SUPPORTING INFORMATION

Redox-Dependent Structural Transformations of the [4Fe-3S] Proximal Cluster in O_2-Tolerant Membrane-Bound [NiFe]-Hydrogenase: a DFT Study

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1. Cα–Cα Distances

In Table S1 below, we used the available MBH X-ray structures[1,2] from *Ralstonia eutropha* (*Re*) and *Hydrogenovibrio marinus* (*Hm*) organisms to map the 9·(9-1)/2 = 36 C_α–C_α distances for nine amino-acid residues present in our model. Comparison of the RED structures from *Re* and *Hm* shows that C_α–C_α distances vary mostly within 0.1 Å between the two analyzed MBH species. Out of these C_α–C_α distances, only three pairs involving C_α of Glu76 (*Re* numbering) deviate by more than 0.1 Å, but all by less than 0.2 Å. The analysis of the reduced (RED) vs superoxidized (S-OX) *Hm* structures indicates that 16 (out of 36) α-carbon atom pairs shift by more than 0.1 Å relative to each other during the two-electron redox process, and 6 of them involve C_α of Cys20. For this RED vs S-OX structural comparison, only 3 C_α–C_α distances change by more than 0.2 Å, and 2 of them involve C_α of Cys20. The latter C_α^{Cys20}–C_α^{Glu76} and C_α^{Cys20}–C_α^{Cys115} distances provide the largest ~0.3 Å C_α–C_α shifts within the considered protein fragment. The above analysis justifies fixations of the C_α atoms during structure optimization of our DFT models (which otherwise lack an actual protein environment), however leaving C_α of Cys20 free to move. This analysis also provides a quantitative measure on how the polypeptide framework around the proximal cluster responds onto Glu76 mobility and coordination of the Cys20 backbone amide to the 'special' Fe4 iron during the redox-dependent structural rearrangement of the [4Fe-3S] core.

Table S1. C_α–C_α Internuclear Distance Chart (Å) from the *Re* and *Hm* MBH X-ray Structures for Nine Amino-Acid Residues Relevant to the Present Modeling of the Proximal Cluster[a]

Residue[b]	**Cys19 (25)**	**Cys20 (26)**	**Ser21 (27)**	**Glu76 (82)**	**Cys115 (121)**	**Cys120 (126)**	**Cys149 (158)**	**His229 (230)**
Cys17 (23)	5.57/5.59 5.56	8.04/**8.15** 8.00	9.26/**9.12** 9.17	9.05/8.98 9.02	9.09/8.99 9.07	10.16/10.08 10.26	9.69/**9.51** 9.76	10.47/10.49 10.46
Cys19 (25)		3.82/3.77 3.79	5.60/**5.42** 5.58	8.87/8.93 8.94	9.97/**10.10** 9.94	11.61/11.68 11.66	7.12/**7.01** 7.13	7.66/7.71 7.61
Cys20 (26)			3.84/3.80 3.81	6.60/**6.94** **6.73**	9.10/**9.42** 9.10	11.88/**12.02** 11.93	7.32/**7.12** 7.30	10.43/**10.31** 10.36
Ser21 (27)				7.62/**7.75** 7.61	12.14/**12.21** 12.08	15.25/15.19 15.26	11.05/**10.81** 11.02	12.60/12.50 12.52
Glu76 (82)					6.84/6.82 6.90	11.10/11.01 **11.23**	10.91/**10.80** **11.07**	15.88/15.92 15.94
Cys115 (121)						4.46/**4.39** 4.51	7.74/7.83 7.81	14.22/14.28 14.21
Cys120 (126)							7.66/7.73 7.76	13.45/13.45 13.52
Cys149 (158)								7.73/7.67 7.74

[a] The distances in the table cells are organized as follows: 1st line – data from RED/S-OX *Hm* structures,[2] PDBs 3AYX (1.18 Å resolution) / 3AYY (1.32 Å resolution), respectively; 2nd line – data from RED *Re* structure,[1] PDB 3RGW (1.50 Å resolution). In **black/red** – RED *Re* and S-OX *Hm* C_α–C_α distances which differ by **>0.1**/**>0.2** Å from the corresponding RED *Hm* C_α–C_α distances, respectively.

[b] The numbering of amino-acid residues corresponds to MBH from the *Re* organism. *Hm* MBH residues numbering are given in parentheses.

2. Reduced Proximal Cluster: PBE vs B3LYP Structures

In Figure S1 below, the proximal cluster from the reduced *Re* MBH structure[1] (PDB 3RGW, 1.50 Å resolution) is compared to our RED_D^{3+} local minima structures, optimized using the PBE and B3LYP functionals. While both the PBE and B3LYP optimizations qualitatively agree with the X-ray structure, there is a noticeable expansion of the $[4Fe\text{-}3S]^{3+}$ core when the B3LYP functional is applied. A comparison of the Fe–Fe and bonding Fe–S internuclear distances in Table S2 further demonstrates that PBE overestimates these distances by 0.1 Å at most (for the Fe4–S3 distance). In contrast, the overestimation of the iron-sulfur core distances by B3LYP is typically more significant, and reaches 0.4 Å (for the Fe1–Fe2 distance).

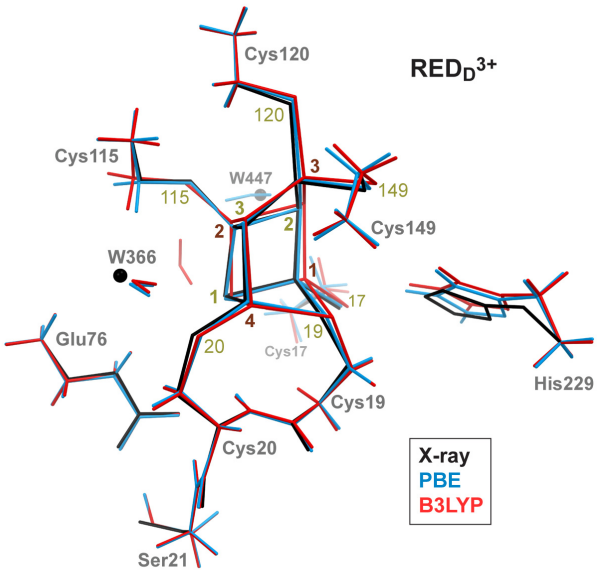

Figure S1. Overlay of the RED_D^{3+} model optimized using the PBE (blue) and B3LYP (red) functionals with the reference *Re* MBH X-ray structure (black). The Fe/S numbers are given in brown/yellow, respectively. All models are shown in 0.05 Å radius tubes.

Table S2. Fe–Fe and Bonding Fe–S Internuclear Distances in the Reduced Structure of the MBH Proximal Cluster from X-ray Data Analysis and Geometry Optimization Using the PBE and B3LYP Functionals

	Internuclear Distance (Å)	
	X-ray (PDB 3RGW[1])	**PBE / B3LYP (RED_D^{3+} Model)**
	Fe – Fe	
Fe1 – Fe2	2.59	2.63 / 3.00
Fe1 – Fe3	3.52	3.59 / 3.70
Fe1 – Fe4	2.67	2.73 / 3.00
Fe2 – Fe3	2.71	2.76 / 2.95
Fe2 – Fe4	2.84	2.76 / 3.18
Fe3 – Fe4	3.96	4.00 / 4.19
	Fe – S (inorganic)	
Fe1 – S1	2.29	2.37 / 2.42
Fe1 – S2	2.27	2.34 / 2.43
Fe2 – S1	2.28	2.31 / 2.45
Fe2 – S2	2.28	2.36 / 2.51
Fe2 – S3	2.27	2.25 / 2.36
Fe3 – S2	2.29	2.25 / 2.28
Fe3 – S3	2.29	2.37 / 2.35
Fe4 – S1	2.28	2.30 / 2.37
Fe4 – S3	2.32	2.42 / 2.65
	Fe – S (Cysteines) [a]	
Fe1 – S17	2.30	2.30 / 2.38
Fe1 – S19	2.31	2.34 / 2.48
Fe2 – S115	2.27	2.33 / 2.40
Fe3 – S120	2.34	2.39 / 2.42
Fe3 – S149	2.30	2.32 / 2.35
Fe4 – S19	2.31	2.38 / 2.48
Fe3 – S20	2.30	2.32 / 2.40

[a] Here, the sulfurs numbering corresponds to the *Re* MBH amino acid sequence; see also Figure S1.

3. Model Structures at the Three Oxidation Levels

In Figure S2 below, the four models RED_D, RED_P, TS, and $S\text{-}OX_{D\text{-}H}$ are superimposed in their PBE-optimized structures at the reduced, oxidized, and superoxidized levels (see Table 1 of the main text for the internuclear distances). The figure shows that the optimized structures are qualitatively similar regardless of the oxidation level. The major redox-dependent change is observed for $S\text{-}OX_{D\text{-}H}$, where the Glu76 carboxylate orientation in the superoxidized $S\text{-}OX_{D\text{-}H}^{5+}$ state is noticeably different from that in the reduced $S\text{-}OX_{D\text{-}H}^{3+}$ and oxidized $S\text{-}OX_{D\text{-}H}^{4+}$ states.

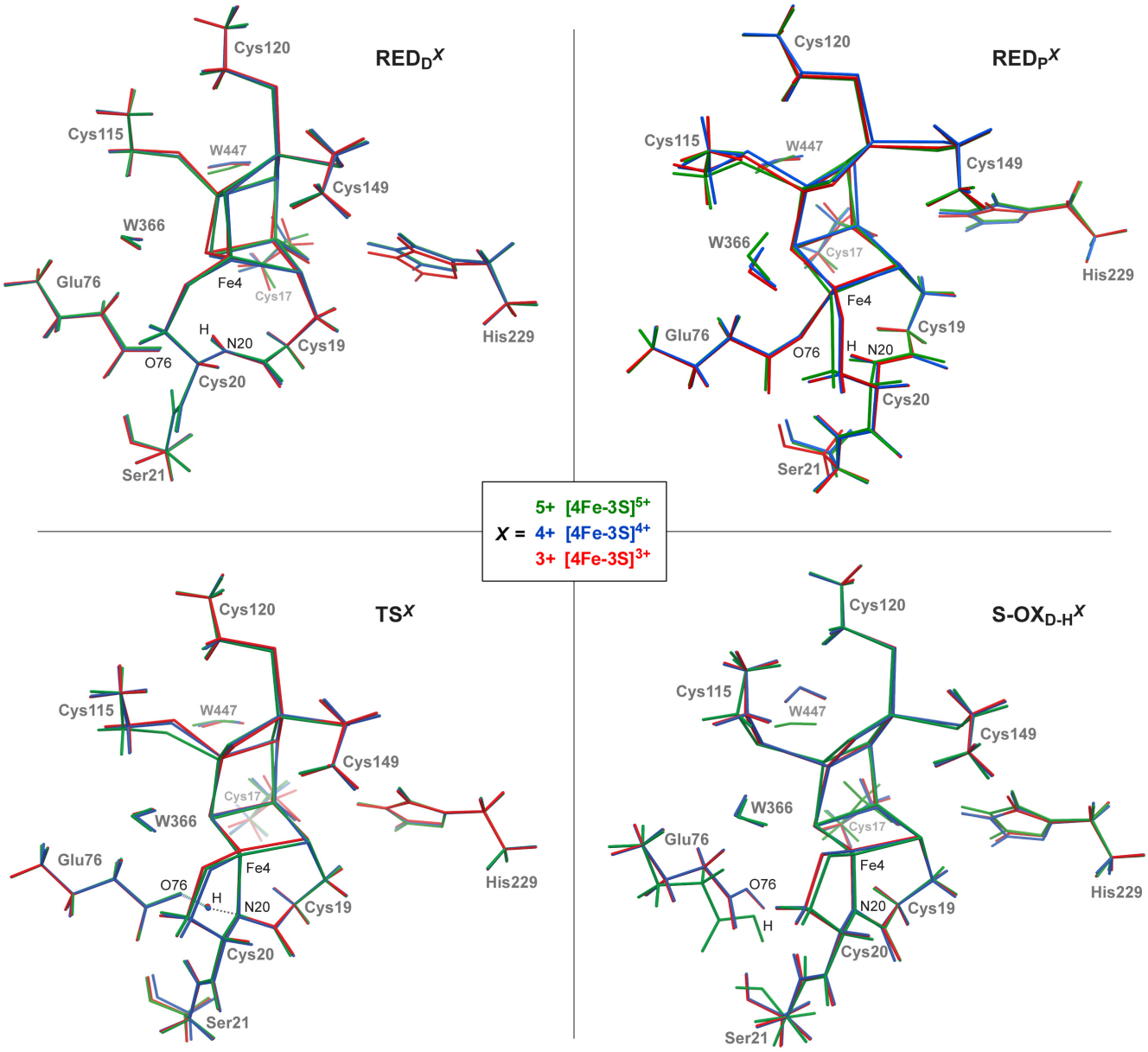

Figure S2. Models RED_D, RED_P, TS, and $S\text{-}OX_{D\text{-}H}$ optimized using the PBE functional at the three oxidation levels of the proximal cluster core: $[4Fe\text{-}3S]^{3+}$ (red), $[4Fe\text{-}3S]^{4+}$ (blue), and $[4Fe\text{-}3S]^{5+}$ (green). All models are shown in 0.05 Å radius tubes.

4. Calculation of the Reorganization Energies

The calculation of the self-exchange inner-sphere contribution λ_i to the reorganization energy of the MBH proximal cluster was done in a manner following Ryde et al:[3,4]

$$\lambda_i = \lambda_{ox} + \lambda_{red}$$
$$\lambda_{ox} = E(\mathrm{Ox}^{\mathrm{Ox}}) - E(\mathrm{Red}^{\mathrm{Ox}})$$
$$\lambda_{red} = E(\mathrm{Red}^{\mathrm{Red}}) - E(\mathrm{Ox}^{\mathrm{Red}})$$

where λ_{ox}, the reorganization energy during oxidation, is the difference between the energies of the oxidized complex in its equilibrium geometry ($\mathrm{Ox}^{\mathrm{Ox}}$) and oxidized complex at the equilibrium structure of the reduced complex ($\mathrm{Red}^{\mathrm{Ox}}$). Similarly, the λ_{red} reorganization energy during reduction is the difference between the energies of the reduced complex in its equilibrium geometry ($\mathrm{Red}^{\mathrm{Red}}$) and reduced complex at the equilibrium structure of the oxidized complex ($\mathrm{Ox}^{\mathrm{Red}}$). For the calculation of the reorganization energies $\lambda_i^{3+\rightarrow4+/4+\rightarrow5+}$ corresponding to one-electron oxidations (see the main text), $\mathrm{Red}^{\mathrm{Red}}$ = $\mathrm{RED_D}^{3+/4+}$ and $\mathrm{Ox}^{\mathrm{Ox}}$ = $\mathrm{RED_D}^{4+/5+}$, respectively. For the two-electron process ($\lambda_i^{3+\rightarrow5+}$), $\mathrm{Red}^{\mathrm{Red}}$ = $\mathrm{RED_D}^{3+}$ and $\mathrm{Ox}^{\mathrm{Ox}}$ = $\mathrm{RED_D}^{5+}$. The λ_i values were obtained at PBE level, resulting in $\lambda_i^{3+\rightarrow4+}$ = 5.3 kcal/mol (= 22.2 kJ/mol), $\lambda_i^{4+\rightarrow5+}$ = 4.6 kcal/mol (= 19.3 kJ/mol), and $\lambda_i^{3+\rightarrow5+}$ = 13.2 kcal/mol (= 55.2 kJ/mol).

5. Evaluation of D3 Dispersion Corrections

Here we provide some more details on the effect of DFT-D3 dispersion corrections[5,6] on energies and structures. Figure S3 gives the mechanistic energy profile analogous to Figure 8 in the main text, but with D3 dispersion corrections added to the PBE and B3LYP energies, respectively, in single-point mode. The effects of the D3 corrections are further analyzed in Table S3. As pointed out in the main text, the main effect pertains to the position of Glu76 relative to the [4Fe-3S] cluster core (distal/proximal for the model names with D/P subscript, respectively). For example, in both $\mathrm{RED_{D/P}}$ and $\mathrm{S\text{-}OX_{D/P}}$ alternatives (at all three $[\mathrm{4Fe\text{-}3S}]^{3+/4+/5+}$ oxidation levels and for both PBE and B3LYP functionals), D3 stabilizes the structures where Fe4-O76 bonding is present ($\mathrm{RED_P}$ and $\mathrm{S\text{-}OX_P}$) by 0.4-3.8 kcal/mol. For the $\mathrm{S\text{-}OX_{D\text{-}H}}$ structure where the Glu76 side chain is most distant from the [4Fe-3S] core (see the main text Figure 5 and Table 1 for the characteristic Fe4-O76 distance), the D3 correction is 0.6-4.2 kcal/mol positive relative to $\mathrm{RED_D}$. The extra relative destabilization of $\mathrm{S\text{-}OX_{D\text{-}H}}$ probably arises from a further opening of the cluster, associated with a loss of the Fe4-S3 bonding. The relative dispersion energy is negative for the TS transition state at the $[\mathrm{4Fe\text{-}3S}]^{5+}$ oxidation level, which leads to a somewhat lower activation barrier of the cluster transformation in the forward direction (cf. Figure S3 vs Figure 8). Both the stabilization of the TS and the destabilization of $\mathrm{S\text{-}OX_{D\text{-}H}}$ relative to $\mathrm{RED_P}$ provide an even more significant decrease of the activation barrier in the reverse direction at the $[\mathrm{4Fe\text{-}3S}]^{4+}$ level, and the back-transformation at the $[\mathrm{4Fe\text{-}3S}]^{3+}$ level becomes essentially barrier-free.

We furthermore evaluated structural effects of the D3 corrections for the superoxidized $[\mathrm{4Fe\text{-}3S}]^{5+}$ oxidation state by optimization of the relevant stationary points at the B3LYP-D3 level (together with the Poisson-Boltzman solvation model[7,8] as implemented in JAGUAR 7.8, using ε = 4.0 and the solvent probe radius 1.4 Å). Structural changes are marginal and are not discussed here in detail. Consequently, the effects on the energy profile remain minor (Table S4).

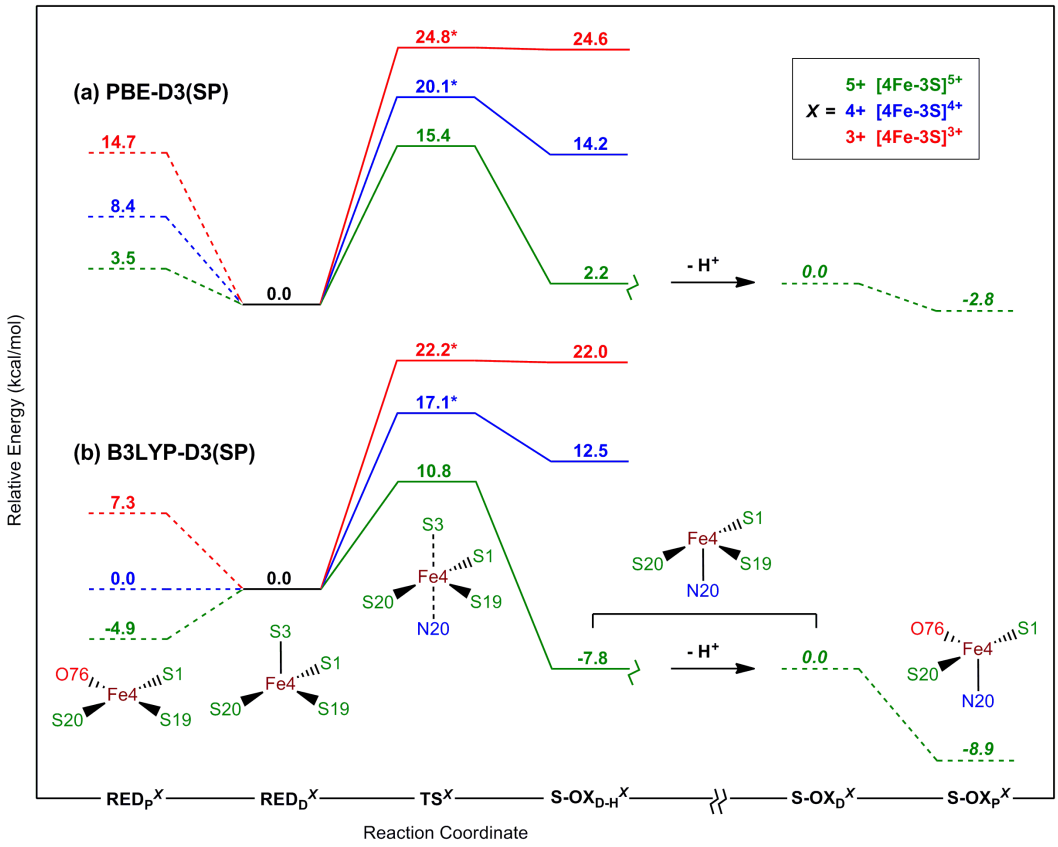

Figure S3. Relative energy profiles obtained for the MBH proximal cluster structural transformations at the superoxidized (green), oxidized (blue), and reduced (red) oxidation levels using (a) PBE and (b) B3LYP density functionals including single-point (SP) D3 dispersion corrections[5,6] (cf. Figure 8 in the main text for the corresponding profiles without D3 corrections). The 'special' Fe4 iron coordination sphere is schematically shown for every state. "-H^+" implies deprotonation of the Glu76 O76 oxygen atom in the S-$OX_{D\text{-}H}^{5+}$ state, and a discontinuity of the PES. The key transformation involving the TS transition state is given as solid line, and the rest of the relative energies are shown as dashed lines. The asterisks (*) denote approximate TS transition states as described in the main text.

Table S3. Relative Single-Point D3 Dispersion Energy Corrections for the Stationary Points at the Three Oxidation Levels[a]

	Relative PBE-D3(SP) / B3LYP-D3(SP) Energies (kcal/mol)					
	RED_P^X	RED_D^X	TS^X	S-$OX_{D\text{-}H}^X$	S-OX_D^X	S-OX_P^X
X **= 3+, [4Fe-3S]$^{3+}$**	-0.4 / -0.6	≡ 0.0 / 0.0	-1.0 / -0.1	1.5 / 4.2	≡ 0.0 / 0.0	- / -
X **= 4+, [4Fe-3S]$^{4+}$**	-1.4 / -0.5	≡ 0.0 / 0.0	-1.6 / 0.2	0.6 / 3.1	≡ 0.0 / 0.0	- / -
X **= 5+, [4Fe-3S]$^{5+}$**	-1.7 / -1.5	≡ 0.0 / 0.0	-1.7 / -1.4	0.8 / 1.7	≡ 0.0 / 0.0	-1.2 / -3.8

[a] Relative to the PBE and B3LYP profiles, respectively, in Figure 8. RED_D and S-OX_D minima are selected as reference points similarly as in Figures 8 and S3. For the total relative energies, see Figure S3.

Table S4. Relative Energies for the B3LYP-D3 Optimized Stationary Points at the Superoxidized Level[a]

Relative B3LYP-D3 Energies / D3 Contribution (kcal/mol)					
RED_P^{5+}	RED_D^{5+}	TS^{5+}	S-$OX_{D\text{-}H}^{5+}$	S-OX_D^{5+}	S-OX_P^{5+}
-1.4 /-0.6	≡ 0.0 / 0.0	14.3 / -0.8	-9.1 / 2.2	≡ 0.0 / 0.0	-6.0 / -3.5

[a] RED_D and S-OX_D minima are selected as reference points similarly as in Figures 8 and S3. For the total relative energies, see Figure S3.

6. Influence of Broken-Symmetry State on Relative Energies

The relative PBE energies of the structure-optimized BS*ab* states (using the present BS notation) at the three relevant oxidation levels of the proximal cluster are summarized in Table S5. For the most relevant BS states BS12, BS13, and BS34 (cf. recent studies[9-11]) B3LYP energies are also included for the $[4Fe\text{-}3S]^{5+}$ superoxidized state. The BS energies are given for the RED_D and $S\text{-}OX_{D\text{-}H}$ models at all three oxidation levels, and also for the two $S\text{-}OX_{D/P}{}^{5+}$ models. The results suggest that the order of the BS states on the energy ladder is generally sensitive to the model, oxidation level, and functional used. At the same time, BS12 can be considered as approximate ground state for all the structures and all the oxidation levels. This holds within a 1.5 kcal/mol tolerance (see BS12 row in Table S5). Using a modified B3LYP functional with 5% exact exchange, BS12 was independently found to be the lowest energy BS state for the $PC3^-$ QM/MM model (related to $S\text{-}OX_P{}^{5+}$ here) by Volbeda et al,[9] and the 2nd lowest energy (1.4 kJ/mol = 0.3 kcal/mol above BS24) BS state for their $PC3^H$ model (related to $S\text{-}OX_{D\text{-}H}{}^{5+}$ here). In another recent DFT study by Pandelia et al,[11] BS12 produced low relative energies in the 0.0-1.7 kcal/mol range for the $[4Fe\text{-}3S]^{4+}$ oxidized models named Semiox1/Semired1_13 (related to $S\text{-}OX_{D\text{-}H}{}^{4+}$ BS12) and $[4Fe\text{-}3S]^{5+}$ superoxidized models Ox1/Ox2_13 (related to $S\text{-}OX_{D\text{-}H}{}^{5+}$/$S\text{-}OX_D{}^{5+}$ BS12), when the PBE functional was used. However, BS12 energies up to +17.7 kcal/mol were reported for their $[4Fe\text{-}3S]^{3+}$ reduced models Red1/Red2_13 (related to $RED_D{}^{3+}$ BS12). At the same time, their BS energies obtained using B3LYP were significantly different. Importantly, variations to the DFT methodology may lead to different spin delocalization patterns within a same BS state (for example, see PBE vs B3LYP results in Table S6). Therefore it cannot be excluded that the electronic structures for particular BS*ab* solutions received here are qualitatively different from those derived by others.[9-11]

Notably, our optimization of several BS states other than BS12 for the $S\text{-}OX_{D\text{-}H}{}^{3+/4+}$ models (cf. Table S5) led to 'closure' of the 'opened' S-OX conformation due to reformation of the Fe4-S3 bonding, and thus to a penta-coordinated 'special' Fe4 site. A qualitative structure dependence on BS configuration has been also reported by Pandelia et al:[11] for their Red2_24 model (related to $RED_D{}^{3+}$ BS34), optimization produced a 'tightly closed' cubane where Fe3-Fe4 is ~2.8 Å vs ~4.0 Å from the X-ray data (cf. Table S2), and coordination of Fe3 to the supernumerary cysteine Cys120 is lost. This contrasts strongly with the available experimental structure of the reduced cluster.

Table S5. Relative Energies of the Broken-Symmetry (BS) states for the RED_D and $S\text{-}OX_{D\text{-}H}$ Proximal Cluster Models at the Three Oxidation $[4Fe\text{-}3S]^{3+/4+/5+}$ Levels and for the $S\text{-}OX_{D/P}$ Models at the Superoxidized $[4Fe\text{-}3S]^{5+}$ Level using the PBE and B3LYP Density Functionals[a]

	PBE / B3LYP Relative Energies (kcal/mol)							
	$[4Fe\text{-}3S]^{3+}$ $S = 1/2$		$[4Fe\text{-}3S]^{4+}$ $S = 0$		$[4Fe\text{-}3S]^{5+}$ $S = 1/2$			
	$RED_D{}^{3+}$	$S\text{-}OX_{D\text{-}H}{}^{3+}$	$RED_D{}^{4+}$	$S\text{-}OX_{D\text{-}H}{}^{4+}$	$RED_D{}^{5+}$	$S\text{-}OX_{D\text{-}H}{}^{5+}$	$S\text{-}OX_D{}^{5+}$	$S\text{-}OX_P{}^{5+}$
BS12	1.5 / –	**0.0** / –	0.8 / –	**0.0** / –	**0.0** / 1.2	**0.0** / **0.0**	**0.0** / **0.0**	**0.0** / **0.0**
BS13	1.2 / –	6.2 / –	**0.0** / –	4.1 / –	6.1 / 2.6	0.2 / 0.7	1.9 / 0.8	4.8 / 0.8
BS14	**0.0** / –	8.8 / –	0.2 / –	6.2[c] / –	6.0 / –	9.8 / –	12.6 / –	10.1 / –
BS23	2.4 / –	10.8[c] / –	= BS14[b]		6.9 / –	9.9 / –	12.0 / –	10.8 / –
BS24	1.4 / –	4.0 / –	= BS13[b]		0.0 / –	0.6 / –	1.6 / –	3.1 / –
BS34	3.4 / –	3.9[c] / –	= BS12[b]		10.9 / **0.0**	1.5 / 8.1	1.3 / 6.8	12.7 / 7.7

[a] All BS states structures were optimized as detailed in the Computational Methods section of the main text. The relative energies are compared within the columns, where **0.0 (**kcal/mol) **marked in bold** designates the most stable BS state.
[b] For the $[4Fe\text{-}3S]^{4+}$ oxidized cluster, the energies of the BS23, BS24, and BS34 states are equal to those of BS14, BS13, and BS12, respectively, due to the $S = 0$ zero total spin.
[c] For these BS states, structure optimization led to reformation of the Fe4-S3 bonding.

