454401 3.020211271 1.517422413
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C -3.480927818 -0.698845509 2.937087789
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C -0.724298663 2.297273778 0.345665888
C 0.000000000 3.475248527 3.636831662
C -0.725907506 2.303878784 5.536024186
C -1.425172024 1.173744266 5.968274590
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C -3.031803808 -1.424150096 4.111841435
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C -2.599155162 -0.725633621 0.631632167
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C 1.171454401 3.020211271 1.517422413
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C -1.423804183 -1.171790305 -0.092627368
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C -2.305696011 -2.597879330 3.663180216
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C 1.174456715 3.029488584 4.362182102
C 2.305696011 2.597879330 3.663180216
C 2.305098596 2.596248174 2.212625459
C 1.423804183 1.171790305 -0.092627368
C 0.699169332 0.000000000 -0.545697760
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C -1.174456715 -3.029488584 4.362182102
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C 1.425172024 1.173744266 5.968274590
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C 2.599155162 0.725633621 0.631632167
C 1.423804183 -1.171790305 -0.092627368
C 0.724298663 -2.297273778 0.345665888
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C 0.000000000 -3.475248527 3.636831662
C 0.725907506 -2.303878784 5.536024186
C 1.425172024 -1.173744266 5.968274590
C 2.599860187 0.725579394 5.242914314
C 3.031803808 1.424150096 4.111841435
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C 3.480927818 0.698845509 2.937087789
C 2.599155162 -0.725633621 0.631632167
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C 1.174456715 -3.029488584 4.362182102
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C 3.031803808 -1.424150096 4.111841435
```

C 3.480927818 -0.698845509 2.937087789  
C 3.032171457 -1.424676614 1.762795423  
C 2.305098596 -2.596248174 2.212625459

————— C<sub>60</sub>@C<sub>60</sub>H<sub>28</sub>: PBE+D3 —————  
R<sub>p</sub> = 12.987 Å and R<sub>t</sub> = 6.286 Å and R<sub>c</sub> = 8.454 Å

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C 1.502172280 -0.705693118 -5.465750698  
C 1.501946858 0.705732133 -5.465928705  
C 2.333633597 1.384777177 -6.373611760  
C 3.143028176 0.697965977 -7.276867514  
C 3.143478737 -0.697877300 -7.276485407  
C 0.708225753 1.522962555 -4.510980038  
C 1.381273473 2.428188481 -3.687290238  
C 0.726129879 3.367746180 -2.875351939  
C -0.726113753 3.367728826 -2.875400529  
C -1.381187191 2.428195708 -3.687416984  
C -0.708069565 1.522953916 -4.511023060  
C 1.476860625 4.296654276 -2.019650242  
C 0.715583993 5.296645354 -1.444603900  
C -0.715699194 5.296604027 -1.444624645  
C -1.476911721 4.296593181 -2.019717372  
C -1.149465957 6.038688219 -0.317607996  
C -0.000122882 6.493652244 0.379660368  
C 1.149270383 6.038758551 -0.317572712  
C -0.000154989 6.753926962 1.744514180  
C -1.309741928 6.734149816 2.356636974  
C -2.438355399 6.293771482 1.672813157  
C -2.372963681 5.823249026 0.307782437  
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C 2.438068051 6.293882659 1.672902684  
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C -3.143153062 0.697875019 -7.276636439  
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C 0.708310840 -1.522961286 -4.510940921  
C 1.381312305 -2.428203421 -3.687245524  
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C -0.726100004 -3.367713069 -2.875387663  
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C -1.476925454 -4.296576762 -2.019718357  
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C -0.000217678 -6.753923508 1.744524397
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C 3.251706349 -4.929934294 -0.402041657
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C 2.438010158 -6.293894746 1.672933096
C 1.309339182 -6.734201177 2.356709913
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H 3.506886878 3.456542763 -1.923846772
H 4.250850875 4.730422334 -0.006284875
H 3.378578752 6.207451274 2.224128287
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C -0.726583244 2.301750260 0.388676391
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C -2.603083088 -0.726997588 5.295564199
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C -0.700275048 0.000022025 -0.499907570
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C -2.307748515 -2.601373765 2.261760228
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## References

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