Most of our calculations are thus based on the BS12 broken-symmetry state of the proximal cluster, as described above and in the main text. In view of the preference of other authors for the Fe spin configurations BS13[9,10] and BS34[11] for the product of the $[4Fe\text{-}3S]^{5+}$ superoxidized proximal cluster transformation (corresponding here to either S-$OX_{D\text{-}H}^{2+}$, S-OX_D^{2+}, or S-OX_P^{2+}), the BS13/34 stationary points at this oxidation level were optimized as well. Here, the B3LYP functional was used and the rest of the computational methods are as detailed in the main text. The relative BS12/BS13/BS34 energies obtained are compared in Figure S4 (where the BS12 profile apparently duplicates the one for $[4Fe\text{-}3S]^{5+}$ in Figure 8b). The behavior of the BS34 vs BS12/BS13 energies can be explained in terms of valence delocalization among the Fe*a* and Fe*b* sites, forming the $[Fe^{2+}\downarrow, Fe^{3+}\downarrow]$ minority spin in the BS*ab* state (see also main text). Electron delocalization into a mixed-valence pair (here, $[Fe^{2+}\downarrow, Fe^{3+}\downarrow] \rightarrow [2Fe^{2.5+}\downarrow]$) commonly stabilizes the energy of an iron-sulfur cluster, by approximately 0.35 V estimated for standard [4Fe-4S] cubane.[10,12-14] When $a = 3$, $b = 4$ (BS34), and the Fe4-S3 bond is lost in the "opened" cluster conformation, four Fe-S bridges separate Fe3 and Fe4, which significantly reduces the Fe3-Fe4 intersite spin coupling and works against electron delocalization. In contrast, when the cluster is "closed" (for all three BS states) *or* when it is "opened" for BS12/BS13, there are only 2 Fe-S bonds separating the two minority-spin sites, which permits effective $[2Fe^{2.5+}\downarrow]$ delocalization. The relative B3LYP spin populations (Table S6) support this interpretation. For BS34 S-$OX_{D\text{-}H}^{5+}$, the Fe4 spin density (-2.98) is significantly lower than for the rest of the Fe sites (>3.63 in absolute value). This indicates a localized solution with ferrous (Fe^{2+} $S = 2$) Fe4, while Fe1/2/3 are ferric (Fe^{3+} $S = 5/2$).

In summary, the B3LYP relative energies in Figure S4 support broken-symmetry states BS12 and BS13 for the products of the 'forward' RED → S-OX transformation, with no change for the mechanistic scenario. While the BS34 PES following the same scenario appears to be acceptable alone, it is less preferred than BS12/BS13 due the ~5-8 kcal/mol higher energies for the stationary points where the cluster is "opened" (shown as absence of the Fe4-S3 bonding in Figure S4). These energy differences match well the abovementioned 0.35 V delocalization energy, which translates to ~8 kcal/mol.

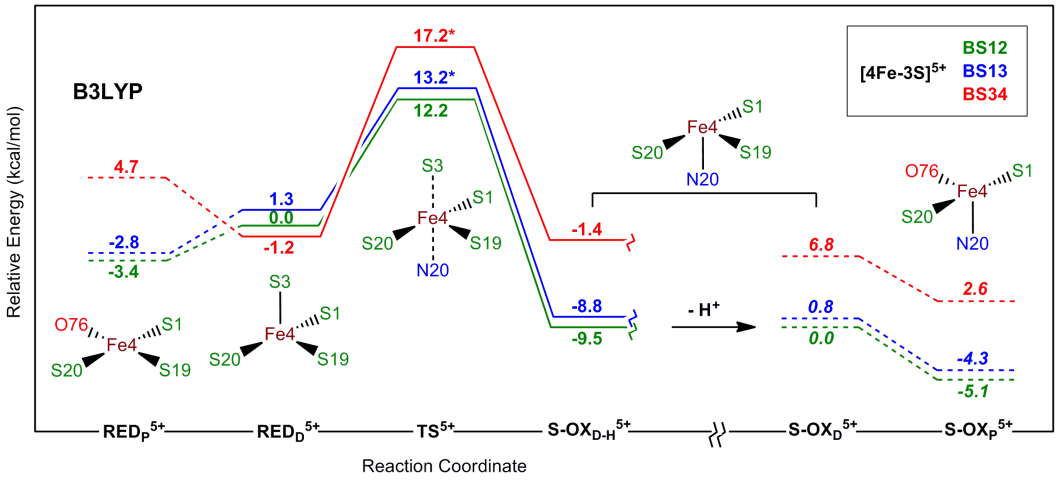

Figure S4. Relative B3LYP energy profiles obtained for the MBH proximal cluster structural transformations at the superoxidized level using BS12 (green), BS13 (blue), and BS34 (red) broken-symmetry states of the $[4Fe\text{-}3S]^{5+}$ core. The 'special' Fe4 iron coordination sphere is schematically shown for every state. "-H^+" implies deprotonation of the Glu76 O76 oxygen in the S-$OX_{D\text{-}H}^{5+}$ state and thus a discontinuity of the potential energy surface. The key transformation involving the TS transition state is given as solid line, and the rest of the relative energies are shown as dashed lines. The asterisks (*) denote approximate TS transition states as described in the main text.

7. Spin Populations for the Fe Sites

Table S6 gives the Mulliken spin populations for the RED_D and S-$OX_{D\text{-}H}$ models, respectively, describing the reactant and the product of the RED → S-OX proximal cluster transformation. The data are provided for the BS states and PBE/B3LYP functional calculations set described in Section 6. The spin populations differ from the nominal integer values (*e.g.*, 4 for the high-spin ferrous Fe^{2+} $S = 2$ sites, and 5 for the high-spin ferric Fe^{3+} $S = 5/2$ sites) due to the mixed-valence character of the iron-sulfur clusters, and due to delocalization of spin density onto ligand atoms (in particular sulfur).

Table S6. Mulliken Spin Populations for the Four Iron Sites of the RED_D and S-$OX_{D\text{-}H}$ Proximal Cluster Models in the Six Broken-Symmetry (BS) States at the Three Oxidation $[4Fe\text{-}3S]^{3+/4+/5+}$ Levels Using the PBE and B3LYP Density Functionals[a]

		PBE / B3LYP Spin Population (*e*)					
		RED_D^X			S-$OX_{D\text{-}H}^X$		
		***X* = 3+** $[4Fe\text{-}3S]^{3+}$ ***S* = 1/2**	***X* = 4+** $[4Fe\text{-}3S]^{4+}$ ***S* = 0**	***X* = 5+** $[4Fe\text{-}3S]^{5+}$ ***S* = 1/2**	***X* = 3+** $[4Fe\text{-}3S]^{3+}$ ***S* = 1/2**	***X* = 4+** $[4Fe\text{-}3S]^{4+}$ ***S* = 0**	***X* = 5+** $[4Fe\text{-}3S]^{5+}$ ***S* = 1/2**
BS12	**Fe1**	-3.01 / -3.59	-3.36 / -3.65	-3.26 / -3.63	-3.10 / -3.59	-3.37 / -3.66	-3.26 / -3.65
	Fe2	-3.12 / -3.61	-3.22 / -3.71	-2.96 / -3.71	-3.33 / -3.61	-3.33 / -3.70	-3.21 / -3.70
	Fe3	3.52 / 3.88	3.52 / 3.80	3.45 / 3.80	3.51 / 3.78	3.45 / 3.78	3.39 / 3.78
	Fe4	3.25 / 3.65	3.06 / 3.65	3.32 / 3.81	3.36 / 3.64	3.16 / 3.64	3.55 / 3.89
BS13	**Fe1**	-2.97 / –	-3.03 / –	-2.32 / -3.60	-3.07 / –	-3.20 / –	-2.84 / -3.63
	Fe2	3.35 / –	3.14 / –	3.04 / 3.77	3.47 / –	3.33 / –	3.26 / 3.74
	Fe3	-3.36 / –	-3.48 / –	-3.36 / -3.77	-3.35 / –	-3.46 / –	-3.42 / -3.77
	Fe4	3.43 / –	3.37 / –	3.33 / 3.83	3.45 / –	3.45 / –	3.61 / 3.91
BS14	**Fe1**	-3.18 / –	-3.35 / –	-2.72 / –	-3.31 / –	-3.39 / –	-3.33 / –
	Fe2	3.27 / –	3.17 / –	2.98 / –	3.46 / –	3.24 / –	3.40 / –
	Fe3	3.55 / –	3.44 / –	3.31 / –	3.59 / –	3.48 / –	3.63 / –
	Fe4	-3.27 / –	-3.38 / –	-2.96 / –	-3.47 / –	-3.55 / –	-3.48 / –
BS23	**Fe1**	3.40 / –	= -BS14[b]	3.32 / –	3.43 / –	= -BS14[b]	3.38 / –
	Fe2	-2.69 / –		-2.84 / –	-2.94 / –		-3.17 / –
	Fe3	-3.38 / –		-3.17 / –	-3.38 / –		-2.92 / –
	Fe4	3.35 / –		3.34 / –	3.54 / –		3.61 / –
BS24	**Fe1**	3.21 / –	= -BS13[b]	3.34 / –	3.27 / –	= -BS13[b]	3.19 / –
	Fe2	-3.08 / –		-2.98 / –	-3.14 / –		-3.21 / –
	Fe3	3.51 / –		3.42 / –	3.55 / –		3.41 / –
	Fe4	-3.05 / –		-3.23 / –	-3.34 / –		-2.79 / –
BS34	**Fe1**	3.42 / –	= -BS12[b]	3.23 / 3.83	3.48 / –	= -BS12[b]	3.31 / 3.63
	Fe2	3.33 / –		2.96 / 3.75	3.40 / –		3.21 / 3.70
	Fe3	-3.32 / –		-2.39 / -3.78	-3.32 / –		-3.32 / -3.75
	Fe4	-2.97 / –		-3.19 / -3.63	-3.24 / –		-2.44 / -2.98

[a] All BS states structures were optimized as detailed in the Computational Methods section of the main text. The relative energies of the BS states are given in Table S5.

[b] For the $[4Fe\text{-}3S]^{4+}$ oxidized cluster, the spin populations of the BS23, BS24, and BS34 states are exactly opposite ("-") to those of BS14, BS13, and BS12, respectively, due to the $S = 0$ zero total spin.

8. Spin Projection and Hyperfine Coupling: Fe4-Bound Cys20 Amide

The spin-coupling model for the superoxidized proximal cluster is provided in Scheme 1 of the main text. This scheme, rationalized based on the proximal cluster topology (see Results, **I**), provides a framework for the quantitative spin-projection procedure, which is in turn used to predict the hyperfine tensor $A^{DFT}(^{14}N20)$ of the Fe4-bound Cys20 amide nitrogen atom N20. Here, we provide only a brief outline of the spin-projection procedure; the detailed methodological background and other application examples are described elsewhere.[15-18] To obtain the spin-projected $A^{DFT}(^{14}N20)$ hyperfine tensor, the 'raw' unrestricted broken-symmetry (UBS) DFT $A^{UBS}(^{14}N20)$ hyperfine tensor (see Table S9 below) is scaled with the $P_{N20} = P_{Fe4}$ projection factor, inherited from the 'special' Fe4 site in view of the terminal Fe4-N20 coordination:

$$A^{DFT}(^{14}N20) = |K_4 / S_4| \cdot S_t \cdot A^{UBS}(^{14}N20) = P_{Fe4} \cdot A^{UBS}(^{14}N20)$$

where $S_4 = 5/2$ and $S_t = 1/2$ are the ferric $Fe4^{3+}$ iron site spin and the total $[4Fe\text{-}3S]^{5+}$ cluster spin, respectively, and K_4 is the spin-projection coefficient for Fe4. The general formulation for K_i (here, $i = 1\ldots4$) via $\boldsymbol{S}_i$ and $\boldsymbol{S}_t$ spin vectors is:

$$K_i = < \boldsymbol{S}_i \cdot \boldsymbol{S}_t > / < \boldsymbol{S}_t \cdot \boldsymbol{S}_t >$$

The K_i values are then obtained using the 'nested' spin-coupling Scheme 1, and the following chain and sum rules:

$$K_i = K_i^t = K_i^q K_q^t$$
$$\sum K_i^{(q)} = 1$$

where q designates a subunit spin system, such as S_{12} and S_{123} in Scheme 1 of the main text and Table S7 below. The final calculation of the K_i values was arranged using an in-house script, which takes the spin-coupling scheme as input. This results in K_i values compiled in Table S8. The key $P_{N20} = P_{Fe4}$ spin-projection factor is then obtained following the first equation above.

Initially applied to the BS12 broken-symmetry state, the spin-coupling Scheme 1 was adapted for the BS13 and BS34 states also relevant for current discussions (see main text), considering collinear spin-vector alignments only, see Table S7. Notably, the construction of the 'nested' Scheme 1 is such that the projection factors $P_{N20} = P_{Fe4}$ in Table S8 are generally invariant to three alternatives for the particular charge and spin distributions (Fe^{3+} $S_i = 5/2$, Fe^{2+} $S_i = 2$, or mixed-valence $Fe^{2.5+}$ $S_i = 9/4$) within the Fe*a* and Fe*b* sites pair, which carries the minority spin in BS*ab*. The final spin-projected $A^{DFT}(^{14}N20)$ values at the B3LYP level are shown in Table S10 for the three structural candidates and the three BS states. The BS12 electronic structure provides the best match to the experimental ^{14}N HFC signals ($A_{iso}^{DFT}(^{14}N20)$ = 16-18 MHz vs 13-15 MHz for N_{C20}[19] and N1[20]). The calculations using BS13 result in an only marginally larger overestimation of the isotropic contribution ($A_{iso}^{DFT}(^{14}N20)$ = 17-19 MHz), as compared to BS12. In contrast, the BS34 state, which the relative energies make less likely (see Section 6 above), gives only a small $A_{iso}^{DFT}(^{14}N20)$ of less than 3.2 MHz. This behavior of the HFC parameters for the Fe4-bound $^{14}N20$ nucleus in BS12/BS13 vs BS34 is due to the difference in the relative orientations of the total $S = 1/2$ and local S_4 spin vectors of the $[4Fe\text{-}3S]^{5+}$ core: while for both BS12 and BS13 these vectors are parallel, for BS34 they are antiparallel. For BS34, this leads to an interplay of various spin-density contributions at the N20 nucleus, which is positive (constructive) for $S\text{-}OX_P^{5+}$ and negative (destructive) for $S\text{-}OX_D^{5+}$ and $S\text{-}OX_{D\text{-}H}^{5+}$ (see Tables S9 and S10).

Yet an alternative spin-coupling approach, easy to test for BS13 and BS34, is to follow the same spin sites starting from Scheme 1 for BS12, instead of using identical Fe*i* sites as done in Table S7. This alternative would result in a nesting scheme different from Scheme 1. The spin-projection factors for these spin-coupling schemes can, however, be directly obtained using permutations of P_{Fei} for BS12 from Table S8. It is easy to show that the new schemes for BS13 give modified $P'_{N20}(BS13) = P'_{Fe4}(BS13) = P_{Fe2}(BS12) \approx 0.27$ *or* $P_{Fe4}(BS12) \approx 0.22$. Similarly for BS34, $P'_{N20}(BS34) = P'_{Fe4}(BS34) = P_{Fe1}(BS12) \approx 0.27$ *or* $P_{Fe2}(BS12) \approx 0.27$. While application of the alternative P'_{N20} factors to the 'raw' $A^{UBS}(^{14}N20)$ hyperfine

tensors in Table S9 may change the final $A^{DFT}(^{14}N20)$ values somewhat, it does not modify our conclusions obtained using the original Scheme 1.

Table S7. Site and Subunit Spin Values S_i for the Spin-Coupling Model of the S = 1/2 Superoxidized Proximal Cluster, Applied to the Broken-Symmetry States BS12, BS13, and BS34[a]

Site/Subunit Spin	BS12	BS13	BS34
$\boldsymbol{S_1}$ =	(a) 9/4 (b) 2 (c) 5/2	(a) 9/4 (b) 2	5/2
$\boldsymbol{S_2}$ =	(a) 9/4 (b) 5/2 (c) 2	5/2	5/2
$\boldsymbol{S_3}$ =	5/2	(a) 9/4 (b) 5/2	(a) 9/4 (b) 2 (c) 5/2
$\boldsymbol{S_4}$ =	5/2	5/2	(a) 9/4 (b) 5/2 (c) 2
$\boldsymbol{S_{12}}$ =	$S_1 + S_2 = 9/2$	$S_2 - S_1$ = (a) 1/4 (b) 1/2	$S_1 + S_2 = 5$
$\boldsymbol{S_{123}}$ =	$S_{12} - S_3 = 2$	$S_3 - S_{12} = 2$	$S_{12} - S_3$ = (a) 11/4 (b) 3 (c) 5/2
$\boldsymbol{S = S_{1234}}$ =	$S_4 - S_{123} = 1/2$	$S_4 - S_{123} = 1/2$	$S_{123} - S_4 = 1/2$

[a] Cf. Scheme 1 of the main text. Options (a)-(c) are to be read in each BS column independently, and they apply to the three (Fe^{3+} S_i = 5/2, Fe^{2+} S_i = 2, or mixed-valence $Fe^{2.5+}$ S_i = 9/4) alternatives for distribution of the Fe oxidation and spin states between the two Fe*a* and Fe*b* sites, carrying the minority spin in BS*ab*. For BS13, the S_1 = 5/2 alternative does not apply as this would lead to S_{12} = 0 and to a collapse of the spin-projection procedure.

Table S8. Assigned Oxidation States, Formal Magnitudes of Spin Vectors S_i, and Calculated Spin-Projection Coefficients K_i for the Four Fe*i* Sites in the BS12, BS13, and BS34 Broken-Symmetry States of the Superoxidized Proximal Cluster[a]

BS State	*i*	Fe$_i$ oxidation state	S_i	K_i	P_{Fei}
BS12	1	(a) 2.5+ (b) 2+ (c) 3+	(a) 9/4 (b) 2 (c) 5/2	(a) -11/9 (b) -88/81 (c) -110/81	22/81
	2	(a) 2.5+ (b) 3+ (c) 2+	(a) 9/4 (b) 5/2 (c) 2	(a) -11/9 (b) -110/81 (c) -88/81	22/81
	3	3+	5/2	10/9	2/9
	4	3+	5/2	7/3	**7/15 ≈ 0.47**
BS13	1	(a) 2.5+ (b) 2+	(a) 9/4 (b) 2	(a) -1/5 (b) -8/27	(a) 1/45 (b) 2/27
	2	3+	5/2	(a) 14/45 (b) 14/27	(a) 14/225 (b) 14/135
	3	(a) 2.5+ (b) 3+	(a) 9/4 (b) 5/2	(a) -13/9 (b) -14/9	(a) 26/81 (b) 14/45
	4	3+	5/2	7/3	**7/15 ≈ 0.47**
BS34	1	3+	5/2	2	2/5
	2	3+	5/2	2	2/5
	3	(a) 2.5+ (b) 2+ (c) 3+	(a) 9/4 (b) 2 (c) 5/2	(a) -1/3 (b) -4/3 (c) -5/3	1/3
	4	(a) 2.5+ (b) 3+ (c) 2+	(a) 9/4 (b) 5/2 (c) 2	(a) -1/3 (b) -5/3 (c) -4/3	**1/3 ≈ 0.33**

[a] Options (a)-(c) are to be read for each BS state independently, and they apply to the three (Fe^{3+} S_i = 5/2, Fe^{2+} S_i = 2, or mixed-valence $Fe^{2.5+}$ S_i = 9/4) alternatives for the distribution of Fe oxidation and spin states between the two Fe*a* and Fe*b* sites, carrying the minority spin in BS*ab*, see also Table S7. The calculated spin populations in Table S6 are consistent with options (a) for BS12 and BS13, and with option (c) for BS34.

Table S9. 'Raw' Unrestricted Broken-Symmetry (UBS) DFT Hyperfine Parameters (MHz) of the Fe4-bound Cys20 Amide Nitrogen Atom N20 in Different Structural Arrangements of the Superoxidized Proximal Cluster Computed using PBE and B3LYP Functionals for the Broken-Symmetry States BS12, BS13, and BS34[a]

BS State	Model	Method	A_{iso}^{UBS}	T^{UBS}	$A^{UBS} = A_{iso}^{UBS} + T^{UBS}$
BS12	$S\text{-}OX_P^{5+}$	PBE	28.8	[-7.4, 0.8, 6.6]	[21.4, 29.6, 35.4]
		B3LYP	38.0	[-8.0, -1.6, 9.5]	[30.0, 36.4, 47.5]
	$S\text{-}OX_D^{5+}$	PBE	26.5	[-9.7, 3.6, 6.1]	[16.9, 30.1, 32.6]
		B3LYP	34.4	[-10.4, 3.1, 7.3]	[24.0, 37.5, 41.7]
	$S\text{-}OX_{D\text{-}H}^{5+}$	PBE	26.2	[-8.3, 1.1, 7.1]	[18.0, 27.4, 33.4]
		B3LYP	35.8	[-9.8, 0.8, 9.0]	[26.1, 36.6, 44.8]
BS13	$S\text{-}OX_P^{5+}$	B3LYP	41.2	[-8.7, -1.8, 10.5]	[32.5, 39.5, 51.7]
	$S\text{-}OX_D^{5+}$	B3LYP	35.2	[-10.8, 3.1, 7.8]	[24.3, 38.2, 43.0]
	$S\text{-}OX_{D\text{-}H}^{5+}$	B3LYP	37.1	[-10.4, 1.1, 9.3]	[26.8, 38.2, 46.4]
BS34	$S\text{-}OX_P^{5+}$	B3LYP	9.5	[-4.5, 0.2, 4.3]	[5.0, 9.7, 13.7]
	$S\text{-}OX_D^{5+}$	B3LYP	-2.5	[-7.0, 2.0, 5.0]	[-9.4, -0.5, 2.5]
	$S\text{-}OX_{D\text{-}H}^{5+}$	B3LYP	-5.3	[-6.1, 2.0, 4.1]	[-11.4, -3.3, -1.3]

[a] HFC calculations using PBE and B3LYP functionals were done as described in Computational Methods. For BS13 and BS34, the HFC calculations were done using B3LYP only. The structures of the $S\text{-}OX_P^{5+}$, $S\text{-}OX_D^{5+}$, and $S\text{-}OX_{D\text{-}H}^{5+}$ models are shown in Figures 4b,c and 5.

Table S10. Spin-Projected ^{14}N Hyperfine Parameters (MHz) of the Fe4-bound Cys20 Amide Nitrogen Atom N20 in Different Structural Arrangements of the Superoxidized Proximal Cluster Computed using B3LYP Functional for the Broken-Symmetry States BS12, BS13, and BS34, Compared to ENDOR and HYSCORE Data[a]

Signal/DFT Model	BS State	A_{iso}	T	$A = A_{iso} + T$
N_{C20} (ENDOR)[19]	–	14.6	[-3.2, -0.5, 3.6]	[11.4, 14.1, 18.2]
N1 (HYSCORE)[20]	–	13.0	[-1.5, -1.5, 3.0]	[11.5, 11.5, 16.0]
$S\text{-}OX_P^{5+}$ (B3LYP)	BS12	17.9	[-3.8, -0.7, 4.5]	[14.1, 17.1, 22.3]
	BS13	19.4	[-4.1, -0.8, 4.9]	[15.3, 18.5, 24.3]
	BS34	3.2	[-1.5, 0.1, 1.4]	[1.7, 3.2, 4.6]
$S\text{-}OX_D^{5+}$ (B3LYP)	BS12	16.2	[-4.9, 1.5, 3.4]	[11.3, 17.6, 19.6]
	BS13	16.5	[-5.1, 1.4, 3.7]	[11.4, 18.0, 20.1]
	BS34	-0.8	[-2.3, 0.7, 1.7]	[-3.1, -0.2, 0.8]
$S\text{-}OX_{D\text{-}H}^{5+}$ (B3LYP)	BS12	16.8	[-4.6, 0.4, 4.2]	[12.3, 17.2, 21.1]
	BS13	17.5	[-4.9, 0.5, 4.4]	[12.6, 18.0, 21.8]
	BS34	-1.8	[-2.0, 0.7, 1.4]	[-3.8, -1.1, -0.4]

[a] HFC calculations using the B3LYP functional as described in Computational Methods. For BS12/BS13/BS34, the projection coefficients P_{N20} = 0.47/0.47/0.33 were used, respectively, see Table S8, based on the 'raw' DFT values in Table S10. The structures of the $S\text{-}OX_P^{5+}$, $S\text{-}OX_D^{5+}$, and $S\text{-}OX_{D\text{-}H}^{5+}$ models are shown in Figures 4b,c and 5.

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10. Coordinates of the Models

On pages S14-S59 below, coordinates of the 46 optimized models are given in XYZ format, including the absolute energies in Hartrees. The XYZ coordinates on every page are preceded by the information on the functional used, the broken-symmetry state, and the model name (as described in the text).

PBE BS12 RED_P^{5+}:

```
  102
Absolute Energy (Hartree): -5805.465226
Fe    11.995566    -1.988627    17.216904
Fe    14.143893    -1.335706    18.563409
Fe    15.084761    -3.619773    17.446122
Fe    10.591984    -1.954406    19.836915
 S    12.084454    -0.488916    19.007401
 S    14.159378    -1.877841    16.330626
 S    14.729043    -3.184174    19.613678
 C    10.010000     1.302000    15.410000
 C    11.115755     0.374627    14.926789
 S    10.743815    -1.357470    15.433182
 H    10.217981     2.342199    15.104598
 H    11.198000     0.381649    13.828862
 H    12.089573     0.665558    15.346678
 H     9.031405     1.012624    14.997159
 H     9.938712     1.277337    16.507967
 C     7.846001    -3.160999    17.912001
 C     9.040156    -3.737112    17.139826
 S    10.644040    -3.704484    18.092227
 H     6.931299    -3.345089    17.325449
 H     8.870857    -4.803342    16.933208
 H     9.181224    -3.197589    16.195744
 H     7.966607    -2.073176    18.041636
 C     8.062092    -3.645290    21.692868
 C     9.199872    -3.062164    22.551431
 S    10.886938    -3.194616    21.793552
 H     8.177662    -4.733463    21.604396
 H     9.012122    -2.009705    22.806587
 H     9.235341    -3.623481    23.496961
 C    16.816000    -0.358000    21.165000
 C    15.752803     0.613167    20.665166
 S    15.476337     0.500798    18.835922
 H    17.790371    -0.161068    20.692007
 H    14.792817     0.443268    21.172819
 H    16.050641     1.657285    20.851657
 H    16.935750    -0.260677    22.257559
 H    16.532193    -1.396823    20.940221
 C    19.442999    -1.915000    17.846000
 C    18.053129    -2.405895    18.251766
 S    17.369922    -3.679204    17.089615
 H    20.171094    -2.740939    17.809894
 H    18.076084    -2.859901    19.254404
 H    17.341037    -1.568547    18.288641
 H    19.421894    -1.437305    16.854158
 H    19.807289    -1.170378    18.574409
 C    13.733000    -7.100000    18.702000
 C    14.796299    -6.844867    17.641821
 S    14.297590    -5.516859    16.455470
 H    13.559409    -6.195735    19.304528
 H    15.755350    -6.554060    18.096459
 H    14.975900    -7.746352    17.034159
 H    12.774759    -7.387243    18.243211
 H    14.048550    -7.912249    19.380012
 C     7.723193    -3.885987    19.248004
 O     7.447266    -5.084111    19.322023
 N     8.067767    -3.114966    20.332131
 H     8.081773    -2.091420    20.233434
 H     8.483848    -8.711204    13.920081
 C     8.899000    -8.791000    12.903000
 H     8.944309    -9.857562    12.632483
 C    10.290866    -8.138723    12.822646
 C    10.289714    -6.656883    13.079865
 N     9.499936    -5.793223    12.333410
 C    11.035833    -5.937775    13.999266
 C     9.770391    -4.578619    12.796119
 N    10.694549    -4.613378    13.800942
 H     8.203195    -8.286667    12.216299
 H    10.978547    -8.622637    13.535358
 H    10.709882    -8.323902    11.816265
 H    11.767378    -6.226845    14.749890
 H     9.332361    -3.646909    12.445284
 H    11.060268    -3.803291    14.308209
 O    13.564387    -1.414197    22.444007
 H    12.685778    -1.854120    22.459442
 H    13.917286    -1.716126    21.584078
 O    14.253487     1.531348    15.976433
 H    14.314183     1.557195    16.953115
 H    14.407122     0.583266    15.799449
 C    11.193999     2.101999    24.316999
 C    10.015791     1.380735    23.628830
 C    10.302933     0.816827    22.222861
 C     9.079748     0.178691    21.553960
 O     7.935375     0.393092    22.017851
 O     9.251557    -0.587825    20.508609
 H    10.896165     2.459335    25.314465
 H    12.060027     1.431978    24.438764
 H    11.528075     2.973051    23.729979
 H     9.677878     0.550773    24.273268
 H     9.155325     2.064580    23.554102
 H    10.653382     1.616586    21.543645
 H    11.120288     0.075735    22.232130
 C     6.642445    -3.412101    22.280207
 O     5.892982    -4.353700    22.553739
 N     6.270703    -2.100723    22.351185
 C     4.874001    -1.683000    22.392000
 C     4.562375    -0.681113    21.274976
 O     5.145837     0.601809    21.481654
 H     6.959190    -1.359184    22.174083
 H     4.264216    -2.593830    22.288455
 H     4.630303    -1.218080    23.364248
 H     4.867275    -1.123348    20.304074
 H     3.471885    -0.522181    21.242047
 H     6.124181     0.504856    21.494522
```

PBE BS12 RED_D^{5+}:

```
  102
Absolute Energy (Hartree): -5805.473503
Fe    11.620732    -2.142340    17.062627
Fe    13.507750    -1.406680    18.766379
Fe    14.829700    -3.495130    17.561591
Fe    11.523077    -3.047769    19.617391
 S    11.302569    -0.882907    19.012912
 S    13.855928    -1.804305    16.501492
 S    13.882784    -3.371979    19.753253
 C    10.010001     1.302000    15.410001
 C    10.981463     0.277413    14.840048
 S    10.466510    -1.446712    15.269268
 H    10.328124     2.320165    15.128938
 H    11.016625     0.322048    13.740694
 H    11.996634     0.450445    15.223245
 H     8.987986     1.144434    15.033374
 H     9.981774     1.245277    16.508344
 C     7.846000    -3.161000    17.912001
 C     8.833905    -4.028430    17.114099
 S    10.634055    -4.181627    17.664341
 H     6.868014    -3.241302    17.410879
 H     8.490294    -5.072470    17.135021
 H     8.892641    -3.691326    16.070615
 H     8.161426    -2.106164    17.905109
 C     8.227328    -3.416006    21.680741
 C     9.463396    -2.883771    22.405607
 S    11.031390    -3.639593    21.761565
 H     8.256740    -4.514732    21.651825
 H     9.521487    -1.790703    22.306089
 H     9.422405    -3.153792    23.470698
 C    16.815997    -0.357999    21.165000
 C    15.466000     0.301940    20.882908
 S    14.996885     0.261342    19.085431
 H    17.618987     0.076344    20.550913
 H    14.663281    -0.170505    21.466727
 H    15.489192     1.371383    21.146000
 H    17.079021    -0.219287    22.227375
 H    16.768303    -1.438130    20.966470
 C    19.443000    -1.915000    17.846000
 C    17.978901    -2.121990    18.269614
 S    17.147425    -3.547512    17.412515
 H    20.049939    -2.809832    18.052523
 H    17.928109    -2.328241    19.347381
 H    17.377777    -1.219827    18.081966
 H    19.520217    -1.688781    16.771580
 H    19.872323    -1.069594    18.408644
 C    13.733000    -7.100000    18.702001
 C    14.823117    -6.693396    17.717247
 S    14.246148    -5.413865    16.506954
 H    13.385194    -6.234386    19.285278
 H    15.707332    -6.295107    18.236862
 H    15.152895    -7.551769    17.110854
 H    12.862998    -7.525944    18.179745
 H    14.116723    -7.858474    19.405619
 C     7.720401    -3.728318    19.313710
 O     7.255490    -4.858144    19.508527
 N     8.245719    -2.955241    20.305278
 H     8.460620    -1.963740    20.152659
 H     8.393797    -8.623329    13.867246
 C     8.899000    -8.790999    12.903000
 H     8.926600    -9.875505    12.713549
 C    10.316510    -8.191582    12.911614
 C    10.336951    -6.695642    13.055590
 N     9.673087    -5.875802    12.153785
 C    10.974370    -5.924516    14.013277
 C     9.909353    -4.635714    12.563817
 N    10.692686    -4.612511    13.682253
 H     8.291350    -8.315526    12.118945
 H    10.913080    -8.637283    13.724280
 H    10.823242    -8.465545    11.968074
 H    11.596710    -6.171090    14.869498
 H     9.540963    -3.725395    12.096216
 H    10.996245    -3.773822    14.185103
 O    12.648392    -0.793225    22.324507
 H    12.319757    -1.717222    22.239770
 H    12.329712    -0.391307    21.496505
 O    14.111740     1.561337    16.105652
 H    14.057164     1.546625    17.080658
 H    14.305784     0.626293    15.905825
 C    11.193999     2.101998    24.316999
 C     9.798929     1.596807    23.918832
 C     9.647620     1.314933    22.415588
 C     8.243751     0.819677    22.010298
 O     7.257086     1.372639    22.576648
 O     8.166172    -0.113455    21.136725
 H    11.257012     2.290257    25.400965
 H    11.968082     1.363811    24.053618
 H    11.438901     3.044605    23.798631
 H     9.576505     0.669221    24.476475
 H     9.022970     2.320340    24.215829
 H     9.847559     2.242586    21.846098
 H    10.397818     0.578999    22.088764
 C     6.869638    -3.113268    22.394482
 O     6.383922    -3.952378    23.166721
 N     6.261137    -1.962082    22.032646
 C     4.874004    -1.682999    22.392000
 C     4.335351    -0.435420    21.680434
 O     4.670613     0.788336    22.302020
 H     6.826687    -1.219939    21.563695
 H     4.268750    -2.568165    22.126023
 H     4.764747    -1.534435    23.482243
 H     4.653219    -0.472904    20.614931
 H     3.233233    -0.501445    21.687503
 H     5.667493     0.915838    22.301187
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PBE BS12 TS^{5+}:

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  102
Absolute Energy (Hartree): -5805.446296
Fe    11.619083    -2.438229    17.274663
Fe    13.712227    -1.702810    18.750942
Fe    15.008559    -3.706192    17.458732
Fe    10.518950    -3.107487    19.787580
 S    11.511849    -1.182829    19.200210
 S    13.787930    -2.057256    16.473151
 S    14.580513    -3.489214    19.654387
 C    10.010000     1.302000    15.409999
 C    11.038384     0.190029    15.207997
 S    10.357788    -1.479654    15.644851
 H    10.451811     2.273340    15.130892
 H    11.362257     0.135389    14.157452
 H    11.931461     0.366279    15.822941
 H     9.113371     1.141828    14.791461
 H     9.695597     1.358291    16.462806
 C     7.846004    -3.160999    17.912001
 C     8.708419    -4.219440    17.204436
 S    10.461158    -4.447348    17.824976
 H     6.872888    -3.127977    17.397678
 H     8.250231    -5.213151    17.315262
 H     8.786926    -3.989868    16.133617
 H     8.326811    -2.172858    17.819011
 C     8.156163    -3.583435    21.662596
 C     9.304494    -3.286344    22.628953
 S    10.902559    -3.914102    21.925508
 H     8.127008    -4.673277    21.510302
 H     9.402036    -2.215540    22.856004
 H     9.129677    -3.824239    23.571741
 C    16.815994    -0.358001    21.165000
 C    15.426087     0.246608    20.992434
 S    14.801093     0.238604    19.245178
 H    17.560774     0.151955    20.534818
 H    14.694162    -0.279173    21.619526
 H    15.419684     1.307961    21.286846
 H    17.132289    -0.266845    22.218229
 H    16.809743    -1.425104    20.901023
 C    19.442999    -1.915001    17.846000
 C    17.973325    -2.237178    18.145414
 S    17.270750    -3.510838    16.993986
 H    20.073226    -2.814155    17.927602
 H    17.865255    -2.628575    19.167788
 H    17.347336    -1.335151    18.075714
 H    19.562453    -1.505897    16.831001
 H    19.817938    -1.166089    18.563919
 C    13.733000    -7.100000    18.701999
 C    14.839861    -6.933706    17.668779
 S    14.429788    -5.646903    16.402626
 H    13.567869    -6.157048    19.244563
 H    15.791980    -6.653336    18.144710
 H    15.007704    -7.868517    17.110421
 H    12.782440    -7.385507    18.225528
 H    14.000061    -7.880004    19.436009
 C     7.588048    -3.532745    19.359746
 O     6.743022    -4.391854    19.626567
 N     8.407266    -2.944905    20.340312
 H     8.574669    -1.594184    20.515661
 H     8.540204    -8.757221    13.943821
 C     8.899000    -8.791000    12.903000
 H     8.998450    -9.847382    12.607958
 C    10.238639    -8.046096    12.757348
 C    10.157643    -6.574032    13.053505
 N     9.307077    -5.738221    12.342860
 C    10.871849    -5.837880    13.984673
 C     9.509670    -4.523905    12.839542
 N    10.448080    -4.531095    13.832267
 H     8.131694    -8.323824    12.267956
 H    10.997019    -8.499716    13.416146
 H    10.606933    -8.179422    11.723639
 H    11.627381    -6.108431    14.717693
 H     9.011243    -3.610590    12.522388
 H    10.764578    -3.712859    14.364676
 O    12.712047    -1.234458    22.434482
 H    12.289779    -2.125816    22.437737
 H    12.633272    -0.998976    21.490156
 O    14.399695     1.305085    16.134749
 H    14.504401     1.401825    17.101206
 H    14.378538     0.333074    16.033130
 C    11.194000     2.102001    24.317000
 C     9.872531     1.589493    23.716658
 C    10.044127     0.967256    22.322906
 C     8.823783     0.216795    21.798812
 O     7.714761     0.313867    22.363433
 O     9.056258    -0.537535    20.753731
 H    11.033342     2.527925    25.319660
 H    11.929011     1.286150    24.405598
 H    11.644282     2.886486    23.686593
 H     9.438595     0.830569    24.389002
 H     9.132525     2.405703    23.671506
 H    10.315863     1.732954    21.573332
 H    10.885309     0.252711    22.325615
 C     6.747725    -3.285585    22.254672
 O     6.157137    -4.152901    22.909042
 N     6.216546    -2.066376    21.968804
 C     4.874003    -1.683000    22.392000
 C     4.397557    -0.415829    21.682065
 O     4.948498     0.786811    22.212913
 H     6.852611    -1.284253    21.773566
 H     4.201233    -2.526750    22.167051
 H     4.827380    -1.515043    23.485006
 H     4.596539    -0.517052    20.594770
 H     3.306431    -0.334664    21.812772
 H     5.926032     0.709689    22.173343
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PBE BS12 S-$OX_{D\text{-}H}^{5+}$:

```
  102
Absolute Energy (Hartree): -5805.471283
Fe    11.481173    -2.302222    17.514887
Fe    13.336822    -1.584907    19.254730
Fe    14.821816    -3.430376    17.801689
Fe    10.230634    -3.085211    19.887140
 S    11.039304    -1.063956    19.408411
 S    13.668500    -1.695171    16.936863
 S    14.273064    -3.436208    19.986177
 C    10.010000     1.302000    15.409999
 C    11.069967     0.211185    15.306524
 S    10.372358    -1.454505    15.716579
 H    10.447148     2.281772    15.152128
 H    11.483973     0.149051    14.288480
 H    11.902572     0.406775    15.996326
 H     9.166939     1.112621    14.727498
 H     9.614213     1.363656    16.434853
 C     7.846001    -3.160999    17.912001
 C     8.749204    -4.192813    17.213969
 S    10.474115    -4.403036    17.917923
 H     6.932993    -3.051897    17.305500
 H     8.297965    -5.195009    17.265721
 H     8.883757    -3.930271    16.156212
 H     8.357629    -2.184706    17.949456
 C     7.978854    -3.840040    21.630080
 C     9.091950    -3.459164    22.620549
 S    10.775234    -3.899774    21.979849
 H     7.923347    -4.940756    21.557403
 H     9.072334    -2.375298    22.812434
 H     8.940429    -3.987643    23.572168
 C    16.815998    -0.358000    21.165001
 C    15.379970    -0.248665    21.671921
 S    14.129304     0.286408    20.404227
 H    17.163323     0.592019    20.729663
 H    15.031025    -1.208877    22.076277
 H    15.301526     0.501711    22.474396
 H    17.489964    -0.627017    21.996486
 H    16.886329    -1.136022    20.397661
 C    19.442999    -1.915000    17.846000
 C    17.985648    -2.127641    18.273504
 S    17.079889    -3.356760    17.222203
 H    20.015133    -2.854473    17.898871
 H    17.949798    -2.491122    19.310852
 H    17.435162    -1.176554    18.229818
 H    19.503693    -1.537733    16.813630
 H    19.926313    -1.179189    18.510342
 C    13.733000    -7.100000    18.702000
 C    14.773680    -6.673917    17.674343
 S    14.183018    -5.280327    16.610343
 H    13.483406    -6.260788    19.369303
 H    15.710153    -6.358859    18.159056
 H    15.016747    -7.501602    16.988657
 H    12.802934    -7.429138    18.213588
 H    14.113308    -7.932895    19.318754
 C     7.427031    -3.619452    19.305618
 O     6.397520    -4.297447    19.476061
 N     8.288785    -3.268175    20.313334
 H     6.834154     0.651567    20.864311
 H     8.463412    -8.748968    13.913718
 C     8.899000    -8.791000    12.903000
 H     8.993629    -9.849112    12.612864
 C    10.264228    -8.080212    12.860550
 C    10.199859    -6.604536    13.146240
 N     9.387940    -5.758639    12.403132
 C    10.902178    -5.873435    14.090839
 C     9.601037    -4.543614    12.893894
 N    10.510616    -4.559860    13.912781
 H     8.194730    -8.302302    12.213649
 H    10.958644    -8.550376    13.575935
 H    10.707810    -8.228216    11.858524
 H    11.633049    -6.146894    14.847786
 H     9.129811    -3.623852    12.554656
 H    10.826777    -3.744905    14.449305
 O    12.055529    -0.928193    22.803322
 H    11.788892    -1.823242    22.492922
 H    12.473704    -0.531497    22.008699
 O    14.416999     1.580800    17.334476
 H    14.445197     1.396718    18.297692
 H    14.349727     0.675474    16.972860
 C    11.194000     2.101999    24.316999
 C     9.698183     1.950058    24.018770
 C     9.452219     1.402164    22.611395
 C     8.002109     1.169267    22.278221
 O     7.069737     1.286327    23.077795
 O     7.815453     0.809431    20.991508
 H    11.359414     2.467605    25.342680
 H    11.711377     1.137556    24.199857
 H    11.667467     2.818570    23.625449
 H     9.237148     1.267828    24.752082
 H     9.180159     2.917517    24.135442
 H     9.868459     2.070489    21.837287
 H     9.998606     0.448760    22.477115
 C     6.615180    -3.431531    22.238067
 O     6.039632    -4.168824    23.047104
 N     6.146138    -2.201108    21.895398
 C     4.874002    -1.683000    22.392000
 C     4.288613    -0.640392    21.449918
 O     5.134668     0.514147    21.284084
 H     6.682968    -1.661797    21.217445
 H     4.178118    -2.529929    22.501614
 H     5.004872    -1.241287    23.398588
 H     4.152826    -1.064086    20.443666
 H     3.299640    -0.328539    21.831006
 H     5.439898     0.825593    22.171408
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PBE BS12 S-OX_D^{5+}:

```
  101
Absolute Energy (Hartree): -5804.950511
Fe    11.537741    -2.371390    17.370847
Fe    13.599181    -1.659391    18.873875
Fe    14.953240    -3.652832    17.510486
Fe    10.273311    -2.994885    19.849403
 S    11.364406    -1.105508    19.303049
 S    13.718808    -2.003150    16.568991
 S    14.497113    -3.516966    19.707044
 C    10.009999     1.302000    15.410000
 C    10.995856     0.161760    15.170354
 S    10.288543    -1.475350    15.672340
 H    10.461089     2.262504    15.106847
 H    11.265571     0.085327    14.105496
 H    11.922415     0.321883    15.738324
 H     9.081153     1.160822    14.835571
 H     9.745681     1.368328    16.475774
 C     7.846002    -3.160999    17.912000
 C     8.729601    -4.214338    17.223017
 S    10.462068    -4.406663    17.908293
 H     6.921104    -3.058652    17.322966
 H     8.276825    -5.213667    17.308464
 H     8.847102    -3.978250    16.156983
 H     8.367482    -2.189050    17.910641
 C     8.062311    -3.702793    21.646403
 C     9.182651    -3.243157    22.586205
 S    10.844282    -3.784902    21.954209
 H     8.031243    -4.807004    21.646103
 H     9.180006    -2.145011    22.655574
 H     9.044133    -3.676185    23.587172
 C    16.816001    -0.358000    21.165000
 C    15.442170     0.282333    20.954033
 S    14.868759     0.238327    19.190086
 H    17.584202     0.125073    20.541025
 H    14.677636    -0.215057    21.567247
 H    15.462507     1.347085    21.235941
 H    17.117870    -0.261809    22.222626
 H    16.791292    -1.427627    20.912890
 C    19.442999    -1.915000    17.846000
 C    18.006633    -2.293493    18.233048
 S    17.228963    -3.476293    17.034879
 H    20.088955    -2.805485    17.790728
 H    17.995665    -2.775895    19.222118
 H    17.363297    -1.402991    18.296853
 H    19.471058    -1.413685    16.866117
 H    19.868371    -1.226795    18.596265
 C    13.733000    -7.100000    18.702001
 C    14.831823    -6.886269    17.668295
 S    14.377228    -5.594643    16.422800
 H    13.532384    -6.165265    19.247116
 H    15.774915    -6.581560    18.148014
 H    15.029817    -7.809678    17.100114
 H    12.793578    -7.419582    18.224666
 H    14.029278    -7.872152    19.433789
 C     7.460016    -3.576946    19.323212
 O     6.422507    -4.232203    19.534453
 N     8.363495    -3.229398    20.288727
 H     8.461376    -8.747166    13.912703
 C     8.899000    -8.790999    12.903000
 H     9.016526    -9.850169    12.624543
 C    10.248683    -8.050670    12.855070
 C    10.151067    -6.573380    13.121314
 N     9.352183    -5.748522    12.341310
 C    10.805309    -5.822078    14.084482
 C     9.526361    -4.525970    12.830397
 N    10.398121    -4.517358    13.881376
 H     8.184856    -8.325109    12.207791
 H    10.950012    -8.495779    13.579622
 H    10.699394    -8.202293    11.856731
 H    11.512621    -6.079154    14.868847
 H     9.051406    -3.617432    12.466894
 H    10.677511    -3.689104    14.423491
 O    13.557285    -2.020845    22.586021
 H    12.631093    -2.333167    22.473527
 H    13.985769    -2.401235    21.792495
 O    14.462149     1.293497    16.107040
 H    14.548327     1.397015    17.076034
 H    14.379414     0.322265    16.024637
 C    11.193999     2.101999    24.316999
 C     9.798202     1.552446    24.010425
 C     9.548869     1.350448    22.511160
 C     8.130661     0.844624    22.175761
 O     7.174407     1.353377    22.844268
 O     8.021844    -0.030775    21.262562
 H    11.354986     2.226106    25.400764
 H    11.979593     1.428277    23.936959
 H    11.347418     3.085502    23.841112
 H     9.661376     0.587225    24.531047
 H     9.019137     2.224101    24.406201
 H     9.687771     2.315305    21.986524
 H    10.285817     0.653123    22.082875
 C     6.672187    -3.311408    22.217687
 O     6.036592    -4.154298    22.877081
 N     6.230176    -2.054023    21.992784
 C     4.874001    -1.683000    22.392000
 C     4.358595    -0.417446    21.687995
 O     4.638630     0.795647    22.357009
 H     6.861430    -1.321913    21.589475
 H     4.223429    -2.544922    22.163843
 H     4.805871    -1.514319    23.484088
 H     4.729108    -0.423601    20.639937
 H     3.257323    -0.495876    21.636496
 H     5.637458     0.919932    22.450199
```

PBE BS12 S-OX_P^{5+}:

```
  101
Absolute Energy (Hartree): -5804.953047
Fe    11.711014    -2.154521    17.422164
Fe    13.815847    -1.447015    18.817900
Fe    14.977189    -3.565208    17.500586
Fe     9.966755    -2.232219    20.161035
 S    11.659583    -0.873786    19.379303
 S    13.883800    -1.845725    16.532381
 S    14.614180    -3.329533    19.705219
 C    10.009999     1.302002    15.410000
 C    10.986725     0.193916    15.033813
 S    10.408747    -1.442349    15.666629
 H    10.361612     2.273944    15.021986
 H    11.084375     0.106638    13.940057
 H    11.983961     0.401712    15.445372
 H     9.006341     1.110618    14.998993
 H     9.918267     1.383977    16.502945
 C     7.846000    -3.161001    17.911998
 C     8.940716    -4.058636    17.317761
 S    10.547129    -4.003522    18.248748
 H     6.961952    -3.202867    17.255711
 H     8.617444    -5.111070    17.338451
 H     9.135657    -3.782694    16.273627
 H     8.204566    -2.118333    17.940451
 C     7.929077    -3.866569    21.614830
 C     8.975137    -3.452722    22.679215
 S    10.707960    -3.385151    22.034050
 H     7.902258    -4.967016    21.531540
 H     8.734623    -2.454656    23.073817
 H     8.944675    -4.166435    23.515188
 C    16.816002    -0.358000    21.165000
 C    15.563000     0.471517    20.891343
 S    15.081752     0.467099    19.100782
 H    17.672359     0.004121    20.574994
 H    14.711070     0.096902    21.477190
 H    15.722281     1.527577    21.162257
 H    17.084190    -0.305469    22.235072
 H    16.639578    -1.412617    20.905446
 C    19.443000    -1.915000    17.846000
 C    17.968487    -2.207787    18.137467
 S    17.263006    -3.510902    17.021950
 H    20.062887    -2.816811    17.972077
 H    17.841329    -2.556587    19.172977
 H    17.355679    -1.300591    18.027019
 H    19.580901    -1.549546    16.816317
 H    19.820786    -1.140749    18.535911
 C    13.733000    -7.100000    18.702001
 C    14.827948    -6.771917    17.693437
 S    14.290418    -5.493693    16.463983
 H    13.427372    -6.197866    19.252839
 H    15.733318    -6.397685    18.195289
 H    15.113707    -7.665013    17.114173
 H    12.840647    -7.503052    18.198861
 H    14.087032    -7.850385    19.430854
 C     7.424887    -3.662561    19.295530
 O     6.439744    -4.426811    19.416458
 N     8.231907    -3.273599    20.313729
 H     8.608930    -8.796862    13.965423
 C     8.899000    -8.791000    12.903000
 H     9.027713    -9.834882    12.576027
 C    10.191564    -7.980050    12.689764
 C    10.071682    -6.517859    13.023841
 N     9.158968    -5.697815    12.373768
 C    10.805623    -5.775233    13.934819
 C     9.346408    -4.487212    12.887257
 N    10.332060    -4.481570    13.832032
 H     8.069302    -8.348210    12.331916
 H    11.009010    -8.413394    13.289008
 H    10.498963    -8.076850    11.632008
 H    11.600967    -6.033512    14.628969
 H     8.799711    -3.586311    12.617895
 H    10.651661    -3.660274    14.362520
 O    13.553388    -1.800188    22.571630
 H    12.598421    -2.020863    22.544946
 H    13.866416    -2.161210    21.716467
 O    14.286425     1.491918    16.094117
 H    14.287357     1.566117    17.069547
 H    14.325908     0.521571    15.977466
 C    11.193999     2.102000    24.317000
 C     9.899780     1.644900    23.630998
 C    10.106591     0.717014    22.425710
 C     8.800859     0.351313    21.709406
 O     7.770520     1.022236    21.958867
 O     8.794865    -0.643869    20.878823
 H    10.978121     2.753046    25.179190
 H    11.783642     1.244507    24.681112
 H    11.836518     2.666312    23.621103
 H     9.255171     1.129969    24.364302
 H     9.321657     2.521221    23.296970
 H    10.771467     1.185324    21.676693
 H    10.617991    -0.218466    22.710772
 C     6.539016    -3.482466    22.177017
 O     5.857887    -4.278804    22.839768
 N     6.172747    -2.191823    21.958492
 C     4.874001    -1.683000    22.392000
 C     4.462204    -0.422626    21.625277
 O     5.075179     0.770036    22.089071
 H     6.817467    -1.597744    21.423389
 H     4.135274    -2.488094    22.237806
 H     4.880911    -1.446036    23.472212
 H     4.637687    -0.591579    20.541797
 H     3.375923    -0.285218    21.761493
 H     6.050678     0.741853    21.904840
```

PBE BS12 RED_P^{4+}:

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  102
Absolute Energy (Hartree): -5805.563046
Fe    11.953040    -2.092723    17.217408
Fe    14.198662    -1.490221    18.467400
Fe    15.192848    -3.786088    17.360242
Fe    10.784936    -2.197343    19.895136
 S    12.160573    -0.565094    19.013856
 S    14.115755    -2.132122    16.227275
 S    14.761558    -3.372772    19.520711
 C    10.009999     1.302000    15.409999
 C    11.085856     0.326286    14.948591
 S    10.638296    -1.391945    15.450875
 H    10.264815     2.334449    15.111785
 H    11.194464     0.339191    13.852498
 H    12.059513     0.582862    15.391121
 H     9.027519     1.051042    14.980253
 H     9.920369     1.272802    16.506469
 C     7.846002    -3.160999    17.912001
 C     9.014125    -3.827392    17.172138
 S    10.639636    -3.843928    18.096820
 H     6.943568    -3.252097    17.285268
 H     8.784004    -4.889175    17.000349
 H     9.176474    -3.331907    16.207437
 H     8.063119    -2.092530    18.070501
 C     7.940232    -3.796173    21.672257
 C     9.081295    -3.284743    22.571791
 S    10.778621    -3.492486    21.858499
 H     8.006040    -4.886236    21.552864
 H     8.930183    -2.227174    22.829254
 H     9.052175    -3.857397    23.511469
 C    16.816000    -0.358001    21.165000
 C    15.844748     0.569365    20.435579
 S    15.770258     0.262880    18.608956
 H    17.839908    -0.240109    20.777364
 H    14.829115     0.473184    20.847749
 H    16.145451     1.622140    20.561642
 H    16.825118    -0.133492    22.245922
 H    16.517361    -1.409179    21.032877
 C    19.442999    -1.915000    17.846000
 C    18.202061    -2.659656    18.335258
 S    17.510519    -3.811805    17.058458
 H    20.246271    -2.608311    17.547173
 H    18.430902    -3.256965    19.232622
 H    17.411061    -1.943285    18.597287
 H    19.198087    -1.281570    16.978628
 H    19.836098    -1.259835    18.643472
 C    13.733000    -7.100000    18.702000
 C    14.910434    -6.972710    17.743214
 S    14.563471    -5.769433    16.381132
 H    13.493066    -6.124472    19.151121
 H    15.819351    -6.637476    18.266876
 H    15.138591    -7.938287    17.262427
 H    12.831841    -7.454709    18.178124
 H    13.962721    -7.811332    19.515368
 C     7.595981    -3.893839    19.225792
 O     7.145027    -5.046084    19.251802
 N     7.997789    -3.212187    20.336908
 H     8.266812    -2.216918    20.270107
 H     8.499482    -8.737470    13.927997
 C     8.899000    -8.791000    12.903000
 H     8.966390    -9.851921    12.614348
 C    10.273142    -8.101846    12.810739
 C    10.244696    -6.624249    13.093469
 N     9.440968    -5.761536    12.360451
 C    10.978485    -5.907457    14.025268
 C     9.691966    -4.550554    12.846182
 N    10.616558    -4.586348    13.849496
 H     8.179037    -8.293440    12.236268
 H    10.983827    -8.581837    13.503219
 H    10.679182    -8.260665    11.794361
 H    11.712681    -6.199387    14.771798
 H     9.238012    -3.619755    12.513703
 H    10.963721    -3.774220    14.372903
 O    13.184785    -1.357762    22.467089
 H    12.435034    -2.000668    22.474014
 H    13.342589    -1.274417    21.506927
 O    14.337609     1.249839    15.873685
 H    14.558587     1.271132    16.831208
 H    14.339217     0.284828    15.710521
 C    11.193999     2.101999    24.316999
 C    10.034537     1.320263    23.662797
 C    10.329773     0.745544    22.263336
 C     9.144822     0.008306    21.618534
 O     7.990242     0.168134    22.112952
 O     9.358687    -0.748640    20.596237
 H    10.905689     2.462786    25.316814
 H    12.089266     1.468689    24.426628
 H    11.480427     2.977012    23.710065
 H     9.747185     0.487215    24.327876
 H     9.142143     1.963866    23.595576
 H    10.618040     1.553410    21.564550
 H    11.194102     0.059134    22.281235
 C     6.528873    -3.510859    22.248991
 O     5.719811    -4.415941    22.485905
 N     6.239604    -2.183484    22.371182
 C     4.874001    -1.683000    22.392000
 C     4.642473    -0.655086    21.277959
 O     5.287132     0.592770    21.510839
 H     6.973297    -1.480394    22.195534
 H     4.210565    -2.553719    22.270584
 H     4.639270    -1.208230    23.362694
 H     4.950436    -1.106291    20.312072
 H     3.562243    -0.439096    21.217140
 H     6.259958     0.436502    21.568146
```

PBE BS12 RED_D^{4+}:

```
  102
Absolute Energy (Hartree): -5805.578695
Fe    11.545398    -2.126363    17.087154
Fe    13.479556    -1.402479    18.712266
Fe    14.816740    -3.526469    17.543978
Fe    11.392572    -3.008381    19.612856
 S    11.265859    -0.809546    19.011197
 S    13.791805    -1.872234    16.437881
 S    13.791667    -3.398348    19.673248
 C    10.010001     1.302000    15.410000
 C    10.965185     0.264659    14.832928
 S    10.406881    -1.456506    15.225616
 H    10.346164     2.320910    15.149540
 H    11.021817     0.339745    13.735559
 H    11.977382     0.408888    15.236261
 H     8.987617     1.166478    15.024128
 H     9.971999     1.225975    16.506914
 C     7.846001    -3.160999    17.912002
 C     8.831774    -4.058733    17.137485
 S    10.629991    -4.195434    17.696800
 H     6.872739    -3.218054    17.398287
 H     8.469563    -5.096412    17.175153
 H     8.884575    -3.743122    16.086696
 H     8.191183    -2.114993    17.902166
 C     8.223364    -3.420667    21.683392
 C     9.446439    -2.875127    22.424416
 S    11.043971    -3.593081    21.801245
 H     8.271319    -4.519114    21.658319
 H     9.480767    -1.779454    22.333366
 H     9.378735    -3.144589    23.489001
 C    16.815995    -0.357999    21.164999
 C    15.471879     0.311488    20.872663
 S    15.023069     0.272683    19.068961
 H    17.629562     0.091582    20.574908
 H    14.663378    -0.166483    21.443808
 H    15.497740     1.376538    21.154169
 H    17.064619    -0.257973    22.235981
 H    16.764866    -1.429178    20.922961
 C    19.443000    -1.915000    17.846000
 C    18.006482    -2.195186    18.318886
 S    17.163954    -3.554687    17.370013
 H    20.077233    -2.810888    17.937366
 H    18.014687    -2.491681    19.377986
 H    17.382282    -1.293162    18.238519
 H    19.457924    -1.593105    16.793182
 H    19.888414    -1.112809    18.458566
 C    13.733000    -7.100000    18.702001
 C    14.816422    -6.733010    17.693866
 S    14.247271    -5.464849    16.467609
 H    13.401975    -6.211552    19.260288
 H    15.711832    -6.336130    18.196461
 H    15.127292    -7.612738    17.107071
 H    12.852062    -7.528637    18.199991
 H    14.112916    -7.843284    19.425054
 C     7.681479    -3.706343    19.317203
 O     7.140850    -4.802373    19.523554
 N     8.255145    -2.963659    20.303969
 H     8.534412    -1.991774    20.137872
 H     8.375158    -8.636580    13.859463
 C     8.899001    -8.790999    12.903000
 H     8.930870    -9.872897    12.698462
 C    10.316162    -8.189755    12.948264
 C    10.334617    -6.693691    13.101269
 N     9.668550    -5.871217    12.203025
 C    10.973314    -5.925225    14.061576
 C     9.904663    -4.632245    12.620545
 N    10.689937    -4.613279    13.736301
 H     8.306955    -8.302736    12.114893
 H    10.893871    -8.640209    13.771838
 H    10.844453    -8.460131    12.015019
 H    11.600643    -6.169679    14.915813
 H     9.532233    -3.719580    12.160859
 H    10.983464    -3.773257    14.248069
 O    12.562312    -0.731925    22.275556
 H    12.238339    -1.664127    22.214018
 H    12.324070    -0.392732    21.391869
 O    14.328643     1.428576    16.041786
 H    14.320635     1.484156    17.018339
 H    14.320567     0.459567    15.907541
 C    11.194000     2.101997    24.316997
 C     9.783286     1.615020    23.951418
 C     9.603443     1.324335    22.453590
 C     8.187525     0.852614    22.063302
 O     7.213305     1.392307    22.670705
 O     8.086823    -0.043767    21.158556
 H    11.289888     2.280228    25.400778
 H    11.951214     1.359152    24.022117
 H    11.434477     3.046556    23.799656
 H     9.560201     0.693250    24.518736
 H     9.023871     2.351104    24.262032
 H     9.814542     2.242642    21.872470
 H    10.337363     0.573819    22.123811
 C     6.857028    -3.128898    22.374342
 O     6.352957    -3.972343    23.133589
 N     6.256921    -1.966873    22.026899
 C     4.874003    -1.682999    22.392000
 C     4.336642    -0.424851    21.696112
 O     4.647038     0.789919    22.347633
 H     6.823659    -1.217375    21.568802
 H     4.262272    -2.562589    22.120615
 H     4.765760    -1.543481    23.484346
 H     4.675247    -0.437752    20.636571
 H     3.234641    -0.501029    21.680475
 H     5.645427     0.928439    22.368855
```

PBE BS12 TS^{4+}:

```
  102
Absolute Energy (Hartree): -5805.544168
Fe    11.623980    -2.442294    17.238374
Fe    13.780260    -1.711522    18.613764
Fe    15.047373    -3.764357    17.349910
Fe    10.506215    -3.011128    19.770257
 S    11.612556    -1.111411    19.153660
 S    13.786389    -2.168392    16.317503
 S    14.588425    -3.557832    19.533637
 C    10.010000     1.302000    15.410000
 C    10.985251     0.156878    15.135909
 S    10.280780    -1.495436    15.602048
 H    10.467997     2.265642    15.126587
 H    11.247171     0.112584    14.067097
 H    11.917675     0.302095    15.698337
 H     9.076179     1.183070    14.837656
 H     9.752250     1.346120    16.478301
 C     7.845999    -3.161003    17.911994
 C     8.730766    -4.198726    17.198267
 S    10.463033    -4.421354    17.884118
 H     6.886450    -3.104858    17.372841
 H     8.266561    -5.193867    17.272104
 H     8.830351    -3.940882    16.135484
 H     8.333041    -2.172306    17.865101
 C     8.088461    -3.672830    21.647160
 C     9.251721    -3.404787    22.609831
 S    10.845391    -3.994860    21.856951
 H     8.049666    -4.759294    21.469012
 H     9.333612    -2.340196    22.875406
 H     9.085437    -3.974597    23.536197
 C    16.815996    -0.358000    21.165002
 C    15.464013     0.244973    20.784742
 S    15.115629     0.184125    18.960466
 H    17.643022     0.155294    20.648605
 H    14.656452    -0.275339    21.317834
 H    15.419295     1.307759    21.072553
 H    16.979117    -0.270315    22.253801
 H    16.854269    -1.423983    20.898272
 C    19.442999    -1.915000    17.846000
 C    17.982408    -2.290977    18.108215
 S    17.335682    -3.551977    16.912463
 H    20.104711    -2.793029    17.920292
 H    17.867995    -2.710079    19.119655
 H    17.329157    -1.407187    18.054787
 H    19.566626    -1.482669    16.840681
 H    19.781716    -1.166808    18.583593
 C    13.733000    -7.100000    18.702000
 C    14.846620    -6.989337    17.668794
 S    14.454801    -5.748258    16.351593
 H    13.568830    -6.128928    19.193781
 H    15.798439    -6.698585    18.140164
 H    15.010936    -7.949853    17.153225
 H    12.783201    -7.401157    18.232688
 H    13.988039    -7.844600    19.477160
 C     7.551168    -3.579137    19.342773
 O     6.717649    -4.474088    19.551911
 N     8.324254    -3.003789    20.346892
 H     8.534039    -1.661583    20.541086
 H     8.512999    -8.753052    13.933850
 C     8.899000    -8.791000    12.903000
 H     9.001398    -9.848737    12.612624
 C    10.245125    -8.050751    12.792313
 C    10.161164    -6.576619    13.079309
 N     9.334370    -5.742003    12.339507
 C    10.850072    -5.838091    14.028381
 C     9.526753    -4.526136    12.839702
 N    10.435825    -4.531733    13.857807
 H     8.151041    -8.320838    12.247184
 H    10.982206    -8.503711    13.475228
 H    10.643016    -8.191979    11.770285
 H    11.582944    -6.106312    14.785291
 H     9.039278    -3.612133    12.507834
 H    10.727953    -3.709299    14.403645
 O    12.703314    -1.365233    22.390677
 H    12.255343    -2.246047    22.405507
 H    12.594911    -1.140245    21.444006
 O    14.379182     1.164119    15.947280
 H    14.434535     1.272159    16.918867
 H    14.316534     0.189562    15.868265
 C    11.194004     2.102004    24.317005
 C     9.874349     1.573152    23.723339
 C    10.057753     0.841160    22.386535
 C     8.808752     0.156711    21.835789
 O     7.689538     0.333706    22.365279
 O     9.030029    -0.618486    20.807689
 H    11.020156     2.606934    25.280432
 H    11.910419     1.282210    24.484748
 H    11.675662     2.825626    23.638838
 H     9.402673     0.881594    24.441903
 H     9.158572     2.403103    23.596190
 H    10.430880     1.527327    21.604442
 H    10.839122     0.064451    22.469191
 C     6.693893    -3.363089    22.253987
 O     6.066453    -4.222722    22.887922
 N     6.207828    -2.115785    22.007299
 C     4.874003    -1.683000    22.392000
 C     4.395403    -0.511964    21.532659
 O     4.962943     0.742790    21.899194
 H     6.858333    -1.368616    21.751401
 H     4.203542    -2.549962    22.274204
 H     4.832268    -1.379795    23.456676
 H     4.584680    -0.756465    20.466294
 H     3.305485    -0.404397    21.660870
 H     5.940679     0.634567    21.931162
```

PBE BS12 S-$OX_{D\text{-}H}^{4+}$:

```
  102
Absolute Energy (Hartree): -5805.556980
Fe    11.331618    -2.207234    17.398482
Fe    13.170514    -1.764325    19.195517
Fe    14.802961    -3.467181    17.659684
Fe    10.331140    -2.990113    19.818027
 S    10.950199    -0.913223    19.256668
 S    13.576550    -1.740305    16.860930
 S    14.303243    -3.576012    19.847808
 C    10.010001     1.301996    15.410000
 C    10.862910     0.129271    14.924623
 S    10.197505    -1.508489    15.477056
 H    10.428212     2.259112    15.051569
 H    10.906732     0.107677    13.824077
 H    11.892821     0.210939    15.301461
 H     8.973668     1.219202    15.046417
 H     9.984465     1.329547    16.510526
 C     7.846002    -3.160994    17.912001
 C     8.699113    -4.247128    17.249806
 S    10.453047    -4.343769    17.871996
 H     6.907729    -3.063738    17.340394
 H     8.259652    -5.243140    17.415380
 H     8.764806    -4.080027    16.165555
 H     8.387149    -2.202013    17.871082
 C     8.055138    -3.731566    21.636335
 C     9.121093    -3.261667    22.630916
 S    10.813347    -3.615169    21.972394
 H     8.063100    -4.836858    21.605087
 H     9.035257    -2.174712    22.792238
 H     8.988602    -3.772578    23.596929
 C    16.815994    -0.358000    21.165000
 C    15.360934    -0.585844    21.553641
 S    14.149420     0.111350    20.330740
 H    17.044348     0.717171    21.079020
 H    15.145518    -1.660009    21.642087
 H    15.133913    -0.112620    22.521724
 H    17.492329    -0.791208    21.923758
 H    17.036988    -0.826231    20.199066
 C    19.442996    -1.915000    17.846000
 C    17.953918    -2.097046    18.176910
 S    17.094539    -3.336814    17.097380
 H    19.996636    -2.861529    17.954021
 H    17.840733    -2.440632    19.215714
 H    17.420984    -1.139269    18.072079
 H    19.578581    -1.558993    16.812442
 H    19.892561    -1.171651    18.526253
 C    13.733000    -7.100000    18.702000
 C    14.837086    -6.687632    17.733258
 S    14.280793    -5.405557    16.517055
 H    13.374245    -6.226089    19.267243
 H    15.703411    -6.277052    18.273887
 H    15.189452    -7.548967    17.142239
 H    12.876024    -7.532503    18.162992
 H    14.106624    -7.851616    19.420185
 C     7.469172    -3.526864    19.345027
 O     6.397325    -4.138302    19.566455
 N     8.380812    -3.195520    20.301265
 H     7.710238     1.455863    19.857352
 H     8.593412    -8.762132    13.960689
 C     8.899001    -8.790999    12.903001
 H     9.027831    -9.845477    12.610869
 C    10.196166    -7.989539    12.684531
 C    10.063612    -6.521212    12.979274
 N     9.180198    -5.719308    12.269698
 C    10.744077    -5.759944    13.916281
 C     9.331389    -4.500427    12.777195
 N    10.266148    -4.472442    13.770906
 H     8.079542    -8.363191    12.306078
 H    11.004475    -8.405627    13.307751
 H    10.517296    -8.113888    11.633925
 H    11.503920    -6.005144    14.654024
 H     8.793457    -3.607070    12.467662
 H    10.537042    -3.635018    14.310605
 O    12.113716    -0.758978    22.764159
 H    11.753686    -1.648580    22.516377
 H    12.590314    -0.481598    21.947302
 O    15.832097     0.700587    17.553966
 H    15.406253     0.606878    18.440189
 H    15.360947     0.002900    17.056396
 C    11.194000     2.101999    24.316999
 C     9.809562     1.939316    23.679075
 C     9.921725     1.671149    22.172219
 C     8.622632     1.330278    21.505913
 O     7.718568     0.667739    22.016138
 O     8.536419     1.810474    20.245744
 H    11.113361     2.289438    25.399738
 H    11.786900     1.189424    24.157316
 H    11.741911     2.947966    23.869594
 H     9.276642     1.095280    24.145433
 H     9.191949     2.837903    23.856272
 H    10.394060     2.508266    21.636356
 H    10.583250     0.790885    22.031462
 C     6.646520    -3.397895    22.184727
 O     5.986397    -4.234999    22.817422
 N     6.220773    -2.112091    22.017203
 C     4.874007    -1.683001    22.391999
 C     4.355590    -0.566133    21.487071
 O     4.884904     0.725592    21.790425
 H     6.842781    -1.462492    21.536892
 H     4.227665    -2.572714    22.320431
 H     4.840493    -1.332713    23.441449
 H     4.543691    -0.849286    20.431212
 H     3.264552    -0.482736    21.619893
 H     5.864613     0.666502    21.787554
```

PBE BS12 RED_P^{3+}:

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  102
Absolute Energy (Hartree): -5805.61138027
Fe    11.885399    -1.809637    17.186639
Fe    14.066042    -1.403700    18.621362
Fe    15.065765    -3.658785    17.450193
Fe    10.844743    -2.194315    19.842115
 S    12.025032    -0.388112    19.044834
 S    14.071023    -1.956376    16.337998
 S    14.645245    -3.307359    19.648723
 C    10.009999     1.302000    15.409999
 C    10.954289     0.306322    14.740288
 S    10.586987    -1.426266    15.275057
 H    10.238577     2.339473    15.103671
 H    10.866473     0.358205    13.641581
 H    11.994164     0.540092    15.011409
 H     8.959593     1.088069    15.155146
 H    10.113956     1.235218    16.504862
 C     7.846002    -3.160999    17.912001
 C     9.012082    -3.796442    17.141721
 S    10.694021    -3.692482    17.949122
 H     6.934581    -3.230363    17.293607
 H     8.813741    -4.869617    16.995216
 H     9.100931    -3.310377    16.160712
 H     8.072032    -2.097626    18.095824
 C     7.929717    -3.831090    21.658798
 C     9.086680    -3.337478    22.553440
 S    10.778155    -3.547440    21.817568
 H     7.975498    -4.923177    21.543060
 H     8.938170    -2.282462    22.823512
 H     9.060646    -3.921069    23.487114
 C    16.816000    -0.358000    21.165000
 C    15.885609     0.671413    20.519472
 S    15.648227     0.417375    18.698353
 H    17.797384    -0.370679    20.665113
 H    14.899507     0.652507    21.011119
 H    16.290206     1.689194    20.647644
 H    16.969818    -0.124410    22.234618
 H    16.380186    -1.365887    21.092868
 C    19.442999    -1.915000    17.846000
 C    18.090756    -2.473444    18.287644
 S    17.432941    -3.781595    17.154116
 H    20.211265    -2.703943    17.776980
 H    18.163726    -2.907713    19.297381
 H    17.345181    -1.664704    18.335220
 H    19.363279    -1.434688    16.857244
 H    19.797983    -1.153664    18.564189
 C    13.733000    -7.100000    18.702000
 C    14.831402    -6.886692    17.666615
 S    14.365982    -5.608676    16.408427
 H    13.457564    -6.148416    19.179710
 H    15.769063    -6.566515    18.147233
 H    15.043366    -7.821683    17.120255
 H    12.823004    -7.505770    18.232239
 H    14.059331    -7.805575    19.488020
 C     7.591408    -3.909735    19.211052
 O     7.106014    -5.051646    19.226867
 N     8.000848    -3.247864    20.326868
 H     8.311050    -2.263313    20.271368
 H     8.322574    -8.627702    13.827210
 C     8.899000    -8.790999    12.903000
 H     9.031900    -9.876284    12.767086
 C    10.258863    -8.069819    12.968206
 C    10.167291    -6.570711    13.073621
 N     9.432328    -5.822197    12.164384
 C    10.787012    -5.729503    13.985727
 C     9.612684    -4.556084    12.531134
 N    10.424948    -4.448500    13.620824
 H     8.301763    -8.405093    12.063448
 H    10.845398    -8.447634    13.821697
 H    10.836719    -8.329505    12.060841
 H    11.445806    -5.911871    14.831854
 H     9.176058    -3.684015    12.049242
 H    10.696495    -3.565313    14.087886
 O    13.048148    -1.341313    22.576752
 H    12.325908    -2.016320    22.509998
 H    13.249060    -1.201684    21.630689
 O    14.346757     1.361112    15.908697
 H    14.491297     1.416367    16.879606
 H    14.261018     0.389431    15.802064
 C    11.193999     2.101999    24.316999
 C    10.007228     1.340810    23.690331
 C    10.268620     0.782796    22.278864
 C     9.095772    -0.009996    21.676940
 O     7.950010     0.125891    22.216534
 O     9.305215    -0.776071    20.672814
 H    10.942240     2.460994    25.327983
 H    12.082459     1.454883    24.395367
 H    11.476620     2.976695    23.707468
 H     9.731684     0.500877    24.351291
 H     9.118820     1.993038    23.658548
 H    10.494060     1.604364    21.572877
 H    11.162769     0.137019    22.270138
 C     6.521312    -3.520476    22.234623
 O     5.706283    -4.414219    22.505759
 N     6.234433    -2.191146    22.314600
 C     4.874001    -1.683000    22.392000
 C     4.660151    -0.504917    21.434475
 O     5.286640     0.698092    21.864505
 H     6.973159    -1.484996    22.150933
 H     4.198464    -2.519664    22.148940
 H     4.626367    -1.342984    23.416682
 H     4.993500    -0.804967    20.419718
 H     3.578439    -0.291595    21.381319
 H     6.263530     0.540743    21.878176
```

PBE BS12 RED_D^{3+}:

```
  102
Absolute Energy (Hartree): -5805.635377
Fe    11.610383    -1.987355    17.132908
Fe    13.591158    -1.398921    18.746470
Fe    14.800340    -3.504571    17.472724
Fe    11.516041    -2.986959    19.669233
 S    11.400804    -0.739646    19.143392
 S    13.828180    -1.767010    16.442838
 S    13.909332    -3.422600    19.665308
 C    10.010000     1.302000    15.410000
 C    10.879183     0.210751    14.791111
 S    10.327814    -1.487056    15.293678
 H    10.379644     2.305796    15.133345
 H    10.851857     0.266209    13.689747
 H    11.925553     0.328423    15.111092
 H     8.962435     1.211478    15.079508
 H    10.019778     1.226639    16.507977
 C     7.846000    -3.161000    17.912000
 C     8.860148    -4.059300    17.173636
 S    10.664619    -4.050657    17.704578
 H     6.886316    -3.211496    17.371576
 H     8.533306    -5.107470    17.254991
 H     8.884651    -3.782026    16.110496
 H     8.202132    -2.118488    17.904418
 C     8.200629    -3.453492    21.681465
 C     9.421179    -2.905881    22.430288
 S    11.029029    -3.639136    21.844107
 H     8.250369    -4.552481    21.657606
 H     9.452753    -1.810966    22.324434
 H     9.328332    -3.155660    23.498223
 C    16.815999    -0.358000    21.165000
 C    15.543795     0.394297    20.769151
 S    15.192850     0.286210    18.947900
 H    17.693943     0.018572    20.616182
 H    14.679258    -0.005555    21.319051
 H    15.633157     1.464695    21.018999
 H    17.009258    -0.250132    22.247634
 H    16.709813    -1.430144    20.942217
 C    19.443000    -1.915000    17.846000
 C    18.018828    -2.251753    18.318975
 S    17.196047    -3.590838    17.326730
 H    20.099063    -2.799795    17.889136
 H    18.047719    -2.579978    19.369667
 H    17.371031    -1.363346    18.277368
 H    19.437295    -1.549931    16.806627
 H    19.881771    -1.128563    18.485051
 C    13.733000    -7.100000    18.702000
 C    14.841540    -6.720939    17.723268
 S    14.278310    -5.513705    16.431754
 H    13.340532    -6.201396    19.199439
 H    15.694348    -6.266632    18.251031
 H    15.218948    -7.609846    17.189974
 H    12.894156    -7.587427    18.180522
 H    14.110761    -7.792615    19.475979
 C     7.633800    -3.699090    19.311632
 O     7.028815    -4.765259    19.513494
 N     8.231229    -2.990124    20.305336
 H     8.603911    -2.053833    20.128420
 H     8.281593    -8.624937    13.800134
 C     8.899000    -8.791000    12.903000
 H     8.956546    -9.875934    12.719226
 C    10.300796    -8.177428    13.079923
 C    10.292733    -6.679747    13.223169
 N     9.681533    -5.869776    12.275656
 C    10.860269    -5.898371    14.218060
 C     9.881404    -4.625551    12.701890
 N    10.589983    -4.592564    13.865807
 H     8.386927    -8.317288    12.052017
 H    10.799875    -8.616684    13.959105
 H    10.918395    -8.452883    12.204257
 H    11.427796    -6.127259    15.117257
 H     9.533798    -3.717877    12.213812
 H    10.840306    -3.740735    14.390621
 O    12.633616    -0.801922    22.347495
 H    12.291237    -1.728730    22.288210
 H    12.398765    -0.469483    21.457727
 O    12.727117     2.010871    17.687076
 H    12.097372     1.290888    17.889189
 H    13.548068     1.641134    18.091623
 C    11.194000     2.102000    24.317000
 C     9.768562     1.648049    23.970377
 C     9.588281     1.288746    22.488382
 C     8.164711     0.842699    22.101625
 O     7.197116     1.389563    22.718480
 O     8.053712    -0.042033    21.190486
 H    11.292017     2.341780    25.389203
 H    11.926216     1.317274    24.072042
 H    11.472851     3.003827    23.745488
 H     9.510240     0.765328    24.582994
 H     9.035654     2.426683    24.239911
 H     9.838961     2.164838    21.860086
 H    10.296086     0.497791    22.198037
 C     6.834849    -3.157984    22.368568
 O     6.311958    -4.002573    23.116190
 N     6.253292    -1.982101    22.034809
 C     4.874001    -1.683000    22.392000
 C     4.347014    -0.420465    21.694393
 O     4.643916     0.791643    22.357354
 H     6.827975    -1.237317    21.577356
 H     4.253782    -2.556907    22.119812
 H     4.758819    -1.540404    23.484106
 H     4.702195    -0.426746    20.640669
 H     3.244987    -0.498269    21.660642
 H     5.643911     0.932410    22.394822
```

PBE BS12 TS^{3+}:

```
  102
Absolute Energy (Hartree): -5805.594318
Fe    11.577668    -2.193232    17.133237
Fe    13.737175    -1.754811    18.615340
Fe    15.009331    -3.785193    17.332056
Fe    10.657516    -3.018669    19.715252
 S    11.592565    -1.000509    19.105549
 S    13.760641    -2.191539    16.291464
 S    14.518013    -3.630789    19.537774
 C    10.010001     1.302001    15.410000
 C    10.827688     0.140668    14.846179
 S    10.181477    -1.510530    15.392978
 H    10.408353     2.270505    15.055738
 H    10.816452     0.161731    13.743075
 H    11.873961     0.229412    15.173326
 H     8.952081     1.232391    15.107490
 H    10.047558     1.299621    16.511630
 C     7.846007    -3.160999    17.912003
 C     8.718609    -4.194763    17.179437
 S    10.523737    -4.226054    17.681425
 H     6.860119    -3.121672    17.418035
 H     8.319788    -5.207365    17.349322
 H     8.702324    -3.992283    16.099210
 H     8.331858    -2.174696    17.824396
 C     8.147928    -3.577255    21.652990
 C     9.269220    -3.236901    22.640155
 S    10.915014    -3.724005    21.940814
 H     8.156146    -4.668870    21.509676
 H     9.281823    -2.165216    22.892968
 H     9.098532    -3.799991    23.570997
 C    16.815991    -0.358002    21.164999
 C    15.504468     0.275223    20.690559
 S    15.204015     0.135599    18.861461
 H    17.684624     0.076206    20.642704
 H    14.661504    -0.189129    21.219218
 H    15.494282     1.350997    20.933792
 H    16.946305    -0.193288    22.250402
 H    16.815228    -1.442133    20.984960
 C    19.442998    -1.915001    17.846000
 C    18.034422    -2.413553    18.186516
 S    17.370192    -3.645179    16.969378
 H    20.165916    -2.746560    17.798323
 H    18.036017    -2.890874    19.179053
 H    17.324894    -1.573048    18.230103
 H    19.455118    -1.402957    16.870399
 H    19.791888    -1.199700    18.612000
 C    13.733001    -7.099999    18.701999
 C    14.881100    -6.965630    17.712128
 S    14.455198    -5.802397    16.339136
 H    13.472220    -6.118558    19.126124
 H    15.788464    -6.587505    18.209435
 H    15.130010    -7.938157    17.253983
 H    12.833213    -7.505789    18.213920
 H    14.007133    -7.774931    19.534532
 C     7.622678    -3.562118    19.358704
 O     6.834410    -4.497520    19.602878
 N     8.381824    -2.941335    20.337470
 H     8.578486    -1.593357    20.503292
 H     8.487316    -8.737489    13.923166
 C     8.899000    -8.791000    12.903000
 H     8.989819    -9.853051    12.622989
 C    10.259555    -8.072741    12.822664
 C    10.187202    -6.595133    13.094887
 N     9.395060    -5.757163    12.321391
 C    10.847955    -5.857789    14.065915
 C     9.582052    -4.540598    12.826694
 N    10.453122    -4.550114    13.875235
 H     8.176737    -8.311989    12.224945
 H    10.969604    -8.529923    13.530954
 H    10.684012    -8.232585    11.813658
 H    11.550906    -6.125138    14.851413
 H     9.114799    -3.622690    12.476760
 H    10.720412    -3.722468    14.435144
 O    12.728638    -1.096220    22.277760
 H    12.258830    -1.969182    22.320342
 H    12.581159    -0.881063    21.332648
 O    14.358800     1.050371    15.865126
 H    14.381774     1.168479    16.838219
 H    14.262995     0.073770    15.806748
 C    11.193999     2.102000    24.316999
 C     9.868063     1.571538    23.738174
 C    10.013984     0.953307    22.339280
 C     8.776513     0.223956    21.817392
 O     7.675816     0.341221    22.408444
 O     8.977908    -0.507322    20.760396
 H    11.051630     2.500101    25.334622
 H    11.952171     1.305321    24.361984
 H    11.607203     2.911663    23.692885
 H     9.457702     0.805217    24.417444
 H     9.117308     2.380106    23.712106
 H    10.288906     1.718705    21.590457
 H    10.847281     0.229840    22.321465
 C     6.734901    -3.308231    22.232174
 O     6.133928    -4.164353    22.899232
 N     6.196782    -2.089287    21.943055
 C     4.874004    -1.682999    22.392000
 C     4.385401    -0.432594    21.661320
 O     4.960924     0.778571    22.142873
 H     6.830712    -1.328257    21.684789
 H     4.187713    -2.527753    22.213348
 H     4.856942    -1.480279    23.481391
 H     4.555257    -0.567753    20.572402
 H     3.297457    -0.339430    21.817941
 H     5.940973     0.669148    22.129866
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PBE BS12 S-$OX_{D\text{-}H}^{3+}$:

```
  102
Absolute Energy (Hartree): -5805.598488
Fe    11.360289    -2.085288    17.348763
Fe    13.174948    -1.711250    19.196925
Fe    14.777869    -3.441182    17.648867
Fe    10.347160    -2.951811    19.820801
 S    10.935901    -0.845066    19.232056
 S    13.616072    -1.668963    16.852967
 S    14.292876    -3.551571    19.853928
 C    10.010001     1.302000    15.410000
 C    10.817863     0.124414    14.856391
 S    10.179034    -1.531576    15.402246
 H    10.417715     2.263203    15.047068
 H    10.805998     0.139727    13.753234
 H    11.867234     0.191169    15.181871
 H     8.953152     1.236627    15.103398
 H    10.043545     1.309180    16.510783
 C     7.846000    -3.161000    17.912001
 C     8.713601    -4.219643    17.219011
 S    10.481697    -4.238956    17.806328
 H     6.901524    -3.050678    17.349936
 H     8.294442    -5.226175    17.384508
 H     8.746662    -4.036606    16.135259
 H     8.386262    -2.200857    17.896702
 C     8.029773    -3.738357    21.633667
 C     9.089934    -3.261513    22.638918
 S    10.797243    -3.624951    22.021622
 H     8.044779    -4.844174    21.598532
 H     8.996643    -2.171335    22.782046
 H     8.931897    -3.758681    23.609684
 C    16.815999    -0.358000    21.165000
 C    15.357094    -0.520881    21.572965
 S    14.161704     0.211067    20.357060
 H    17.086157     0.706420    21.056842
 H    15.106161    -1.587781    21.668452
 H    15.165476    -0.037516    22.544855
 H    17.489383    -0.809448    21.917196
 H    16.995989    -0.849193    20.201492
 C    19.442999    -1.915000    17.846000
 C    17.950591    -2.087411    18.159774
 S    17.108407    -3.336063    17.082638
 H    19.989073    -2.864848    17.968397
 H    17.822258    -2.417700    19.201696
 H    17.425653    -1.125991    18.042251
 H    19.590980    -1.573958    16.808350
 H    19.895470    -1.166401    18.520152
 C    13.733000    -7.100000    18.702000
 C    14.843969    -6.669438    17.745795
 S    14.279778    -5.410779    16.507365
 H    13.342594    -6.224346    19.243736
 H    15.687723    -6.230229    18.300211
 H    15.232965    -7.531901    17.178032
 H    12.897559    -7.561262    18.152557
 H    14.111928    -7.830869    19.439994
 C     7.479746    -3.578606    19.336604
 O     6.460834    -4.294879    19.521508
 N     8.338364    -3.177649    20.309482
 H     7.709621     1.457234    19.859803
 H     8.436296    -8.693140    13.897585
 C     8.899000    -8.790999    12.903000
 H     9.041887    -9.863504    12.693795
 C    10.236410    -8.027755    12.843114
 C    10.104159    -6.540582    13.028496
 N     9.306679    -5.774873    12.188481
 C    10.712152    -5.727717    13.973395
 C     9.436214    -4.527064    12.631896
 N    10.277234    -4.446595    13.701630
 H     8.192840    -8.382952    12.164214
 H    10.927090    -8.418459    13.608097
 H    10.713000    -8.228363    11.864924
 H    11.403500    -5.927398    14.789146
 H     8.947098    -3.648471    12.216770
 H    10.500975    -3.578572    14.225611
 O    12.093022    -0.754732    22.750796
 H    11.727999    -1.637891    22.476068
 H    12.570824    -0.451624    21.942391
 O    15.818690     0.731469    17.541434
 H    15.398213     0.652565    18.433320
 H    15.325908     0.032460    17.060880
 C    11.194000     2.102000    24.317000
 C     9.800876     1.961944    23.693896
 C     9.899057     1.692795    22.187655
 C     8.594458     1.366349    21.526907
 O     7.674684     0.735328    22.049286
 O     8.524401     1.825332    20.258473
 H    11.130129     2.289147    25.401369
 H    11.769863     1.180198    24.147283
 H    11.750851     2.938742    23.863146
 H     9.259738     1.125156    24.163969
 H     9.197886     2.869651    23.878317
 H    10.379087     2.522740    21.647448
 H    10.552135     0.806265    22.040641
 C     6.630931    -3.405321    22.192510
 O     5.977516    -4.212357    22.873762
 N     6.197600    -2.129525    21.974010
 C     4.874001    -1.683000    22.392000
 C     4.329091    -0.560534    21.509975
 O     4.860239     0.731089    21.808494
 H     6.808758    -1.516302    21.434233
 H     4.212641    -2.564205    22.347249
 H     4.878652    -1.331382    23.442460
 H     4.486295    -0.834676    20.446529
 H     3.241324    -0.482797    21.673857
 H     5.840979     0.673146    21.801569
```

B3LYP BS12 RED_P^{5+}:

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  102
Absolute Energy (Hartree): -5809.230569
Fe    11.996253    -1.986833    16.819601
Fe    14.332601    -1.291389    18.419983
Fe    15.278455    -3.779951    17.294166
Fe    10.680733    -1.888262    19.844274
 S    12.186027    -0.493629    18.867427
 S    14.373645    -1.924258    16.185263
 S    14.778141    -3.236937    19.473436
 C    10.010000     1.302000    15.409999
 C    11.028760     0.454851    14.656936
 S    10.763581    -1.355261    14.942689
 H    10.176638     2.367363    15.211385
 H    10.951187     0.619743    13.580047
 H    12.042790     0.713909    14.962706
 H     8.988196     1.054070    15.109991
 H    10.095917     1.142188    16.487255
 C     7.846003    -3.160999    17.912003
 C     9.041898    -3.680558    17.111533
 S    10.656997    -3.609627    18.032942
 H     6.935038    -3.359886    17.339701
 H     8.900617    -4.735121    16.875269
 H     9.151225    -3.112084    16.191385
 H     7.928442    -2.081204    18.056909
 C     8.059762    -3.654522    21.681261
 C     9.207056    -3.083758    22.534978
 S    10.884057    -3.260812    21.766114
 H     8.160033    -4.734975    21.606575
 H     9.037461    -2.037382    22.783593
 H     9.242444    -3.637300    23.474638
 C    16.815999    -0.358001    21.165000
 C    15.862785     0.651463    20.538937
 S    15.792338     0.492578    18.693471
 H    17.832732    -0.221746    20.787714
 H    14.856210     0.536782    20.942117
 H    16.187941     1.674336    20.742629
 H    16.835546    -0.236452    22.253979
 H    16.507162    -1.380039    20.941592
 C    19.442999    -1.915001    17.846000
 C    18.233372    -2.703815    18.330380
 S    17.594789    -3.890430    17.053191
 H    20.266625    -2.574746    17.557374
 H    18.478906    -3.287300    19.220765
 H    17.427386    -2.022800    18.590901
 H    19.185356    -1.296207    16.982692
 H    19.802743    -1.252080    18.641004
 C    13.733000    -7.099999    18.701999
 C    14.824363    -6.984262    17.645684
 S    14.440342    -5.713574    16.352229
 H    13.589910    -6.149482    19.219243
 H    15.784144    -6.728954    18.098069
 H    14.953758    -7.928992    17.111963
 H    12.777568    -7.381572    18.252152
 H    13.999588    -7.861190    19.444592
 C     7.747623    -3.899455    19.236709
 O     7.484163    -5.089565    19.304067
 N     8.078547    -3.134130    20.320696
 H     8.072345    -2.125793    20.214375
 H     8.572716    -8.602759    13.929798
 C     8.899000    -8.791000    12.903000
 H     9.026614    -9.870251    12.777970
 C    10.208108    -8.043484    12.596612
 C    10.092016    -6.548178    12.676574
 N     9.212426    -5.845032    11.872493
 C    10.792631    -5.672474    13.472699
 C     9.385540    -4.575778    12.182312
 N    10.331639    -4.415034    13.143964
 H     8.103616    -8.458428    12.232015
 H    10.993984    -8.373347    13.282796
 H    10.542094    -8.317897    11.588234
 H    11.558615    -5.822212    14.216495
 H     8.860271    -3.739531    11.746280
 H    10.636406    -3.530261    13.540886
 O    13.660111    -1.524331    22.436325
 H    12.803235    -1.976388    22.478222
 H    14.053902    -1.884214    21.629330
 O    14.439072     1.544464    15.769153
 H    14.579921     1.535557    16.727742
 H    14.584625     0.619993    15.527256
 C    11.193999     2.101999    24.316999
 C     9.999367     1.460652    23.586042
 C    10.337397     0.825433    22.225927
 C     9.138573     0.186356    21.527315
 O     7.988533     0.388939    21.930714
 O     9.362262    -0.593651    20.503985
 H    10.875521     2.516829    25.276851
 H    11.983714     1.369926    24.509406
 H    11.631848     2.913710    23.727847
 H     9.557439     0.693085    24.229720
 H     9.216754     2.209688    23.436956
 H    10.748110     1.571537    21.534162
 H    11.119753     0.064921    22.319282
 C     6.651001    -3.397304    22.273046
 O     5.923276    -4.321139    22.612948
 N     6.266178    -2.096287    22.273208
 C     4.874001    -1.683000    22.392000
 C     4.554487    -0.514254    21.460893
 O     5.144720     0.711913    21.869976
 H     6.943414    -1.364435    22.081054
 H     4.254012    -2.548300    22.147190
 H     4.637686    -1.386331    23.421288
 H     4.842265    -0.776362    20.433015
 H     3.473309    -0.352424    21.473191
 H     6.107113     0.655550    21.763065
```

B3LYP BS12 RED_D^{5+}:

```
  102
Absolute Energy (Hartree): -5809.22519252
Fe    11.525631    -2.093621    16.746536
Fe    13.599835    -1.170388    18.688659
Fe    14.895215    -3.550063    17.460684
Fe    11.433588    -3.043718    19.609516
 S    11.299226    -0.853154    18.929061
 S    13.951565    -1.715071    16.432222
 S    13.854401    -3.262030    19.658185
 C    10.010001     1.302001    15.410001
 C    10.857136     0.357461    14.566395
 S    10.414066    -1.422353    14.842013
 H    10.283232     2.343204    15.204453
 H    10.707454     0.546209    13.501280
 H    11.917257     0.495217    14.781343
 H     8.946048     1.178082    15.193464
 H    10.159593     1.116926    16.475994
 C     7.846000    -3.161000    17.912000
 C     8.797782    -4.038820    17.086580
 S    10.606197    -4.179972    17.597666
 H     6.860808    -3.216153    17.440300
 H     8.445159    -5.069057    17.110488
 H     8.826322    -3.697198    16.053764
 H     8.176678    -2.120883    17.906876
 C     8.219355    -3.419327    21.682083
 C     9.436604    -2.885706    22.435478
 S    11.026314    -3.616262    21.815591
 H     8.254987    -4.507409    21.657537
 H     9.487027    -1.801076    22.354064
 H     9.377437    -3.168363    23.487154
 C    16.815997    -0.357999    21.165000
 C    15.532545     0.447648    20.982325
 S    14.989350     0.573358    19.208887
 H    17.627925     0.035046    20.549367
 H    14.715186     0.024175    21.563841
 H    15.676559     1.481714    21.302708
 H    17.128165    -0.315730    22.214459
 H    16.657260    -1.405038    20.903298
 C    19.443000    -1.915000    17.846000
 C    17.984493    -2.161112    18.254940
 S    17.226271    -3.624097    17.391377
 H    20.068957    -2.783113    18.068077
 H    17.926565    -2.358653    19.324564
 H    17.370796    -1.284312    18.047096
 H    19.523306    -1.700731    16.777454
 H    19.838911    -1.056723    18.398385
 C    13.733000    -7.100000    18.702001
 C    14.789595    -6.776587    17.651545
 S    14.233351    -5.483255    16.442224
 H    13.490909    -6.221843    19.302686
 H    15.716950    -6.437186    18.115243
 H    15.025161    -7.657412    17.050343
 H    12.809886    -7.454211    18.237292
 H    14.100426    -7.883895    19.373639
 C     7.734599    -3.725449    19.313159
 O     7.271704    -4.843868    19.507343
 N     8.263406    -2.958950    20.304746
 H     8.431256    -1.965832    20.160789
 H     8.490686    -8.520135    13.880717
 C     8.899000    -8.791000    12.903000
 H     9.019089    -9.877952    12.872734
 C    10.241115    -8.081639    12.653674
 C    10.138124    -6.584227    12.626613
 N     9.375718    -5.925939    11.678109
 C    10.731511    -5.666948    13.461620
 C     9.510465    -4.642009    11.943216
 N    10.322630    -4.429360    13.011427
 H     8.167911    -8.505380    12.143212
 H    10.962237    -8.372180    13.423675
 H    10.651366    -8.427053    11.696939
 H    11.392039    -5.776651    14.306412
 H     9.048695    -3.831117    11.400489
 H    10.563913    -3.526349    13.412186
 O    12.670455    -0.716374    22.358602
 H    12.363459    -1.637445    22.326429
 H    12.299018    -0.336563    21.552924
 O    14.357549     1.633340    15.846588
 H    14.233418     1.795412    16.789502
 H    14.450230     0.671629    15.799155
 C    11.193999     2.101998    24.316999
 C     9.802865     1.598155    23.904635
 C     9.642214     1.381688    22.391642
 C     8.252932     0.851095    21.992867
 O     7.261420     1.399278    22.533445
 O     8.197387    -0.103158    21.157209
 H    11.252569     2.253309    25.399450
 H    11.967705     1.384123    24.032165
 H    11.427167     3.057458    23.834348
 H     9.599544     0.651986    24.420509
 H     9.029150     2.295586    24.236266
 H     9.792251     2.336310    21.870329
 H    10.404553     0.694551    22.021237
 C     6.858623    -3.116491    22.371674
 O     6.368727    -3.951269    23.130571
 N     6.256360    -1.965270    22.021002
 C     4.874004    -1.682999    22.392000
 C     4.327681    -0.436478    21.691240
 O     4.663348     0.781058    22.318898
 H     6.818787    -1.227944    21.573262
 H     4.268767    -2.557084    22.127412
 H     4.776142    -1.540849    23.475016
 H     4.637396    -0.456547    20.633937
 H     3.234805    -0.502486    21.706738
 H     5.642369     0.926676    22.302907
```

B3LYP BS12 TS^{5+}:

```
  102
Absolute Energy (Hartree): -5809.205688
Fe    11.595155    -2.451499    16.971364
Fe    13.926348    -1.611388    18.640232
Fe    15.163172    -3.821750    17.253118
Fe    10.461663    -3.122771    19.844648
 S    11.638939    -1.303764    19.157963
 S    13.930516    -2.048602    16.341187
 S    14.804173    -3.485483    19.492440
 C    10.010000     1.302000    15.409999
 C    10.883616     0.159833    14.898366
 S    10.210597    -1.512825    15.351036
 H    10.432152     2.265158    15.101826
 H    10.950510     0.183667    13.808681
 H    11.895533     0.251619    15.290949
 H     8.992300     1.232346    15.016312
 H     9.952998     1.289334    16.501127
 C     7.846005    -3.161000    17.912001
 C     8.674642    -4.266973    17.238963
 S    10.427598    -4.475459    17.846460
 H     6.890755    -3.094094    17.386254
 H     8.195099    -5.235054    17.384645
 H     8.745192    -4.073866    16.170125
 H     8.359986    -2.201915    17.811857
 C     8.117163    -3.632635    21.663453
 C     9.258190    -3.376639    22.651044
 S    10.888681    -3.957435    21.973503
 H     8.061939    -4.709362    21.498893
 H     9.349382    -2.324168    22.916868
 H     9.069205    -3.945690    23.561455
 C    16.815992    -0.358001    21.165001
 C    15.525787     0.397401    20.862588
 S    15.041157     0.372321    19.068843
 H    17.652880     0.039594    20.585363
 H    14.703463    -0.004655    21.451669
 H    15.629817     1.455384    21.114152
 H    17.060057    -0.265021    22.229383
 H    16.707763    -1.418581    20.931529
 C    19.442998    -1.915001    17.846000
 C    17.982254    -2.316659    18.025427
 S    17.441577    -3.609984    16.806821
 H    20.111256    -2.771113    17.975815
 H    17.815048    -2.720616    19.024059
 H    17.330792    -1.450163    17.913295
 H    19.620416    -1.495804    16.852010
 H    19.716367    -1.155898    18.586989
 C    13.733000    -7.099999    18.701999
 C    14.797009    -7.042298    17.614042
 S    14.409174    -5.789052    16.304801
 H    13.647307    -6.139503    19.212839
 H    15.777588    -6.808687    18.033490
 H    14.879918    -8.001606    17.097523
 H    12.755460    -7.348937    18.281272
 H    13.988776    -7.863101    19.446653
 C     7.540810    -3.504476    19.354790
 O     6.637663    -4.283089    19.612752
 N     8.388342    -2.981269    20.349174
 H     8.561476    -1.635981    20.557598
 H     8.616360    -8.692705    13.955033
 C     8.899000    -8.791000    12.903000
 H     9.056114    -9.852442    12.689910
 C    10.165139    -7.972789    12.596698
 C     9.987270    -6.494274    12.785766
 N     9.055047    -5.779456    12.055002
 C    10.659111    -5.646775    13.635219
 C     9.167791    -4.530853    12.462374
 N    10.125951    -4.393984    13.415913
 H     8.061336    -8.437811    12.296959
 H    10.990880    -8.314300    13.228099
 H    10.466948    -8.164226    11.559660
 H    11.448569    -5.813570    14.350244
 H     8.588352    -3.692886    12.105368
 H    10.377043    -3.527155    13.891247
 O    12.799397    -1.215639    22.450673
 H    12.401045    -2.096664    22.538515
 H    12.649493    -1.022509    21.515060
 O    14.468164     1.324136    15.798680
 H    14.504560     1.486018    16.750383
 H    14.458831     0.357485    15.744655
 C    11.194001     2.102001    24.317001
 C     9.874289     1.590695    23.714497
 C    10.058285     0.966579    22.323997
 C     8.849197     0.205624    21.797996
 O     7.720923     0.365613    22.272672
 O     9.121686    -0.628669    20.834357
 H    11.026300     2.545163    25.302674
 H    11.914807     1.287342    24.429376
 H    11.652929     2.865536    23.680820
 H     9.441192     0.841081    24.384426
 H     9.144524     2.404179    23.661972
 H    10.310052     1.733847    21.581364
 H    10.902297     0.272885    22.329093
 C     6.723485    -3.299750    22.258110
 O     6.123681    -4.153220    22.902686
 N     6.221276    -2.071906    21.995145
 C     4.874003    -1.683000    22.392000
 C     4.413080    -0.407549    21.690699
 O     4.940582     0.784518    22.255593
 H     6.851385    -1.309180    21.771838
 H     4.204998    -2.510060    22.139166
 H     4.805231    -1.531894    23.476890
 H     4.640603    -0.480715    20.617199
 H     3.327362    -0.335141    21.793894
 H     5.908228     0.749698    22.198772
```

B3LYP BS12 S-OX$_{D\text{-}H}^{5+}$:

```
  102
Absolute Energy (Hartree): -5809.24025960
Fe    11.431968    -2.238273    17.198543
Fe    13.409174    -1.340926    19.264550
Fe    14.888681    -3.371298    17.678317
Fe    10.199123    -3.172080    19.960211
 S    11.046329    -1.129825    19.394829
 S    13.757652    -1.464196    16.932580
 S    14.380330    -3.248446    19.926380
 C    10.009994     1.302000    15.409996
 C    10.871821     0.177407    14.841325
 S    10.261430    -1.509288    15.311317
 H    10.395811     2.277061    15.090546
 H    10.876774     0.212036    13.749482
 H    11.904333     0.269423    15.179982
 H     8.974246     1.215380    15.071067
 H    10.010890     1.275912    16.502464
 C     7.846002    -3.161001    17.912001
 C     8.718063    -4.215370    17.214644
 S    10.449774    -4.405012    17.884025
 H     6.944267    -3.021259    17.310313
 H     8.255192    -5.200022    17.293557
 H     8.825006    -3.973715    16.158736
 H     8.368853    -2.203294    17.960574
 C     7.898599    -3.931977    21.616977
 C     8.991466    -3.611102    22.650745
 S    10.696697    -4.042799    22.055202
 H     7.810334    -5.018789    21.519871
 H     8.979649    -2.547646    22.896272
 H     8.806330    -4.178031    23.563081
 C    16.816008    -0.358005    21.165007
 C    15.428821    -0.019008    21.697300
 S    14.228704     0.545197    20.394897
 H    17.264715     0.491985    20.644963
 H    14.989227    -0.876859    22.204944
 H    15.473411     0.805862    22.412191
 H    17.476050    -0.645405    21.991415
 H    16.751983    -1.193898    20.471499
 C    19.442998    -1.915000    17.846000
 C    17.979963    -2.134274    18.223007
 S    17.164737    -3.412999    17.158131
 H    20.020593    -2.838862    17.940967
 H    17.907497    -2.472723    19.256642
 H    17.422380    -1.202261    18.127288
 H    19.536641    -1.562408    16.815386
 H    19.891944    -1.162650    18.503559
 C    13.733001    -7.099998    18.701997
 C    14.754598    -6.644750    17.666156
 S    14.137567    -5.270473    16.583787
 H    13.488386    -6.288381    19.390378
 H    15.676499    -6.312568    18.146430
 H    15.013427    -7.463610    16.990569
 H    12.805189    -7.426492    18.225463
 H    14.132593    -7.936791    19.286567
 C     7.394904    -3.622186    19.293193
 O     6.338967    -4.242461    19.432237
 N     8.252812    -3.342363    20.319525
 H     6.865481     0.648986    20.847157
 H     8.606452    -8.676840    13.950652
 C     8.899000    -8.791000    12.903000
 H     9.043410    -9.856915    12.703259
 C    10.179771    -7.993902    12.601706
 C    10.022018    -6.511318    12.776457
 N     9.115456    -5.786657    12.023215
 C    10.688981    -5.669362    13.635190
 C     9.238460    -4.537771    12.427388
 N    10.179034    -4.410568    13.399312
 H     8.072954    -8.433095    12.284007
 H    10.993785    -8.341907    13.244913
 H    10.489356    -8.199509    11.569667
 H    11.458874    -5.841908    14.369729
 H     8.678194    -3.693322    12.055418
 H    10.434145    -3.546495    13.877001
 O    12.107895    -1.003345    22.892791
 H    11.828998    -1.875515    22.569702
 H    12.430052    -0.546964    22.102587
 O    16.111209     0.995159    17.585155
 H    15.632750     0.954814    18.430577
 H    15.635621     0.346353    17.049014
 C    11.193997     2.102004    24.316999
 C     9.698935     1.963441    24.012686
 C     9.451777     1.447811    22.595262
 C     8.000434     1.237122    22.253168
 O     7.064404     1.445805    23.007499
 O     7.830435     0.784173    21.001918
 H    11.352992     2.465725    25.336350
 H    11.701878     1.140872    24.210612
 H    11.672783     2.809785    23.632659
 H     9.238165     1.275462    24.728271
 H     9.193037     2.925214    24.145606
 H     9.865234     2.132280    21.845708
 H     9.978122     0.500459    22.434606
 C     6.540516    -3.489192    22.200497
 O     5.911679    -4.237820    22.941039
 N     6.142934    -2.225039    21.919041
 C     4.874001    -1.683000    22.392000
 C     4.289366    -0.672863    21.416635
 O     5.126527     0.478017    21.230397
 H     6.720461    -1.675509    21.298741
 H     4.181774    -2.517575    22.521147
 H     4.999875    -1.213330    23.376645
 H     4.170874    -1.120601    20.428677
 H     3.302663    -0.359056    21.775175
 H     5.349043     0.868625    22.093872
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B3LYP BS12 S-OX_D^{5+}:

```
  101
Absolute Energy (Hartree): -5808.715271
Fe    11.474251    -2.279664    17.082994
Fe    13.660294    -1.469992    18.790771
Fe    15.027288    -3.664681    17.383603
Fe    10.257362    -2.984835    19.902795
 S    11.369801    -1.086241    19.238274
 S    13.824508    -1.886395    16.481936
 S    14.551059    -3.394086    19.604525
 C    10.010001     1.301992    15.409999
 C    10.879904     0.194841    14.822540
 S    10.250557    -1.497829    15.247089
 H    10.410339     2.285595    15.137678
 H    10.903773     0.257945    13.732053
 H    11.905110     0.287479    15.180219
 H     8.981827     1.235361    15.044021
 H     9.983664     1.234238    16.500161
 C     7.846003    -3.160989    17.912006
 C     8.724221    -4.209669    17.213739
 S    10.460991    -4.365807    17.881855
 H     6.921321    -3.057275    17.338707
 H     8.276817    -5.200261    17.307682
 H     8.821182    -3.977137    16.154577
 H     8.350099    -2.191330    17.915529
 C     8.027277    -3.746275    21.647178
 C     9.134544    -3.311705    22.615372
 S    10.820504    -3.810945    22.003260
 H     7.979291    -4.839551    21.636467
 H     9.124511    -2.227687    22.731797
 H     8.983922    -3.780465    23.588137
 C    16.815994    -0.358001    21.164999
 C    15.471179     0.338231    20.968477
 S    14.948914     0.426219    19.189521
 H    17.603862     0.134871    20.589162
 H    14.690756    -0.170579    21.532663
 H    15.517202     1.372724    21.316599
 H    17.098299    -0.333693    22.224210
 H    16.762121    -1.401219    20.851391
 C    19.442998    -1.915001    17.846000
 C    17.968014    -2.231593    18.095234
 S    17.316709    -3.512201    16.920696
 H    20.064301    -2.808268    17.955747
 H    17.826188    -2.614038    19.106243
 H    17.355974    -1.333575    17.999481
 H    19.597042    -1.517655    16.839208
 H    19.794163    -1.165559    18.563977
 C    13.733000    -7.100000    18.701999
 C    14.802212    -6.918020    17.631322
 S    14.349626    -5.636557    16.369155
 H    13.594272    -6.179859    19.271761
 H    15.758441    -6.637666    18.078448
 H    14.959137    -7.845769    17.075292
 H    12.770969    -7.367244    18.257570
 H    14.022505    -7.895510    19.399162
 C     7.460738    -3.597780    19.318994
 O     6.434845    -4.258009    19.503566
 N     8.343730    -3.261157    20.298313
 H     8.582537    -8.653166    13.940716
 C     8.899002    -8.790998    12.903000
 H     9.038226    -9.862082    12.727787
 C    10.194098    -8.011223    12.617582
 C    10.048216    -6.524332    12.764327
 N     9.173234    -5.800693    11.973470
 C    10.699081    -5.677595    13.630684
 C     9.299110    -4.547367    12.363906
 N    10.211877    -4.416806    13.361108
 H     8.091210    -8.438179    12.257433
 H    10.989253    -8.356075    13.285516
 H    10.525175    -8.237642    11.596466
 H    11.444196    -5.849159    14.390570
 H     8.760063    -3.701868    11.964104
 H    10.458924    -3.548400    13.836403
 O    13.671521    -2.120334    22.669542
 H    12.735557    -2.352543    22.559183
 H    14.080251    -2.516443    21.886575
 O    14.470662     1.441657    15.931579
 H    14.435687     1.615758    16.881075
 H    14.424331     0.474779    15.892511
 C    11.193997     2.101998    24.316998
 C     9.825869     1.501862    23.985139
 C     9.530116     1.454097    22.480969
 C     8.126409     0.906216    22.168101
 O     7.170913     1.416858    22.817444
 O     8.030460    -0.002146    21.301933
 H    11.374006     2.118316    25.397000
 H    12.001881     1.527265    23.853790
 H    11.271618     3.131765    23.951053
 H     9.766845     0.485411    24.393477
 H     9.031014     2.073725    24.472025
 H     9.586606     2.472062    22.072544
 H    10.274274     0.852317    21.953324
 C     6.645524    -3.333419    22.210452
 O     6.004252    -4.158231    22.868025
 N     6.219458    -2.077766    21.982290
 C     4.874006    -1.683001    22.391999
 C     4.364908    -0.418061    21.687285
 O     4.629574     0.788368    22.368862
 H     6.853010    -1.364705    21.588826
 H     4.212589    -2.526428    22.171884
 H     4.820044    -1.511958    23.475093
 H     4.748225    -0.406442    20.655491
 H     3.273750    -0.496491    21.621685
 H     5.608856     0.939048    22.454657
```

B3LYP BS12 S-OX_P^{5+}:

```
  101
Absolute Energy (Hartree): -5808.723471
Fe    11.644734    -2.137679    17.131186
Fe    13.894409    -1.390905    18.638486
Fe    15.092436    -3.695685    17.301286
Fe    10.025411    -2.208168    20.124008
 S    11.727739    -0.802278    19.194715
 S    13.965913    -1.897777    16.341053
 S    14.678736    -3.340376    19.518612
 C    10.009999     1.302001    15.409999
 C    10.893451     0.212901    14.813437
 S    10.312495    -1.477393    15.297310
 H    10.370190     2.295439    15.116466
 H    10.888140     0.260985    13.721715
 H    11.923667     0.340021    15.145935
 H     8.973907     1.199343    15.075183
 H    10.016899     1.245609    16.501291
 C     7.845998    -3.161001    17.912001
 C     8.932628    -4.069386    17.328064
 S    10.548698    -3.951722    18.230571
 H     6.955848    -3.227086    17.280285
 H     8.616677    -5.113081    17.384028
 H     9.110228    -3.822886    16.283101
 H     8.186453    -2.122559    17.903364
 C     7.968894    -3.799424    21.624871
 C     9.008750    -3.345250    22.674708
 S    10.745347    -3.351567    22.039385
 H     7.971983    -4.892124    21.560863
 H     8.781085    -2.333207    23.010010
 H     8.962480    -4.008750    23.538842
 C    16.816002    -0.358000    21.165000
 C    15.607433     0.493769    20.786624
 S    15.264429     0.483392    18.962697
 H    17.722100    -0.005621    20.664441
 H    14.719910     0.144165    21.314025
 H    15.768694     1.539835    21.058873
 H    16.982890    -0.314885    22.248106
 H    16.654143    -1.400741    20.887577
 C    19.443000    -1.915000    17.846000
 C    17.991863    -2.312405    18.088978
 S    17.395551    -3.575812    16.870318
 H    20.112816    -2.776681    17.923310
 H    17.871224    -2.736482    19.086796
 H    17.341035    -1.440690    18.026466
 H    19.571141    -1.477147    16.852210
 H    19.760980    -1.171459    18.585826
 C    13.733000    -7.100000    18.702001
 C    14.855776    -6.914560    17.689105
 S    14.422175    -5.706038    16.350568
 H    13.466699    -6.150771    19.169549
 H    15.770310    -6.570963    18.176413
 H    15.087549    -7.857668    17.187205
 H    12.834702    -7.498612    18.223613
 H    14.039765    -7.798810    19.489825
 C     7.449031    -3.630112    19.311921
 O     6.472644    -4.384891    19.454371
 N     8.252862    -3.220162    20.313933
 H     8.567882    -8.666126    13.937704
 C     8.899001    -8.790999    12.903000
 H     9.034031    -9.860377    12.714231
 C    10.204222    -8.017060    12.648181
 C    10.075137    -6.531320    12.822997
 N     9.204801    -5.782066    12.050983
 C    10.745465    -5.708221    13.697559
 C     9.352427    -4.537264    12.461408
 N    10.275274    -4.436499    13.452420
 H     8.102770    -8.424273    12.250886
 H    10.988271    -8.383221    13.317984
 H    10.545328    -8.228033    11.626889
 H    11.497135    -5.902101    14.445481
 H     8.822029    -3.677499    12.081044
 H    10.536747    -3.579074    13.940175
 O    13.711568    -1.891873    22.540120
 H    12.756672    -2.056059    22.563102
 H    13.980216    -2.294216    21.700856
 O    14.473085     1.471363    15.845168
 H    14.483605     1.599538    16.804211
 H    14.456335     0.506035    15.765293
 C    11.193998     2.102000    24.317000
 C     9.933187     1.755009    23.516965
 C    10.178080     0.757267    22.380477
 C     8.925092     0.416712    21.573570
 O     7.900334     1.109675    21.700887
 O     8.977734    -0.592498    20.778699
 H    10.969478     2.816615    25.114784
 H    11.631592     1.211412    24.778846
 H    11.961234     2.546757    23.675140
 H     9.173597     1.346059    24.192207
 H     9.497101     2.666105    23.098030
 H    10.918478     1.145984    21.670484
 H    10.608475    -0.177685    22.754402
 C     6.584589    -3.438534    22.199271
 O     5.977960    -4.211060    22.938896
 N     6.152449    -2.188690    21.916376
 C     4.874003    -1.683000    22.391999
 C     4.795025    -0.159956    22.312836
 O     5.691597     0.491967    23.194065
 H     6.702774    -1.641025    21.264428
 H     4.049432    -2.112508    21.805177
 H     4.738308    -2.006405    23.426602
 H     4.960918     0.163771    21.276446
 H     3.773948     0.132886    22.584898
 H     6.500537     0.709458    22.691205
```

B3LYP BS12 RED_P^{4+}:

```
  102
Absolute Energy (Hartree): -5809.354334
Fe    11.952058    -2.104944    16.927282
Fe    14.311383    -1.469272    18.357995
Fe    15.330818    -3.913148    17.200663
Fe    10.806006    -2.242760    19.955832
 S    12.246142    -0.624863    18.900119
 S    14.284041    -2.127492    16.105022
 S    14.838041    -3.440056    19.367626
 C    10.010000     1.302000    15.410001
 C    11.004242     0.381533    14.708410
 S    10.661350    -1.400321    15.069850
 H    10.217151     2.350941    15.164362
 H    10.949579     0.508115    13.624195
 H    12.022574     0.615761    15.019177
 H     8.982630     1.076509    15.111840
 H    10.082433     1.186729    16.493816
 C     7.845998    -3.160997    17.911999
 C     8.993842    -3.811123    17.131001
 S    10.641433    -3.826753    18.001920
 H     6.934618    -3.237531    17.310934
 H     8.756730    -4.858366    16.939999
 H     9.121657    -3.296802    16.181448
 H     8.062313    -2.103162    18.079482
 C     7.933818    -3.825533    21.661261
 C     9.071665    -3.361163    22.592486
 S    10.781617    -3.630872    21.935034
 H     7.961352    -4.908037    21.548719
 H     8.948317    -2.308926    22.846351
 H     8.987678    -3.929106    23.521395
 C    16.816000    -0.358001    21.165001
 C    15.923920     0.606783    20.387767
 S    15.898422     0.273116    18.564974
 H    17.849766    -0.305640    20.812779
 H    14.899041     0.575690    20.762289
 H    16.278672     1.634015    20.504402
 H    16.805001    -0.107834    22.232494
 H    16.469751    -1.387338    21.054358
 C    19.443001    -1.914999    17.846000
 C    18.265023    -2.776099    18.282943
 S    17.679068    -3.925118    16.946551
 H    20.297292    -2.524488    17.534401
 H    18.531388    -3.387570    19.148558
 H    17.432672    -2.136998    18.566407
 H    19.165220    -1.268524    17.009631
 H    19.768951    -1.273040    18.672805
 C    13.733000    -7.100000    18.702000
 C    14.812090    -7.135621    17.625353
 S    14.542537    -5.894517    16.274166
 H    13.704930    -6.129417    19.198754
 H    15.799984    -6.960824    18.056169
 H    14.836444    -8.112481    17.134840
 H    12.744650    -7.281297    18.273402
 H    13.925184    -7.870186    19.459202
 C     7.606037    -3.898873    19.219498
 O     7.115132    -5.023607    19.242459
 N     8.044007    -3.248888    20.328717
 H     8.291384    -2.262271    20.266135
 H     8.544443    -8.614137    13.922299
 C     8.898999    -8.791001    12.903001
 H     9.012332    -9.870328    12.763011
 C    10.229658    -8.060441    12.650939
 C    10.137482    -6.565273    12.758838
 N     9.309103    -5.827481    11.931284
 C    10.812914    -5.722001    13.610054
 C     9.487739    -4.569307    12.284278
 N    10.389016    -4.449900    13.292899
 H     8.129913    -8.433446    12.214269
 H    10.987364    -8.417944    13.354785
 H    10.589727    -8.321787    11.647868
 H    11.537481    -5.901750    14.387702
 H     8.997332    -3.712616    11.847377
 H    10.681274    -3.578883    13.732789
 O    13.192914    -1.316882    22.495499
 H    12.516020    -2.017463    22.516935
 H    13.307369    -1.167459    21.547504
 O    14.533383     1.302022    15.698583
 H    14.699746     1.309421    16.654917
 H    14.544845     0.354469    15.500632
 C    11.193998     2.101999    24.316998
 C    10.005069     1.399548    23.632655
 C    10.334033     0.780776    22.263590
 C     9.180873     0.007090    21.615254
 O     8.020009     0.147688    22.059722
 O     9.446899    -0.772922    20.633599
 H    10.901366     2.496878    25.294197
 H    12.026396     1.407291    24.465284
 H    11.564591     2.936929    23.713358
 H     9.633115     0.608891    24.292731
 H     9.176482     2.104588    23.518468
 H    10.636480     1.556951    21.548830
 H    11.189476     0.103659    22.338991
 C     6.539540    -3.488387    22.237469
 O     5.770383    -4.356516    22.641056
 N     6.223403    -2.173520    22.187867
 C     4.874004    -1.683001    22.392000
 C     4.644633    -0.351098    21.678993
 O     5.306114     0.745167    22.292399
 H     6.941095    -1.478840    21.982372
 H     4.177075    -2.436472    22.012686
 H     4.653528    -1.548253    23.459655
 H     4.929074    -0.451327    20.621850
 H     3.574807    -0.125541    21.715581
 H     6.265284     0.637377    22.170146
```

B3LYP BS12 RED_D^{4+}:

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  102
Absolute Energy (Hartree): -5809.355191
Fe    11.478342    -2.139004    16.823686
Fe    13.575592    -1.266469    18.572118
Fe    14.895057    -3.601806    17.397151
Fe    11.240960    -3.114426    19.669740
 S    11.318247    -0.851414    18.918778
 S    13.880027    -1.829789    16.294923
 S    13.942788    -3.318902    19.532553
 C    10.010001     1.302001    15.410002
 C    10.843139     0.312576    14.604146
 S    10.320929    -1.437713    14.911803
 H    10.324911     2.331184    15.199436
 H    10.732597     0.492694    13.532070
 H    11.900700     0.415185    14.850589
 H     8.947633     1.211433    15.167327
 H    10.126187     1.124151    16.480970
 C     7.846001    -3.160999    17.912000
 C     8.746939    -4.074703    17.065531
 S    10.544056    -4.251151    17.566582
 H     6.849599    -3.153965    17.460015
 H     8.348959    -5.088893    17.092947
 H     8.751500    -3.732574    16.031623
 H     8.235452    -2.141044    17.912936
 C     8.197771    -3.475893    21.687948
 C     9.391221    -2.982045    22.509133
 S    11.010718    -3.699971    21.947262
 H     8.221700    -4.563663    21.646624
 H     9.445109    -1.894325    22.470084
 H     9.254523    -3.288574    23.547500
 C    16.815995    -0.357999    21.164999
 C    15.489967     0.352420    20.893904
 S    15.065944     0.457192    19.086461
 H    17.641342     0.112177    20.623959
 H    14.671941    -0.146093    21.412620
 H    15.529867     1.384951    21.248827
 H    17.042824    -0.321453    22.237078
 H    16.759398    -1.405817    20.867747
 C    19.443000    -1.915000    17.846000
 C    17.975691    -2.195568    18.194190
 S    17.252282    -3.599096    17.216248
 H    20.071145    -2.790302    18.034651
 H    17.885969    -2.450878    19.250348
 H    17.365217    -1.310197    18.019559
 H    19.552751    -1.639228    16.793829
 H    19.818686    -1.087038    18.456943
 C    13.733000    -7.100001    18.702001
 C    14.857696    -6.818964    17.714238
 S    14.364398    -5.613046    16.393827
 H    13.410197    -6.182760    19.196835
 H    15.740123    -6.427337    18.223710
 H    15.157262    -7.731344    17.192510
 H    12.865181    -7.531626    18.197416
 H    14.068173    -7.805816    19.471308
 C     7.719634    -3.725003    19.312051
 O     7.191318    -4.815967    19.503742
 N     8.296708    -3.000110    20.313076
 H     8.489499    -2.008817    20.182731
 H     8.461999    -8.546050    13.875060
 C     8.899000    -8.791000    12.903000
 H     9.005198    -9.878297    12.839942
 C    10.257420    -8.091781    12.721964
 C    10.171660    -6.593104    12.745237
 N     9.428737    -5.895333    11.809066
 C    10.762012    -5.711427    13.620369
 C     9.573053    -4.622457    12.122519
 N    10.371832    -4.455799    13.207854
 H     8.198558    -8.468369    12.129094
 H    10.949592    -8.418147    13.503825
 H    10.693935    -8.410101    11.767016
 H    11.408032    -5.854917    14.471719
 H     9.125791    -3.787644    11.604440
 H    10.609085    -3.565450    13.644258
 O    12.581011    -0.796803    22.267862
 H    12.247992    -1.715117    22.271011
 H    12.292184    -0.476863    21.402476
 O    14.426596     1.525493    15.896532
 H    14.411679     1.667553    16.852418
 H    14.398886     0.559546    15.824839
 C    11.194000     2.101997    24.316997
 C     9.800139     1.593383    23.919457
 C     9.650660     1.307172    22.417714
 C     8.248124     0.820136    22.009932
 O     7.265997     1.371756    22.571499
 O     8.170921    -0.098319    21.140406
 H    11.259860     2.274766    25.396168
 H    11.963891     1.377258    24.039451
 H    11.428105     3.046213    23.812948
 H     9.584452     0.673027    24.475747
 H     9.032275     2.312850    24.216719
 H     9.853896     2.224846    21.849161
 H    10.387994     0.569866    22.097151
 C     6.822570    -3.164343    22.336105
 O     6.296805    -3.998731    23.074359
 N     6.245730    -1.992655    22.002397
 C     4.874004    -1.682999    22.392000
 C     4.333478    -0.434108    21.689730
 O     4.674126     0.783790    22.314313
 H     6.821093    -1.258824    21.564891
 H     4.251464    -2.550330    22.146142
 H     4.794192    -1.529493    23.475572
 H     4.642297    -0.458242    20.632427
 H     3.239771    -0.494548    21.706178
 H     5.656790     0.919620    22.310136
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B3LYP BS12 TS^{4+}:

```
  102
Absolute Energy (Hartree): -5809.328255
Fe    11.632354    -2.479252    16.936609
Fe    14.005939    -1.734079    18.485770
Fe    15.263560    -3.979092    17.160528
Fe    10.565552    -3.216584    19.859551
 S    11.821603    -1.315163    19.083076
 S    13.997566    -2.262390    16.186952
 S    14.866523    -3.636159    19.371538
 C    10.010005     1.301991    15.409996
 C    10.918520     0.200580    14.864574
 S    10.290225    -1.504464    15.251190
 H    10.406208     2.288103    15.139729
 H    10.993622     0.271851    13.776636
 H    11.924327     0.308729    15.268818
 H     8.996274     1.217003    15.008030
 H     9.947737     1.246948    16.499144
 C     7.845996    -3.160993    17.912012
 C     8.669044    -4.214122    17.154370
 S    10.418791    -4.473177    17.744442
 H     6.882681    -3.054924    17.405173
 H     8.181135    -5.186383    17.236049
 H     8.722987    -3.947081    16.100206
 H     8.361218    -2.197389    17.875275
 C     8.040058    -3.726326    21.652552
 C     9.145260    -3.459813    22.682958
 S    10.795788    -4.054519    22.082750
 H     7.991773    -4.805328    21.495752
 H     9.209511    -2.402014    22.941197
 H     8.904978    -4.012157    23.593046
 C    16.815987    -0.358001    21.165000
 C    15.569878     0.362992    20.651483
 S    15.315671     0.208637    18.818936
 H    17.719165     0.016170    20.674744
 H    14.682127    -0.007906    21.161496
 H    15.639112     1.434415    20.855390
 H    16.920981    -0.200073    22.244988
 H    16.748233    -1.432239    20.985124
 C    19.442998    -1.915000    17.846000
 C    18.080620    -2.541855    18.117985
 S    17.587950    -3.781321    16.828262
 H    20.233717    -2.670729    17.802483
 H    18.078698    -3.056814    19.080372
 H    17.313188    -1.770856    18.159440
 H    19.444403    -1.371053    16.897266
 H    19.697249    -1.205630    18.641876
 C    13.733001    -7.100000    18.701999
 C    14.889597    -7.154449    17.710530
 S    14.647856    -6.028223    16.255512
 H    13.625695    -6.099129    19.120399
 H    15.832379    -6.888295    18.193160
 H    15.002521    -8.161094    17.299656
 H    12.789791    -7.366336    18.217739
 H    13.903968    -7.801606    19.527864
 C     7.555429    -3.595227    19.341120
 O     6.689590    -4.451031    19.525819
 N     8.337274    -3.073415    20.357001
 H     8.641314    -1.749291    20.550707
 H     8.558647    -8.648915    13.932492
 C     8.899004    -8.790995    12.902999
 H     9.043070    -9.862766    12.735800
 C    10.200490    -8.012057    12.644307
 C    10.055828    -6.523770    12.780552
 N     9.202775    -5.800084    11.965788
 C    10.694042    -5.674601    13.654166
 C     9.330042    -4.544466    12.349625
 N    10.222245    -4.412740    13.364820
 H     8.106011    -8.441773    12.237219
 H    10.979629    -8.354814    13.331651
 H    10.554627    -8.243523    11.631951
 H    11.420797    -5.845750    14.431565
 H     8.807181    -3.697862    11.930982
 H    10.467181    -3.541608    13.838341
 O    12.783815    -1.416291    22.411541
 H    12.267536    -2.238636    22.510294
 H    12.714962    -1.263265    21.457004
 O    14.424538     1.126040    15.739969
 H    14.475382     1.237607    16.700651
 H    14.400299     0.161745    15.645077
 C    11.193997     2.101996    24.316997
 C     9.908964     1.512633    23.703998
 C    10.137921     0.846019    22.339114
 C     8.938964     0.080066    21.785205
 O     7.799647     0.254919    22.239864
 O     9.223158    -0.757178    20.837644
 H    10.994267     2.536425    25.300835
 H    11.961324     1.330833    24.433371
 H    11.612321     2.888836    23.680991
 H     9.493853     0.768962    24.392027
 H     9.147348     2.293562    23.612170
 H    10.426440     1.588225    21.584577
 H    10.972902     0.142398    22.394061
 C     6.642243    -3.379781    22.213860
 O     5.986675    -4.215202    22.833774
 N     6.191740    -2.125971    21.971875
 C     4.874011    -1.682999    22.391999
 C     4.474003    -0.357902    21.746909
 O     5.066526     0.782558    22.352797
 H     6.855270    -1.396453    21.734649
 H     4.156543    -2.460442    22.112718
 H     4.815332    -1.571085    23.483331
 H     4.690439    -0.399814    20.669370
 H     3.393693    -0.233372    21.862207
 H     6.031321     0.702055    22.274851
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B3LYP BS12 S-$OX_{D\text{-}H}^{4+}$:

```
  102
Absolute Energy (Hartree): -5809.340220
Fe    11.439531    -2.269201    17.108921
Fe    13.489820    -1.348121    18.888088
Fe    14.931798    -3.499837    17.483974
Fe    10.350722    -3.104354    19.917441
 S    11.205314    -0.993203    19.170500
 S    13.774259    -1.702117    16.560904
 S    14.399553    -3.266771    19.691332
 C    10.010001     1.301995    15.410000
 C    10.835674     0.188743    14.768455
 S    10.225398    -1.498590    15.225519
 H    10.396626     2.286237    15.118457
 H    10.793604     0.260831    13.678603
 H    11.883046     0.265979    15.063408
 H     8.962014     1.240899    15.102764
 H    10.046596     1.230277    16.499838
 C     7.846007    -3.160993    17.912001
 C     8.692202    -4.205035    17.172202
 S    10.443866    -4.385243    17.781324
 H     6.907819    -3.037455    17.361760
 H     8.233200    -5.190782    17.271423
 H     8.747016    -3.965694    16.110687
 H     8.366529    -2.201335    17.921788
 C     7.978398    -3.812464    21.626720
 C     9.028323    -3.394643    22.670631
 S    10.758575    -3.811119    22.154031
 H     7.953931    -4.906679    21.575145
 H     8.968331    -2.316019    22.838061
 H     8.812792    -3.898651    23.615255
 C    16.815994    -0.358000    21.165001
 C    15.410944     0.219855    21.307538
 S    14.565852     0.612708    19.698422
 H    17.464109     0.312611    20.594333
 H    14.768524    -0.455020    21.872112
 H    15.438827     1.168126    21.850618
 H    17.263534    -0.510966    22.154264
 H    16.780896    -1.319484    20.655890
 C    19.442989    -1.915000    17.845999
 C    17.967063    -2.172780    18.142565
 S    17.241071    -3.465476    17.032565
 H    20.038089    -2.825147    17.966145
 H    17.845406    -2.510236    19.171441
 H    17.394477    -1.255520    18.011599
 H    19.580872    -1.552780    16.823411
 H    19.838539    -1.155996    18.530427
 C    13.732999    -7.100001    18.702002
 C    14.813462    -6.781675    17.674612
 S    14.296817    -5.488898    16.449896
 H    13.480505    -6.215148    19.289526
 H    15.728551    -6.445293    18.165454
 H    15.063838    -7.670079    17.088583
 H    12.817473    -7.444619    18.214568
 H    14.076425    -7.884334    19.387565
 C     7.476175    -3.622191    19.324457
 O     6.463715    -4.333164    19.469620
 N     8.314118    -3.245498    20.314709
 H     7.809002     1.481979    19.773882
 H     8.537705    -8.645302    13.924704
 C     8.899002    -8.790998    12.903001
 H     9.039271    -9.863996    12.740043
 C    10.211110    -8.021084    12.671276
 C    10.073218    -6.532282    12.808660
 N     9.239128    -5.802844    11.979221
 C    10.694630    -5.688443    13.699534
 C     9.361886    -4.549163    12.371075
 N    10.232627    -4.424432    13.405264
 H     8.122546    -8.437586    12.220266
 H    10.974078    -8.371163    13.373119
 H    10.583294    -8.253438    11.665502
 H    11.405867    -5.860222    14.491223
 H     8.849179    -3.699461    11.946180
 H    10.464504    -3.556197    13.891773
 O    12.297012    -0.860603    22.526216
 H    11.847081    -1.723524    22.417362
 H    12.438617    -0.580161    21.612326
 O    16.300778     0.689565    16.838229
 H    15.940091     0.752139    17.739831
 H    15.759725    -0.015566    16.455755
 C    11.194000     2.101998    24.316999
 C     9.828657     1.876851    23.658470
 C     9.954371     1.706003    22.141377
 C     8.665860     1.361301    21.450282
 O     7.759970     0.709351    21.938962
 O     8.610818     1.830299    20.193915
 H    11.090984     2.224676    25.398972
 H    11.850212     1.248397    24.126714
 H    11.681812     2.999337    23.923234
 H     9.357978     0.982865    24.074733
 H     9.158760     2.715655    23.880402
 H    10.383054     2.590560    21.665049
 H    10.638533     0.874332    21.929094
 C     6.588227    -3.438959    22.177149
 O     5.925474    -4.230927    22.846232
 N     6.179143    -2.163905    21.954455
 C     4.874009    -1.683001    22.391999
 C     4.337032    -0.561552    21.508323
 O     4.907760     0.715163    21.777545
 H     6.798364    -1.557936    21.433934
 H     4.194688    -2.537971    22.367647
 H     4.909974    -1.324135    23.429418
 H     4.462416    -0.843259    20.453009
 H     3.265384    -0.453592    21.696736
 H     5.874984     0.649253    21.743940
```

B3LYP BS12 RED_P^{3+}:

```
  102
Absolute Energy (Hartree): -5809.420243
Fe    12.015167    -1.943727    16.943422
Fe    14.438970    -1.448356    18.539508
Fe    15.323392    -3.905394    17.189172
Fe    10.839665    -2.210890    19.923018
 S    12.245419    -0.566374    18.957194
 S    14.279812    -2.139261    16.108652
 S    14.877187    -3.574655    19.379109
 C    10.010000     1.302000    15.409999
 C    10.930223     0.351151    14.644440
 S    10.592435    -1.423820    15.052264
 H    10.216361     2.346345    15.141563
 H    10.799872     0.480050    13.565566
 H    11.971096     0.575564    14.882328
 H     8.958243     1.092449    15.195140
 H    10.164450     1.190265    16.485377
 C     7.846001    -3.161000    17.912002
 C     9.009017    -3.792534    17.136609
 S    10.669820    -3.757065    17.970063
 H     6.937673    -3.242060    17.305833
 H     8.784918    -4.844587    16.950753
 H     9.112864    -3.280913    16.181968
 H     8.052138    -2.102584    18.087238
 C     7.929755    -3.827244    21.660308
 C     9.060410    -3.345933    22.594397
 S    10.776347    -3.587611    21.945868
 H     7.967011    -4.910617    21.554072
 H     8.916986    -2.295835    22.846980
 H     8.977067    -3.913993    23.524020
 C    16.816000    -0.358001    21.165000
 C    16.116149     0.754663    20.385912
 S    16.009240     0.399182    18.571752
 H    17.835635    -0.505764    20.797520
 H    15.107539     0.916413    20.775857
 H    16.659555     1.697327    20.502621
 H    16.868280    -0.112713    22.233954
 H    16.282876    -1.304605    21.060535
 C    19.442999    -1.915000    17.846000
 C    18.357754    -2.884324    18.299350
 S    17.717996    -3.965221    16.934307
 H    20.294838    -2.437654    17.397870
 H    18.731067    -3.536709    19.093972
 H    17.515783    -2.325254    18.696405
 H    19.043491    -1.214674    17.107601
 H    19.812485    -1.329019    18.696937
 C    13.733000    -7.100000    18.702000
 C    14.942986    -7.068697    17.772178
 S    14.668969    -5.990940    16.287428
 H    13.444397    -6.087140    18.985941
 H    15.826043    -6.698590    18.297571
 H    15.178484    -8.071747    17.403323
 H    12.874943    -7.564322    18.207416
 H    13.953981    -7.669910    19.613684
 C     7.596668    -3.897756    19.217366
 O     7.085151    -5.015985    19.241159
 N     8.036273    -3.253451    20.327298
 H     8.314714    -2.274243    20.266982
 H     8.438278    -8.594019    13.875077
 C     8.899001    -8.790999    12.903000
 H     9.014187    -9.873874    12.792450
 C    10.258039    -8.078819    12.785096
 C    10.180484    -6.580987    12.876733
 N     9.405719    -5.837399    12.003170
 C    10.831776    -5.740789    13.750813
 C     9.592933    -4.578681    12.354582
 N    10.447795    -4.465306    13.402045
 H     8.213145    -8.437631    12.129544
 H    10.935428    -8.442390    13.563665
 H    10.715331    -8.354520    11.825963
 H    11.517184    -5.925136    14.562810
 H     9.137496    -3.716955    11.890558
 H    10.730516    -3.589230    13.846939
 O    13.197036    -1.211640    22.403270
 H    12.572247    -1.956443    22.454290
 H    13.164606    -0.985497    21.461201
 O    14.450191     1.220566    15.776891
 H    14.688993     1.273656    16.718258
 H    14.409809     0.258999    15.642021
 C    11.193999     2.102000    24.317000
 C     9.988498     1.407088    23.652451
 C    10.284844     0.806941    22.267442
 C     9.125675     0.020856    21.639828
 O     7.970792     0.166695    22.114150
 O     9.376731    -0.760443    20.664051
 H    10.927570     2.481201    25.308256
 H    12.030132     1.405296    24.430520
 H    11.548476     2.946108    23.716413
 H     9.635857     0.606245    24.311178
 H     9.154923     2.111123    23.570386
 H    10.554799     1.594373    21.552042
 H    11.153245     0.145077    22.311315
 C     6.532356    -3.495133    22.231026
 O     5.753524    -4.365242    22.615203
 N     6.222700    -2.177517    22.201920
 C     4.874001    -1.683000    22.392000
 C     4.615885    -0.413687    21.579793
 O     5.259555     0.738529    22.101838
 H     6.943679    -1.480615    22.010296
 H     4.181862    -2.473637    22.088353
 H     4.671095    -1.463304    23.449682
 H     4.898543    -0.593244    20.532677
 H     3.541961    -0.203969    21.604174
 H     6.224084     0.618969    22.022013
```

B3LYP BS12 RED_D^{3+}:

```
  102
Absolute Energy (Hartree): -5809.432754
Fe    11.572305    -2.003615    16.857712
Fe    13.800488    -1.209977    18.708159
Fe    14.857859    -3.625925    17.377181
Fe    11.386042    -3.051236    19.659482
 S    11.398572    -0.790486    18.940751
 S    13.927823    -1.852027    16.280496
 S    14.012292    -3.396559    19.561031
 C    10.010001     1.301999    15.409998
 C    10.645573     0.254498    14.499339
 S    10.202196    -1.477558    14.981977
 H    10.252523     2.315217    15.065076
 H    10.310073     0.394914    13.467198
 H    11.733480     0.355310    14.504890
 H     8.921764     1.196482    15.427811
 H    10.374235     1.199579    16.434141
 C     7.845999    -3.161000    17.912002
 C     8.785084    -4.067422    17.096664
 S    10.585495    -4.163428    17.588395
 H     6.856552    -3.179367    17.444117
 H     8.407044    -5.089759    17.138882
 H     8.778705    -3.739140    16.057921
 H     8.216420    -2.134716    17.904139
 C     8.219959    -3.425386    21.688346
 C     9.415717    -2.890096    22.483148
 S    11.040684    -3.627535    21.960600
 H     8.267389    -4.513509    21.669155
 H     9.456761    -1.803535    22.395569
 H     9.275637    -3.146900    23.534978
 C    16.816001    -0.358000    21.165001
 C    15.656853     0.592839    20.859545
 S    15.234387     0.687561    19.048897
 H    17.725771    -0.058360    20.636870
 H    14.767901     0.286929    21.412366
 H    15.911667     1.609066    21.174189
 H    17.028319    -0.368720    22.241731
 H    16.568279    -1.374587    20.856355
 C    19.442999    -1.915000    17.846000
 C    18.012316    -2.290130    18.266704
 S    17.272743    -3.640882    17.226984
 H    20.112351    -2.778780    17.903336
 H    18.012974    -2.631419    19.303859
 H    17.357891    -1.419868    18.212849
 H    19.464381    -1.538479    16.819506
 H    19.836300    -1.132315    18.504908
 C    13.733000    -7.099999    18.701999
 C    14.858818    -6.865392    17.701915
 S    14.393446    -5.686058    16.346671
 H    13.418389    -6.159810    19.157790
 H    15.746429    -6.474706    18.203756
 H    15.144170    -7.801131    17.212437
 H    12.860756    -7.544913    18.216077
 H    14.062866    -7.776695    19.500588
 C     7.702787    -3.700157    19.319467
 O     7.142989    -4.775030    19.532351
 N     8.285828    -2.971955    20.307588
 H     8.567289    -2.010378    20.140173
 H     8.421129    -8.569352    13.861223
 C     8.899000    -8.791000    12.903000
 H     8.953542    -9.878647    12.791348
 C    10.297301    -8.153903    12.828547
 C    10.274219    -6.655765    12.920615
 N     9.576390    -5.887730    12.004537
 C    10.877034    -5.840107    13.850175
 C     9.759226    -4.637526    12.386209
 N    10.540002    -4.554094    13.492232
 H     8.259981    -8.394856    12.110514
 H    10.929987    -8.548491    13.629383
 H    10.769511    -8.450651    11.883158
 H    11.501440    -6.044747    14.706114
 H     9.349443    -3.761384    11.907206
 H    10.777109    -3.690097    13.981416
 O    12.668130    -0.721588    22.204037
 H    12.350712    -1.644561    22.234560
 H    12.363870    -0.433489    21.330005
 O    12.385667     2.457322    18.768727
 H    11.801713     1.695726    18.897498
 H    13.266647     2.040672    18.804960
 C    11.194001     2.102001    24.317001
 C     9.783374     1.612101    23.954281
 C     9.589869     1.344744    22.454916
 C     8.171399     0.888020    22.065921
 O     7.206950     1.415394    22.684969
 O     8.065169     0.020446    21.152133
 H    11.295560     2.253205    25.397123
 H    11.952197     1.381447    24.000159
 H    11.418267     3.054418    23.824209
 H     9.572463     0.688257    24.506942
 H     9.033274     2.337523    24.282726
 H     9.802626     2.261159    21.888173
 H    10.302946     0.596422    22.106377
 C     6.848189    -3.127632    22.348650
 O     6.341260    -3.955246    23.109627
 N     6.247841    -1.972155    22.000332
 C     4.873998    -1.683000    22.392000
 C     4.326568    -0.418129    21.722489
 O     4.633946     0.783299    22.394308
 H     6.803784    -1.232619    21.546286
 H     4.255535    -2.546648    22.121011
 H     4.789180    -1.559072    23.479179
 H     4.656838    -0.400318    20.671746
 H     3.233464    -0.496606    21.714340
 H     5.615402     0.941463    22.405485
```

B3LYP BS12 TS^{3+}:

```
  102
Absolute Energy (Hartree): -5809.397255
Fe    11.705407    -2.318735    16.886860
Fe    14.100061    -1.624894    18.582811
Fe    15.226464    -3.958326    17.129645
Fe    10.662364    -3.057025    19.770871
 S    11.749350    -1.111904    18.948820
 S    14.005908    -2.265447    16.119419
 S    14.920194    -3.657792    19.355592
 C    10.009999     1.302001    15.410000
 C    10.816451     0.195159    14.725549
 S    10.225885    -1.513600    15.156248
 H    10.384677     2.290535    15.115580
 H    10.753841     0.300226    13.638322
 H    11.867290     0.281226    15.003779
 H     8.949043     1.241902    15.147148
 H    10.095866     1.213443    16.495895
 C     7.846006    -3.160999    17.912001
 C     8.686402    -4.204935    17.161338
 S    10.456616    -4.354290    17.707550
 H     6.867460    -3.090871    17.426053
 H     8.229783    -5.189050    17.282168
 H     8.697973    -3.964171    16.098351
 H     8.336231    -2.185775    17.847931
 C     8.107452    -3.622698    21.651749
 C     9.201705    -3.287982    22.672783
 S    10.880207    -3.765641    22.063765
 H     8.106185    -4.704762    21.513953
 H     9.199683    -2.227454    22.929129
 H     8.995605    -3.848959    23.586982
 C    16.815996    -0.358001    21.165000
 C    15.715791     0.558718    20.631278
 S    15.440151     0.385146    18.805090
 H    17.762999    -0.178357    20.647408
 H    14.780292     0.360401    21.155425
 H    15.976789     1.605674    20.813603
 H    16.971458    -0.190373    22.239010
 H    16.543690    -1.405341    21.022321
 C    19.442998    -1.915001    17.846000
 C    18.062507    -2.525876    18.057801
 S    17.602859    -3.790226    16.780454
 H    20.232439    -2.673221    17.894066
 H    18.003177    -3.012279    19.033630
 H    17.305240    -1.744454    18.042793
 H    19.511699    -1.422171    16.871875
 H    19.646741    -1.163920    18.618721
 C    13.733000    -7.100000    18.702000
 C    14.903682    -7.150132    17.725031
 S    14.652624    -6.065468    16.240710
 H    13.607060    -6.090834    19.095177
 H    15.829343    -6.840325    18.215914
 H    15.051730    -8.166890    17.348811
 H    12.799309    -7.381284    18.206887
 H    13.899962    -7.784026    19.544342
 C     7.605988    -3.577401    19.352627
 O     6.797037    -4.486141    19.570954
 N     8.362569    -2.988440    20.342343
 H     8.618010    -1.651038    20.513624
 H     8.564251    -8.662821    13.936049
 C     8.899000    -8.791000    12.903000
 H     9.046887    -9.860310    12.721801
 C    10.194877    -8.001292    12.646628
 C    10.041457    -6.514893    12.795828
 N     9.165630    -5.793243    12.003390
 C    10.691479    -5.665607    13.661674
 C     9.291928    -4.538729    12.396204
 N    10.204083    -4.407322    13.391741
 H     8.100082    -8.436510    12.246847
 H    10.977774    -8.344167    13.329482
 H    10.547724    -8.224588    11.631520
 H    11.437500    -5.830629    14.421943
 H     8.752179    -3.693042    11.997659
 H    10.445926    -3.533606    13.871604
 O    12.812404    -1.104323    22.230595
 H    12.305523    -1.934046    22.332341
 H    12.680116    -0.920488    21.286899
 O    14.384297     1.064298    15.717862
 H    14.400807     1.193485    16.678364
 H    14.354885     0.095005    15.646954
 C    11.193999     2.101999    24.316999
 C     9.880170     1.571438    23.709082
 C    10.073243     0.929373    22.327370
 C     8.864529     0.175739    21.777302
 O     7.737149     0.327737    22.275941
 O     9.127311    -0.616863    20.789699
 H    11.020515     2.537858    25.305726
 H    11.927145     1.297638    24.421520
 H    11.641295     2.873978    23.682705
 H     9.448662     0.827309    24.386419
 H     9.145119     2.380614    23.645236
 H    10.352155     1.683542    21.581048
 H    10.910021     0.227282    22.351151
 C     6.698644    -3.329232    22.216408
 O     6.082518    -4.173089    22.866363
 N     6.191256    -2.101077    21.946207
 C     4.874003    -1.682999    22.392000
 C     4.407866    -0.408769    21.692437
 O     4.991660     0.779272    22.209492
 H     6.829838    -1.358577    21.685828
 H     4.176672    -2.500001    22.183819
 H     4.850953    -1.512017    23.477510
 H     4.583789    -0.506316    20.611098
 H     3.329389    -0.306493    21.844867
 H     5.959375     0.699194    22.147210
```

B3LYP BS12 S-$OX_{D\text{-}H}^{3+}$:

```
  102
Absolute Energy (Hartree): -5809.404462
Fe    11.443586    -2.092675    17.067678
Fe    13.442871    -1.502387    19.217432
Fe    14.907626    -3.587564    17.529041
Fe    10.358694    -3.002187    19.871058
 S    11.068110    -0.891426    19.086483
 S    13.813378    -1.752437    16.672609
 S    14.380950    -3.562196    19.741053
 C    10.010001     1.301999    15.409999
 C    10.740892     0.196228    14.646120
 S    10.173710    -1.509694    15.102360
 H    10.361164     2.292225    15.091755
 H    10.588359     0.316019    13.569298
 H    11.814583     0.260263    14.834347
 H     8.929774     1.249542    15.242389
 H    10.191285     1.204064    16.483240
 C     7.846002    -3.160998    17.912003
 C     8.704098    -4.198489    17.178734
 S    10.467560    -4.271621    17.752961
 H     6.903650    -3.042182    17.364726
 H     8.270388    -5.193563    17.308307
 H     8.722063    -3.976646    16.110932
 H     8.364821    -2.201254    17.916683
 C     7.984343    -3.785841    21.625946
 C     9.027813    -3.337950    22.665219
 S    10.762869    -3.710316    22.143003
 H     7.977517    -4.881467    21.583550
 H     8.936538    -2.259847    22.824917
 H     8.825087    -3.840827    23.614275
 C    16.815997    -0.358000    21.165000
 C    15.407011    -0.132341    21.690946
 S    14.225999     0.496695    20.410162
 H    17.235960     0.563893    20.751172
 H    15.005779    -1.060702    22.099916
 H    15.413493     0.603933    22.500146
 H    17.480638    -0.709620    21.965590
 H    16.812087    -1.107648    20.376395
 C    19.442997    -1.915000    17.846000
 C    17.970267    -2.186959    18.147528
 S    17.267584    -3.527128    17.084902
 H    20.051826    -2.810678    18.003982
 H    17.856202    -2.493981    19.188020
 H    17.383122    -1.279106    17.999319
 H    19.579208    -1.594737    16.808770
 H    19.827927    -1.122355    18.498964
 C    13.733000    -7.100000    18.702000
 C    14.838157    -6.871264    17.676574
 S    14.401638    -5.601818    16.394764
 H    13.454435    -6.161049    19.182617
 H    15.757855    -6.553092    18.171591
 H    15.062352    -7.796032    17.136123
 H    12.837832    -7.510993    18.227578
 H    14.064872    -7.802783    19.477287
 C     7.478831    -3.616899    19.326278
 O     6.473792    -4.345265    19.473860
 N     8.305086    -3.219387    20.313382
 H     7.719848     1.578003    19.829895
 H     8.399988    -8.569671    13.850488
 C     8.899001    -8.790999    12.903000
 H     9.036037    -9.874955    12.833859
 C    10.247395    -8.056565    12.808589
 C    10.128640    -6.560726    12.853725
 N     9.446344    -5.854326    11.878103
 C    10.634470    -5.689266    13.790526
 C     9.545568    -4.586124    12.233007
 N    10.255776    -4.432272    13.378473
 H     8.235151    -8.477195    12.093614
 H    10.902913    -8.380945    13.622052
 H    10.743182    -8.349116    11.873946
 H    11.215499    -5.840491    14.686270
 H     9.122914    -3.746258    11.702425
 H    10.441548    -3.544770    13.857563
 O    12.156738    -0.764334    22.817335
 H    11.777968    -1.628707    22.558576
 H    12.554331    -0.414219    22.001212
 O    15.845735     0.812289    17.478910
 H    15.474687     0.813186    18.380685
 H    15.319824     0.115147    17.051083
 C    11.194000     2.101997    24.316998
 C     9.806441     1.935546    23.688281
 C     9.891449     1.772236    22.168338
 C     8.582319     1.463776    21.504383
 O     7.667472     0.838498    22.011299
 O     8.518752     1.933547    20.248676
 H    11.119823     2.218213    25.403016
 H    11.808259     1.226439    24.099620
 H    11.704671     2.986042    23.920924
 H     9.312963     1.055017    24.107102
 H     9.170411     2.795630    23.931631
 H    10.334366     2.646141    21.685323
 H    10.546912     0.923627    21.932078
 C     6.594799    -3.426118    22.178749
 O     5.938528    -4.212477    22.863531
 N     6.177436    -2.155028    21.947893
 C     4.874002    -1.682999    22.392000
 C     4.314540    -0.567854    21.512784
 O     4.835507     0.724727    21.804026
 H     6.781200    -1.562835    21.393542
 H     4.201938    -2.544643    22.376306
 H     4.912757    -1.320975    23.428602
 H     4.463254    -0.833906    20.456472
 H     3.236903    -0.497549    21.686439
 H     5.805669     0.695957    21.785162
```

B3LYP BS13 RED_P^{5+}:

```
  102
Absolute Energy (Hartree): -5809.229700
Fe    11.924735    -1.642022    16.814990
Fe    14.314678    -1.210678    18.446662
Fe    15.188821    -3.714179    17.333470
Fe    10.703293    -1.864824    19.839198
 S    12.149096    -0.309409    18.850352
 S    14.324139    -1.802767    16.220942
 S    14.697418    -3.159080    19.512564
 C    10.010010     1.301998    15.410005
 C    10.872353     0.453578    14.481967
 S    10.711557    -1.355419    14.844186
 H    10.112670     2.366121    15.165739
 H    10.578795     0.596451    13.439375
 H    11.920782     0.738217    14.577269
 H     8.954073     1.030978    15.324518
 H    10.311589     1.165773    16.451191
 C     7.845995    -3.161002    17.912002
 C     9.057533    -3.614244    17.098332
 S    10.690108    -3.433139    17.962094
 H     6.941144    -3.397184    17.343789
 H     8.976068    -4.678057    16.874279
 H     9.116856    -3.050831    16.169636
 H     7.877725    -2.079286    18.063848
 C     8.064532    -3.656799    21.678068
 C     9.221594    -3.091447    22.522851
 S    10.890606    -3.279524    21.736787
 H     8.159811    -4.737806    21.604429
 H     9.059514    -2.044333    22.772948
 H     9.263868    -3.645429    23.462027
 C    16.815994    -0.357996    21.164994
 C    15.869566     0.679872    20.577668
 S    15.775074     0.564198    18.731744
 H    17.830426    -0.225225    20.780494
 H    14.866203     0.567721    20.990021
 H    16.210678     1.693004    20.802392
 H    16.850422    -0.264835    22.256540
 H    16.490718    -1.369374    20.919002
 C    19.442998    -1.915001    17.846001
 C    18.153954    -2.583760    18.310071
 S    17.504890    -3.817977    17.085707
 H    20.235014    -2.647310    17.663480
 H    18.309146    -3.113511    19.252598
 H    17.384180    -1.833276    18.474510
 H    19.282485    -1.352356    16.922988
 H    19.798331    -1.215291    18.610669
 C    13.733001    -7.100000    18.701998
 C    14.814768    -6.938273    17.641325
 S    14.399443    -5.652452    16.372686
 H    13.584575    -6.169886    19.253440
 H    15.772151    -6.673483    18.093055
 H    14.959148    -7.868855    17.087110
 H    12.776694    -7.377091    18.251674
 H    14.015379    -7.882732    19.415756
 C     7.783723    -3.912521    19.229896
 O     7.568187    -5.113098    19.289438
 N     8.077793    -3.139910    20.317240
 H     8.065368    -2.132747    20.207349
 H     8.555611    -8.591223    13.922001
 C     8.899001    -8.790999    12.903000
 H     9.028541    -9.871645    12.792187
 C    10.212837    -8.046328    12.610469
 C    10.093421    -6.550811    12.675268
 N     9.233270    -5.855998    11.843597
 C    10.769619    -5.667700    13.484424
 C     9.394055    -4.584145    12.150777
 N    10.313221    -4.414341    13.136146
 H     8.114992    -8.466130    12.215060
 H    10.987428    -8.369462    13.312478
 H    10.562954    -8.329831    11.610201
 H    11.515381    -5.809589    14.250015
 H     8.877799    -3.752292    11.695943
 H    10.603377    -3.524859    13.535970
 O    13.612088    -1.486880    22.467340
 H    12.770872    -1.969633    22.493399
 H    14.038723    -1.843195    21.675583
 O    14.236175     1.632273    15.891392
 H    14.404351     1.661902    16.844330
 H    14.406011     0.704084    15.678980
 C    11.194000     2.102000    24.317000
 C    10.000308     1.448959    23.594967
 C    10.335259     0.831351    22.226163
 C     9.140543     0.183032    21.530135
 O     7.989543     0.379729    21.932173
 O     9.368250    -0.599255    20.507911
 H    10.881460     2.503654    25.284386
 H    11.997010     1.380366    24.492861
 H    11.611838     2.925309    23.729457
 H     9.577454     0.669353    24.237076
 H     9.205096     2.187381    23.460598
 H    10.727468     1.591535    21.539268
 H    11.130838     0.083301    22.305809
 C     6.656323    -3.396036    22.273602
 O     5.929980    -4.320684    22.614830
 N     6.267971    -2.095760    22.271902
 C     4.874001    -1.683000    22.392000
 C     4.554354    -0.512884    21.462930
 O     5.143681     0.712984    21.874599
 H     6.944488    -1.363216    22.079496
 H     4.254728    -2.548364    22.145630
 H     4.638280    -1.388545    23.421980
 H     4.842809    -0.772865    20.434763
 H     3.473111    -0.351562    21.475035
 H     6.105969     0.656965    21.768197
```

B3LYP BS13 RED_D^{5+}:

```
  102
Absolute Energy (Hartree): -5809.22307888
Fe    11.479486    -1.792342    16.842119
Fe    13.757652    -1.021849    18.628726
Fe    14.845946    -3.493455    17.421973
Fe    11.436299    -2.988278    19.621653
 S    11.427402    -0.694039    19.003932
 S    13.923991    -1.578238    16.397860
 S    13.880626    -3.189879    19.584545
 C    10.010005     1.301999    15.410002
 C    10.599117     0.292805    14.430950
 S    10.250490    -1.464543    14.909136
 H    10.229243     2.324411    15.082644
 H    10.173406     0.426628    13.433892
 H    11.678781     0.426533    14.350993
 H     8.925499     1.190027    15.488148
 H    10.432527     1.169547    16.408645
 C     7.846000    -3.160999    17.912003
 C     8.837977    -4.013115    17.108221
 S    10.648434    -3.988573    17.587702
 H     6.864006    -3.266336    17.442607
 H     8.549138    -5.061826    17.172456
 H     8.835360    -3.707432    16.063381
 H     8.133020    -2.108164    17.886594
 C     8.251273    -3.375022    21.684352
 C     9.457754    -2.823524    22.441484
 S    11.065954    -3.535442    21.843352
 H     8.300300    -4.462534    21.666552
 H     9.497487    -1.739535    22.350718
 H     9.392487    -3.097130    23.495102
 C    16.815992    -0.357999    21.164998
 C    15.623789     0.567059    20.933529
 S    15.156273     0.712801    19.140359
 H    17.684793    -0.049844    20.579469
 H    14.755863     0.225607    21.495260
 H    15.857629     1.586272    21.247806
 H    17.092280    -0.338383    22.225028
 H    16.565023    -1.386995    20.902915
 C    19.442998    -1.915001    17.846000
 C    17.952030    -2.079217    18.172212
 S    17.174365    -3.514813    17.283348
 H    20.010212    -2.806956    18.123857
 H    17.821050    -2.251850    19.239242
 H    17.397843    -1.177272    17.911476
 H    19.596522    -1.731406    16.779814
 H    19.848220    -1.063555    18.402101
 C    13.733002    -7.099999    18.701998
 C    14.838405    -6.699419    17.731287
 S    14.278155    -5.475729    16.449332
 H    13.363240    -6.237545    19.258982
 H    15.692797    -6.274676    18.260184
 H    15.196991    -7.564421    17.169342
 H    12.887188    -7.547206    18.174552
 H    14.115228    -7.833627    19.420331
 C     7.754069    -3.704351    19.322901
 O     7.299210    -4.821463    19.538870
 N     8.295891    -2.924978    20.302093
 H     8.426693    -1.925898    20.154814
 H     8.454653    -8.531222    13.867977
 C     8.899000    -8.791000    12.903000
 H     9.025571    -9.877116    12.866745
 C    10.244658    -8.071761    12.707688
 C    10.128308    -6.575439    12.693882
 N     9.382333    -5.915752    11.733635
 C    10.686554    -5.660766    13.555917
 C     9.492215    -4.633473    12.019387
 N    10.273414    -4.423485    13.110314
 H     8.194267    -8.501215    12.120178
 H    10.941069    -8.365505    13.498929
 H    10.689572    -8.404340    11.761923
 H    11.326015    -5.771103    14.416825
 H     9.032686    -3.822066    11.475458
 H    10.480842    -3.521286    13.535900
 O    12.795228    -0.660791    22.396951
 H    12.465954    -1.574019    22.358085
 H    12.391701    -0.255678    21.619336
 O    13.937197     1.817124    15.905152
 H    13.773430     1.971292    16.842721
 H    14.152610     0.874681    15.869124
 C    11.194000     2.101999    24.316999
 C     9.797286     1.607441    23.910006
 C     9.641950     1.365804    22.400665
 C     8.246749     0.858481    21.989401
 O     7.259820     1.402072    22.542032
 O     8.183976    -0.072585    21.127836
 H    11.259643     2.250942    25.399294
 H    11.961386     1.380111    24.024990
 H    11.430244     3.056816    23.834558
 H     9.580420     0.672908    24.441381
 H     9.030935     2.319541    24.226983
 H     9.821184     2.305005    21.860711
 H    10.392320     0.655043    22.051185
 C     6.883964    -3.086469    22.371356
 O     6.412855    -3.918921    23.144281
 N     6.257716    -1.951359    22.008126
 C     4.874003    -1.682999    22.391999
 C     4.317354    -0.430530    21.710827
 O     4.657575     0.780915    22.347693
 H     6.805988    -1.210200    21.550549
 H     4.271974    -2.556726    22.118934
 H     4.784943    -1.556390    23.477358
 H     4.615357    -0.438348    20.650003
 H     3.224898    -0.499296    21.737566
 H     5.635526     0.929895    22.320299
```

B3LYP BS13 TS^{5+}:

```
  102
Absolute Energy (Hartree): -5809.204097
Fe    11.585692    -2.245036    17.011893
Fe    13.943012    -1.544307    18.659940
Fe    15.129806    -3.787157    17.305702
Fe    10.472064    -3.047151    19.822187
 S    11.618106    -1.135043    19.128522
 S    13.943647    -1.961174    16.375480
 S    14.749114    -3.436491    19.536742
 C    10.009999     1.302002    15.409999
 C    10.837178     0.159470    14.823431
 S    10.197409    -1.523471    15.289355
 H    10.417922     2.267576    15.090345
 H    10.831819     0.204403    13.731922
 H    11.874536     0.242264    15.148554
 H     8.967451     1.244997    15.084750
 H    10.025659     1.270892    16.502355
 C     7.846008    -3.161000    17.912000
 C     8.709623    -4.248053    17.253455
 S    10.478287    -4.353226    17.826823
 H     6.888639    -3.128881    17.386959
 H     8.272347    -5.231928    17.426445
 H     8.756273    -4.074744    16.179624
 H     8.331262    -2.188435    17.797541
 C     8.143118    -3.600059    21.663726
 C     9.293291    -3.332503    22.637444
 S    10.919614    -3.899829    21.936134
 H     8.093253    -4.677899    21.504891
 H     9.378943    -2.279136    22.901156
 H     9.122746    -3.903055    23.550475
 C    16.815992    -0.358002    21.165000
 C    15.553408     0.443018    20.869220
 S    15.074301     0.426989    19.076530
 H    17.665145     0.011311    20.584555
 H    14.717876     0.068527    21.458266
 H    15.694912     1.496893    21.119661
 H    17.067052    -0.278339    22.228973
 H    16.668482    -1.412875    20.927987
 C    19.442998    -1.915001    17.845999
 C    17.980980    -2.300110    18.054656
 S    17.410295    -3.604606    16.862903
 H    20.105128    -2.775081    17.980055
 H    17.826774    -2.688841    19.061466
 H    17.335367    -1.429415    17.939732
 H    19.608342    -1.514349    16.842379
 H    19.734388    -1.145983    18.569654
 C    13.733000    -7.100000    18.702000
 C    14.774780    -7.018346    17.593719
 S    14.375947    -5.727788    16.324045
 H    13.670073    -6.157361    19.248000
 H    15.765602    -6.805477    17.999563
 H    14.838394    -7.962882    17.048172
 H    12.743262    -7.320507    18.294438
 H    13.995123    -7.892373    19.412908
 C     7.550526    -3.493253    19.358166
 O     6.654520    -4.274827    19.630325
 N     8.399924    -2.954989    20.344140
 H     8.548084    -1.606297    20.549793
 H     8.620397    -8.683024    13.955175
 C     8.899000    -8.791001    12.903000
 H     9.056151    -9.854351    12.699288
 C    10.162761    -7.974020    12.584171
 C     9.982002    -6.494610    12.762014
 N     9.052492    -5.786311    12.021639
 C    10.645085    -5.641090    13.612418
 C     9.158615    -4.535489    12.425043
 N    10.109339    -4.391377    13.384416
 H     8.058484    -8.444322    12.297091
 H    10.991380    -8.308907    13.215434
 H    10.460718    -8.173916    11.547644
 H    11.429470    -5.801806    14.334327
 H     8.578756    -3.700972    12.060687
 H    10.353058    -3.521017    13.859178
 O    12.812475    -1.154073    22.404670
 H    12.422145    -2.039384    22.483582
 H    12.638179    -0.940459    21.477569
 O    14.452862     1.402242    15.814037
 H    14.465367     1.559961    16.766870
 H    14.447627     0.435799    15.756748
 C    11.194001     2.102001    24.317001
 C     9.870560     1.594012    23.720005
 C    10.042738     0.999796    22.314565
 C     8.832164     0.241733    21.787809
 O     7.703534     0.406743    22.258542
 O     9.103354    -0.596047    20.825798
 H    11.035516     2.521382    25.314534
 H    11.923100     1.291753    24.401412
 H    11.638052     2.883739    23.692468
 H     9.450694     0.827668    24.379470
 H     9.134837     2.403293    23.693158
 H    10.279725     1.784488    21.585373
 H    10.891507     0.312771    22.296386
 C     6.749174    -3.275707    22.266900
 O     6.165153    -4.131282    22.922744
 N     6.227227    -2.057277    21.995779
 C     4.874003    -1.683000    22.392000
 C     4.398451    -0.416935    21.683855
 O     4.915245     0.783671    22.240368
 H     6.845138    -1.288352    21.761253
 H     4.215127    -2.519583    22.143850
 H     4.804845    -1.526998    23.476007
 H     4.624262    -0.494360    20.610304
 H     3.312300    -0.355189    21.789183
 H     5.882982     0.759354    22.179942
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B3LYP BS13 S-$OX_{D\text{-}H}^{5+}$:

```
  102
Absolute Energy (Hartree): -5809.23920700
Fe    11.388167    -1.987739    17.237515
Fe    13.446892    -1.291792    19.292207
Fe    14.867259    -3.355336    17.719400
Fe    10.225864    -3.130283    19.934959
 S    11.039902    -1.007240    19.410720
 S    13.772824    -1.397037    16.979482
 S    14.355407    -3.218991    19.969961
 C    10.009998     1.301999    15.409998
 C    10.806826     0.182595    14.743841
 S    10.255876    -1.516505    15.246188
 H    10.369365     2.281781    15.074580
 H    10.699801     0.232160    13.657565
 H    11.869711     0.277316    14.972757
 H     8.946404     1.224965    15.168335
 H    10.110845     1.255231    16.497339
 C     7.845999    -3.161004    17.911998
 C     8.752398    -4.191628    17.224190
 S    10.503961    -4.255011    17.847411
 H     6.934559    -3.060242    17.317348
 H     8.340889    -5.195700    17.339307
 H     8.822583    -3.972649    16.159948
 H     8.336192    -2.184754    17.941419
 C     7.946560    -3.879470    21.627696
 C     9.052123    -3.539667    22.640825
 S    10.747242    -3.988632    22.027121
 H     7.864018    -4.967945    21.545423
 H     9.046182    -2.470970    22.862809
 H     8.879874    -4.087284    23.567186
 C    16.816005    -0.358004    21.165004
 C    15.458126     0.087210    21.693229
 S    14.272553     0.615689    20.365623
 H    17.297982     0.431689    20.583608
 H    14.981494    -0.707066    22.267230
 H    15.555983     0.957844    22.345875
 H    17.475736    -0.624306    21.998801
 H    16.697884    -1.233298    20.529884
 C    19.442998    -1.915001    17.845999
 C    17.979555    -2.109737    18.236758
 S    17.142879    -3.392758    17.194101
 H    20.010018    -2.844026    17.952944
 H    17.909358    -2.431658    19.275722
 H    17.433251    -1.172197    18.130839
 H    19.533566    -1.580905    16.809044
 H    19.905241    -1.157165    18.487793
 C    13.733001    -7.099998    18.701997
 C    14.763623    -6.621011    17.685875
 S    14.143470    -5.244013    16.607535
 H    13.460205    -6.297716    19.390430
 H    15.674702    -6.282813    18.182096
 H    15.042172    -7.429484    17.005717
 H    12.820929    -7.441744    18.206585
 H    14.138689    -7.932597    19.288301
 C     7.420056    -3.613598    19.303323
 O     6.376019    -4.247835    19.463972
 N     8.284246    -3.306442    20.318425
 H     6.845961     0.705562    20.848913
 H     8.569889    -8.651814    13.936677
 C     8.899000    -8.790999    12.903000
 H     9.039700    -9.862276    12.730966
 C    10.197902    -8.012581    12.632096
 C    10.049590    -6.525666    12.775492
 N     9.180020    -5.805422    11.975903
 C    10.691237    -5.675399    13.645542
 C     9.299939    -4.551073    12.364445
 N    10.203606    -4.416237    13.369225
 H     8.099579    -8.438848    12.246977
 H    10.985465    -8.357329    13.309134
 H    10.540221    -8.239921    11.615041
 H    11.430789    -5.841411    14.412155
 H     8.763088    -3.707832    11.956889
 H    10.445000    -3.546455    13.845225
 O    12.237399    -1.019907    22.908033
 H    11.922362    -1.879065    22.582283
 H    12.472208    -0.531650    22.107291
 O    16.170524     1.049287    17.556266
 H    15.683611     1.009671    18.396678
 H    15.689392     0.413374    17.010424
 C    11.193998     2.102007    24.317004
 C     9.697806     1.963244    24.019643
 C     9.442695     1.482662    22.591497
 C     7.989775     1.264971    22.258806
 O     7.061742     1.433398    23.032635
 O     7.809947     0.855440    20.994566
 H    11.357949     2.445552    25.342479
 H    11.705511     1.145418    24.189325
 H    11.665757     2.825315    23.644187
 H     9.245128     1.255352    24.720692
 H     9.188070     2.918802    24.179689
 H     9.842829     2.189415    21.855779
 H     9.974537     0.544187    22.400130
 C     6.590070    -3.444199    22.223517
 O     5.992757    -4.185683    22.996878
 N     6.152408    -2.200513    21.912797
 C     4.874001    -1.683000    22.392000
 C     4.283649    -0.662632    21.431182
 O     5.113956     0.495173    21.260385
 H     6.700664    -1.651645    21.266095
 H     4.188453    -2.525908    22.503553
 H     4.991942    -1.230064    23.385215
 H     4.166519    -1.097279    20.437152
 H     3.295254    -0.360047    21.794569
 H     5.348389     0.865758    22.129649
```

B3LYP BS13 S-OX_D^{5+}:

```
  101
Absolute Energy (Hartree): -5808.71407563
Fe    11.430683    -2.001697    17.075524
Fe    13.720262    -1.357336    18.802571
Fe    14.987135    -3.594658    17.409359
Fe    10.289026    -2.785267    19.880303
 S    11.409717    -0.830891    19.170271
 S    13.821893    -1.757882    16.508313
 S    14.537229    -3.298066    19.633068
 C    10.010002     1.301991    15.410000
 C    10.769162     0.192131    14.687034
 S    10.188322    -1.509505    15.153422
 H    10.391264     2.284977    15.109641
 H    10.642562     0.281427    13.605210
 H    11.837295     0.265031    14.897985
 H     8.941117     1.262421    15.181888
 H    10.123806     1.208749    16.492615
 C     7.845996    -3.160990    17.912003
 C     8.797546    -4.187560    17.279516
 S    10.548102    -4.154957    17.908817
 H     6.913531    -3.166518    17.342003
 H     8.426407    -5.200535    17.445853
 H     8.863386    -4.021825    16.205064
 H     8.272846    -2.157911    17.842200
 C     8.114772    -3.605757    21.664973
 C     9.213112    -3.087959    22.600304
 S    10.903688    -3.566949    21.984357
 H     8.126794    -4.700646    21.682194
 H     9.168544    -1.999892    22.659163
 H     9.091988    -3.514003    23.596588
 C    16.815999    -0.357999    21.164999
 C    15.553247     0.469515    20.942794
 S    15.029480     0.519193    19.165445
 H    17.648194     0.021111    20.566413
 H    14.729021     0.076343    21.536082
 H    15.714424     1.510411    21.232981
 H    17.107125    -0.321954    22.221400
 H    16.646763    -1.400777    20.893542
 C    19.442999    -1.915000    17.846000
 C    17.962193    -2.193505    18.105981
 S    17.277458    -3.471327    16.948623
 H    20.043087    -2.821836    17.962052
 H    17.815135    -2.560186    19.121958
 H    17.370764    -1.283278    18.000601
 H    19.601406    -1.531997    16.834269
 H    19.816045    -1.166603    18.553961
 C    13.733000    -7.100000    18.702000
 C    14.815964    -6.847392    17.658721
 S    14.334824    -5.570687    16.400090
 H    13.486561    -6.185035    19.242760
 H    15.747808    -6.530170    18.130140
 H    15.030106    -7.758513    17.094375
 H    12.816153    -7.466115    18.233340
 H    14.071065    -7.850031    19.426833
 C     7.493404    -3.527227    19.348218
 O     6.474434    -4.181752    19.586113
 N     8.390953    -3.142650    20.297292
 H     8.569995    -8.638174    13.934731
 C     8.899002    -8.790998    12.903000
 H     9.036426    -9.864848    12.743679
 C    10.200220    -8.019102    12.623906
 C    10.054795    -6.530623    12.752412
 N     9.189888    -5.816142    11.942659
 C    10.692208    -5.674327    13.619780
 C     9.308455    -4.558880    12.323663
 N    10.206904    -4.417355    13.331569
 H     8.100904    -8.443747    12.242624
 H    10.986385    -8.358455    13.305222
 H    10.542357    -8.258180    11.609285
 H    11.427244    -5.835805    14.391778
 H     8.773224    -3.718179    11.908893
 H    10.440230    -3.543405    13.806310
 O    13.698443    -1.848254    22.653462
 H    12.763740    -2.081906    22.531564
 H    14.123410    -2.291644    21.906064
 O    14.410444     1.585160    15.970590
 H    14.387597     1.744642    16.923171
 H    14.370854     0.618609    15.918620
 C    11.193998     2.101998    24.316998
 C     9.832497     1.504908    23.955050
 C     9.490006     1.629756    22.462975
 C     8.109913     1.028776    22.146478
 O     7.123365     1.570148    22.718145
 O     8.065636     0.037572    21.369919
 H    11.406026     1.998437    25.386221
 H    12.000544     1.606144    23.768419
 H    11.234816     3.168679    24.070707
 H     9.815686     0.445123    24.237239
 H     9.041509     1.990743    24.534261
 H     9.473533     2.691794    22.188133
 H    10.248756     1.133758    21.852048
 C     6.716417    -3.256010    22.229510
 O     6.102568    -4.113526    22.870419
 N     6.245277    -2.014545    22.015653
 C     4.874005    -1.683002    22.391999
 C     4.350254    -0.411774    21.712214
 O     4.597769     0.783671    22.419386
 H     6.861695    -1.275766    21.641067
 H     4.248829    -2.538571    22.117507
 H     4.776829    -1.552710    23.477903
 H     4.737244    -0.373261    20.682472
 H     3.260428    -0.504326    21.641639
 H     5.570202     0.986246    22.447463
```

B3LYP BS13 S-OX_P^{5+}:

```
  101
Absolute Energy (Hartree): -5808.722147
Fe    11.501696    -1.765231    17.063048
Fe    13.871280    -1.205524    18.662372
Fe    14.983108    -3.529035    17.318309
Fe    10.019546    -2.130387    20.090100
 S    11.675883    -0.545482    19.134633
 S    13.883083    -1.657515    16.379669
 S    14.599066    -3.176746    19.532466
 C    10.009999     1.302000    15.409996
 C    10.541814     0.181698    14.522279
 S    10.120000    -1.498794    15.175144
 H    10.244234     2.281866    14.976520
 H    10.112131     0.249744    13.519311
 H    11.626113     0.258986    14.421630
 H     8.925668     1.227339    15.528532
 H    10.462141     1.260677    16.403520
 C     7.845998    -3.161001    17.912004
 C     8.990499    -4.040823    17.389461
 S    10.626927    -3.719056    18.197848
 H     6.969356    -3.299581    17.273749
 H     8.751307    -5.094283    17.552052
 H     9.123573    -3.887537    16.319746
 H     8.136346    -2.107994    17.864072
 C     8.014703    -3.735405    21.634673
 C     9.059253    -3.250138    22.666101
 S    10.786597    -3.242172    22.005461
 H     8.037430    -4.828805    21.584226
 H     8.818524    -2.237760    22.991890
 H     9.034344    -3.903378    23.538871
 C    16.816001    -0.358000    21.165001
 C    15.652788     0.564809    20.817905
 S    15.309148     0.612242    18.998027
 H    17.736881    -0.038078    20.669941
 H    14.749622     0.250872    21.340772
 H    15.871999     1.593984    21.113410
 H    16.989671    -0.356207    22.247865
 H    16.600147    -1.381604    20.856456
 C    19.442999    -1.915001    17.846000
 C    17.966541    -2.228547    18.084709
 S    17.287509    -3.451584    16.862960
 H    20.058392    -2.817042    17.910837
 H    17.820038    -2.649249    19.080282
 H    17.366755    -1.320027    18.025429
 H    19.597849    -1.471453    16.858579
 H    19.802318    -1.202782    18.597163
 C    13.733000    -7.100000    18.702001
 C    14.780231    -6.799091    17.633841
 S    14.224175    -5.523710    16.404985
 H    13.455483    -6.192278    19.241343
 H    15.713238    -6.457625    18.085312
 H    15.010436    -7.696401    17.053414
 H    12.824188    -7.510111    18.254387
 H    14.121227    -7.830248    19.421976
 C     7.458227    -3.594431    19.324911
 O     6.482389    -4.343180    19.496816
 N     8.275047    -3.169755    20.312132
 H     8.568345    -8.651856    13.936079
 C     8.899001    -8.790997    12.902999
 H     9.049894    -9.861644    12.733819
 C    10.189464    -7.998955    12.630981
 C    10.019531    -6.514034    12.768142
 N     9.156650    -5.807124    11.949554
 C    10.626411    -5.655079    13.654587
 C     9.247064    -4.551639    12.345181
 N    10.124671    -4.404413    13.369932
 H     8.096214    -8.447580    12.246101
 H    10.978849    -8.330492    13.312367
 H    10.537205    -8.226853    11.615705
 H    11.350110    -5.811417    14.438197
 H     8.704765    -3.716258    11.928719
 H    10.335725    -3.529579    13.856300
 O    13.709740    -1.718414    22.561965
 H    12.758993    -1.905576    22.534874
 H    14.040992    -2.158518    21.765833
 O    13.907083     1.771078    16.150818
 H    13.937370     1.808234    17.116966
 H    14.041423     0.827483    15.978563
 C    11.193998     2.101999    24.316999
 C     9.918482     1.782916    23.527581
 C    10.133902     0.761927    22.407121
 C     8.884741     0.456071    21.580987
 O     7.856345     1.138583    21.732991
 O     8.949691    -0.516064    20.741934
 H    10.996645     2.833175    25.107040
 H    11.607323     1.204374    24.787579
 H    11.970287     2.514638    23.664872
 H     9.148977     1.407077    24.210630
 H     9.508827     2.700882    23.096776
 H    10.903970     1.103365    21.705200
 H    10.513690    -0.185972    22.803182
 C     6.630360    -3.394383    22.220597
 O     6.052632    -4.168506    22.981552
 N     6.165309    -2.160194    21.922019
 C     4.874004    -1.683000    22.391998
 C     4.762338    -0.161831    22.321966
 O     5.638166     0.505786    23.212989
 H     6.693067    -1.612423    21.252231
 H     4.061809    -2.125855    21.797690
 H     4.740401    -2.016353    23.423424
 H     4.925862     0.173720    21.288849
 H     3.734082     0.106497    22.591790
 H     6.453165     0.725059    22.721327
```

B3LYP BS34 RED_P^{5+}:

```
  102
Absolute Energy (Hartree): -5809.21772720
Fe    11.897552    -1.997701    16.715136
Fe    14.046319    -1.245788    18.477818
Fe    15.160407    -3.690901    17.336298
Fe    10.756883    -2.231083    19.914049
 S    11.840946    -0.524137    18.737596
 S    14.296824    -1.840369    16.220033
 S    14.560695    -3.189678    19.507939
 C    10.010001     1.301999    15.409999
 C    10.986145     0.458884    14.595882
 S    10.702468    -1.361673    14.816565
 H    10.200478     2.369068    15.245409
 H    10.878391     0.663141    13.528448
 H    12.014821     0.689219    14.875404
 H     8.974788     1.092088    15.128041
 H    10.118726     1.098245    16.477541
 C     7.846006    -3.160996    17.912006
 C     9.035997    -3.712537    17.121444
 S    10.696936    -3.723357    17.987532
 H     6.960768    -3.254616    17.276085
 H     8.859130    -4.760946    16.879230
 H     9.161584    -3.141792    16.204659
 H     7.995744    -2.101781    18.132609
 C     7.844824    -3.929235    21.628175
 C     9.059347    -3.542919    22.492675
 S    10.676684    -3.854926    21.652055
 H     7.820312    -5.007489    21.483848
 H     9.009378    -2.500795    22.802238
 H     9.054802    -4.158666    23.394024
 C    16.815996    -0.358001    21.164999
 C    15.650432     0.537574    20.753731
 S    15.409404     0.584424    18.915867
 H    17.749011    -0.028311    20.701428
 H    14.720453     0.209852    21.219460
 H    15.827755     1.571130    21.058694
 H    16.944559    -0.327460    22.252917
 H    16.631828    -1.392137    20.871508
 C    19.442999    -1.915001    17.846000
 C    18.059872    -2.421452    18.244395
 S    17.472410    -3.812467    17.165578
 H    20.193624    -2.708135    17.907290
 H    18.064751    -2.786649    19.272722
 H    17.331207    -1.614011    18.185363
 H    19.442077    -1.527509    16.823908
 H    19.750625    -1.104226    18.515366
 C    13.733000    -7.099999    18.701999
 C    14.780230    -6.917511    17.609670
 S    14.329508    -5.608998    16.374597
 H    13.604697    -6.181883    19.278431
 H    15.751082    -6.659846    18.036247
 H    14.907455    -7.837337    17.034051
 H    12.762089    -7.367807    18.278407
 H    14.039221    -7.897626    19.388610
 C     7.613286    -3.979951    19.168312
 O     7.241496    -5.146106    19.125619
 N     7.923210    -3.321609    20.311644
 H     8.158092    -2.334725    20.272205
 H     8.566045    -8.566401    13.920215
 C     8.899000    -8.791000    12.903000
 H     9.041984    -9.872499    12.821800
 C    10.199446    -8.038823    12.571709
 C    10.066702    -6.543089    12.601296
 N     9.189116    -5.875259    11.765734
 C    10.747884    -5.635006    13.377789
 C     9.343531    -4.595163    12.038649
 N    10.276465    -4.393648    13.005480
 H     8.101669    -8.497327    12.216412
 H    10.988118    -8.336374    13.269331
 H    10.537697    -8.343234    11.573572
 H    11.506431    -5.753941    14.134636
 H     8.813074    -3.779151    11.571660
 H    10.564946    -3.494436    13.382154
 O    13.267186    -1.836310    22.457145
 H    12.483253    -2.410264    22.429953
 H    13.763957    -2.113151    21.674053
 O    14.399445     1.564143    15.720556
 H    14.343079     1.667589    16.679246
 H    14.554529     0.614955    15.614651
 C    11.193998     2.101998    24.316998
 C    10.028823     1.358290    23.646792
 C    10.403268     0.631592    22.346181
 C     9.235861    -0.108816    21.701891
 O     8.075700     0.082192    22.102852
 O     9.481247    -0.939617    20.743473
 H    10.862804     2.588660    25.238454
 H    12.009506     1.418385    24.571541
 H    11.604521     2.874525    23.658941
 H     9.615454     0.627896    24.349929
 H     9.216850     2.059607    23.436404
 H    10.785467     1.337385    21.597946
 H    11.215590    -0.085181    22.504389
 C     6.475912    -3.550868    22.244124
 O     5.663950    -4.409415    22.570170
 N     6.220987    -2.220959    22.278097
 C     4.874000    -1.682999    22.392000
 C     4.674607    -0.449873    21.511343
 O     5.324667     0.712983    22.003945
 H     6.965222    -1.550950    22.096250
 H     4.179015    -2.474429    22.100714
 H     4.642148    -1.408898    23.429011
 H     4.987120    -0.681568    20.483186
 H     3.606496    -0.216451    21.489327
 H     6.285048     0.580420    21.953997
```

B3LYP BS34 RED_D^{5+}:

```
  102
Absolute Energy (Hartree): -5809.227169
Fe    11.500343    -2.065810    16.779976
Fe    13.723247    -1.116887    18.687338
Fe    14.878153    -3.532579    17.463988
Fe    11.232678    -2.933348    19.662042
 S    11.369160    -0.711556    18.719129
 S    13.844502    -1.726068    16.362282
 S    13.959182    -3.164036    19.611683
 C    10.010000     1.302003    15.410002
 C    10.885898     0.341501    14.617959
 S    10.412611    -1.434164    14.877722
 H    10.305557     2.333875    15.193181
 H    10.786577     0.509971    13.543989
 H    11.935637     0.465480    14.881839
 H     8.955230     1.186277    15.149231
 H    10.116554     1.137286    16.483717
 C     7.846000    -3.161005    17.911998
 C     8.783942    -4.013031    17.047474
 S    10.590180    -4.116192    17.549664
 H     6.847718    -3.210092    17.467473
 H     8.449624    -5.049965    17.069402
 H     8.773076    -3.664092    16.016795
 H     8.170335    -2.118440    17.919378
 C     8.207403    -3.463066    21.689732
 C     9.398282    -2.951851    22.502271
 S    11.026021    -3.603108    21.886995
 H     8.242444    -4.550205    21.650499
 H     9.421366    -1.863496    22.490537
 H     9.298716    -3.294382    23.533133
 C    16.815999    -0.357999    21.165000
 C    15.577802     0.510642    20.975203
 S    15.046638     0.670392    19.199790
 H    17.657447     0.003609    20.569580
 H    14.736463     0.115956    21.542917
 H    15.766286     1.535012    21.302782
 H    17.111749    -0.347101    22.219943
 H    16.609545    -1.391782    20.884150
 C    19.443000    -1.915000    17.846000
 C    17.977524    -2.161704    18.227816
 S    17.194202    -3.510026    17.215890
 H    20.045024    -2.817140    17.981878
 H    17.906388    -2.458078    19.274411
 H    17.389940    -1.252413    18.100053
 H    19.531784    -1.599756    16.803465
 H    19.861379    -1.125827    18.479103
 C    13.732999    -7.100000    18.702000
 C    14.802559    -6.765058    17.670715
 S    14.249447    -5.483149    16.448701
 H    13.460784    -6.222048    19.290255
 H    15.716338    -6.410048    18.149648
 H    15.062177    -7.643932    17.076359
 H    12.826184    -7.475595    18.221981
 H    14.100926    -7.871325    19.387961
 C     7.764679    -3.745623    19.308398
 O     7.312703    -4.870385    19.486818
 N     8.293572    -2.987459    20.312601
 H     8.406866    -1.981766    20.193343
 H     8.536332    -8.518088    13.897924
 C     8.899000    -8.791000    12.903001
 H     8.993751    -9.880051    12.861734
 C    10.244640    -8.108911    12.603929
 C    10.164990    -6.610617    12.583359
 N     9.400392    -5.939182    11.645359
 C    10.774444    -5.705339    13.418976
 C     9.550375    -4.658672    11.914866
 N    10.374001    -4.461294    12.978036
 H     8.144552    -8.484391    12.174826
 H    10.988530    -8.414645    13.345703
 H    10.611303    -8.457989    11.631178
 H    11.439595    -5.824950    14.258850
 H     9.093393    -3.840057    11.379730
 H    10.627594    -3.566328    13.381597
 O    12.692099    -0.719690    22.240631
 H    12.340187    -1.629173    22.219480
 H    12.294508    -0.311267    21.463192
 O    14.250996     1.649262    15.848051
 H    14.130832     1.811121    16.791589
 H    14.359698     0.689550    15.798231
 C    11.193999     2.101999    24.316998
 C     9.809122     1.581572    23.903441
 C     9.665160     1.329475    22.394663
 C     8.274404     0.813887    21.982711
 O     7.282548     1.371108    22.513730
 O     8.217012    -0.137541    21.143891
 H    11.250377     2.254960    25.399257
 H    11.978402     1.395334    24.032702
 H    11.415943     3.059779    23.833470
 H     9.605263     0.645881    24.437750
 H     9.029692     2.282866    24.212708
 H     9.842345     2.266554    21.850085
 H    10.419383     0.617808    22.057123
 C     6.829591    -3.160499    22.340276
 O     6.306274    -4.005026    23.066450
 N     6.249827    -1.989265    22.010596
 C     4.874003    -1.682997    22.392000
 C     4.332316    -0.444270    21.673802
 O     4.678977     0.782117    22.278395
 H     6.827044    -1.251934    21.583432
 H     4.257746    -2.555831    22.151256
 H     4.789277    -1.519618    23.473385
 H     4.635948    -0.484908    20.615253
 H     3.239026    -0.501836    21.696568
 H     5.659817     0.914526    22.269437
```

B3LYP BS34 TS^{5+}:

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  102
Absolute Energy (Hartree): -5809.197921
Fe    11.667090    -2.386456    17.021643
Fe    14.139625    -1.803821    18.673263
Fe    15.299836    -3.996803    17.218742
Fe    10.467702    -3.153346    19.903818
 S    11.910111    -1.493599    19.353549
 S    14.031589    -2.208684    16.373421
 S    15.050859    -3.672491    19.475892
 C    10.010001     1.302001    15.409999
 C    10.919375     0.194159    14.885849
 S    10.304051    -1.492504    15.357953
 H    10.381989     2.281395    15.088075
 H    10.964877     0.216893    13.794942
 H    11.935054     0.323189    15.259551
 H     8.987815     1.185359    15.039913
 H     9.977138     1.293314    16.502280
 C     7.846008    -3.161000    17.912002
 C     8.698148    -4.217871    17.205292
 S    10.422711    -4.356088    17.881326
 H     6.878884    -3.095569    17.407926
 H     8.247299    -5.205540    17.307181
 H     8.786505    -3.986480    16.145445
 H     8.343793    -2.190823    17.842741
 C     8.073876    -3.673096    21.680362
 C     9.109843    -3.277273    22.732089
 S    10.821498    -3.557472    22.114899
 H     8.094991    -4.757779    21.564266
 H     9.007083    -2.235436    23.034628
 H     8.974344    -3.894887    23.621807
 C    16.815990    -0.358002    21.165000
 C    15.620410     0.493880    20.751349
 S    15.123128     0.274293    18.978933
 H    17.688421    -0.143454    20.542891
 H    14.760153     0.281410    21.384511
 H    15.851606     1.556745    20.850990
 H    17.077913    -0.150473    22.208525
 H    16.586132    -1.421018    21.076002
 C    19.442997    -1.915001    17.845999
 C    18.006428    -2.394082    17.987702
 S    17.567085    -3.721760    16.766328
 H    20.155427    -2.730246    18.002486
 H    17.832232    -2.801207    18.983526
 H    17.314728    -1.563549    17.852316
 H    19.627189    -1.492703    16.854261
 H    19.651974    -1.135698    18.587465
 C    13.733000    -7.099999    18.701999
 C    14.817169    -7.200636    17.635892
 S    14.600258    -5.975768    16.261625
 H    13.756961    -6.127349    19.193678
 H    15.808680    -7.057497    18.069056
 H    14.803803    -8.184358    17.160653
 H    12.740208    -7.236399    18.266196
 H    13.879691    -7.873273    19.465737
 C     7.569650    -3.559038    19.353500
 O     6.678723    -4.360677    19.588381
 N     8.403522    -3.050514    20.365192
 H     8.625407    -1.706833    20.533991
 H     8.618675    -8.697312    13.956069
 C     8.899000    -8.791000    12.903000
 H     9.057714    -9.851253    12.685369
 C    10.162961    -7.969296    12.596514
 C     9.985051    -6.491151    12.789952
 N     9.050380    -5.774145    12.064420
 C    10.662192    -5.645274    13.636752
 C     9.167137    -4.526013    12.472102
 N    10.129999    -4.391475    13.421362
 H     8.059166    -8.437043    12.300376
 H    10.990818    -8.311689    13.224666
 H    10.462617    -8.157188    11.558182
 H    11.454377    -5.813662    14.347989
 H     8.587480    -3.686927    12.118116
 H    10.390066    -3.525509    13.892786
 O    13.077691    -1.112464    22.575325
 H    12.489778    -1.840901    22.825924
 H    12.963217    -1.094901    21.614029
 O    14.467518     1.147877    15.728351
 H    14.550800     1.309931    16.677621
 H    14.484412     0.181188    15.674802
 C    11.194001     2.102001    24.317001
 C     9.939761     1.454711    23.701012
 C    10.142345     0.893929    22.281329
 C     8.956520     0.080888    21.772016
 O     7.861177     0.136642    22.344326
 O     9.181309    -0.680376    20.740036
 H    10.983776     2.459199    25.328726
 H    12.018740     1.386211    24.372303
 H    11.536151     2.956277    23.724055
 H     9.609194     0.639053    24.351689
 H     9.117937     2.176835    23.690418
 H    10.326382     1.700291    21.560716
 H    11.027403     0.253628    22.240137
 C     6.639563    -3.372262    22.179028
 O     5.976970    -4.242391    22.732931
 N     6.198110    -2.110623    21.970130
 C     4.874002    -1.683000    22.392000
 C     4.557109    -0.254157    21.957305
 O     5.167889     0.742255    22.765730
 H     6.877956    -1.365649    21.837337
 H     4.139526    -2.368879    21.957392
 H     4.764970    -1.748476    23.482053
 H     4.816804    -0.126169    20.896487
 H     3.479027    -0.102332    22.053281
 H     6.128093     0.676636    22.649421
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B3LYP BS34 S-$OX_{D\text{-}H}^{5+}$:

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  102
Absolute Energy (Hartree): -5809.227495
Fe    11.454315    -2.081939    17.148284
Fe    13.658212    -1.288407    19.172940
Fe    14.939773    -3.387630    17.574299
Fe    10.212243    -3.015945    19.943366
 S    11.298589    -1.106075    19.436925
 S    13.829283    -1.475340    16.824041
 S    14.583490    -3.204831    19.840351
 C    10.009995     1.302001    15.409997
 C    10.789894     0.206293    14.689096
 S    10.285387    -1.500280    15.205374
 H    10.327095     2.292127    15.062353
 H    10.624923     0.265122    13.610683
 H    11.861232     0.313580    14.865045
 H     8.936004     1.202944    15.231136
 H    10.177050     1.250608    16.488681
 C     7.846007    -3.161002    17.912001
 C     8.745803    -4.163313    17.194477
 S    10.452358    -4.196487    17.907907
 H     6.913317    -3.055914    17.351386
 H     8.343836    -5.174901    17.271178
 H     8.841652    -3.910841    16.139916
 H     8.333387    -2.184111    17.946365
 C     7.938896    -3.888328    21.647714
 C     8.920488    -3.367546    22.708631
 S    10.656324    -3.422277    22.112344
 H     7.949541    -4.982605    21.645099
 H     8.690584    -2.331596    22.962120
 H     8.843655    -3.964503    23.618666
 C    16.816000    -0.358004    21.165005
 C    15.524223     0.377692    21.485210
 S    14.471620     0.733247    19.997713
 H    17.423107     0.198101    20.446227
 H    14.917506    -0.183723    22.195352
 H    15.730745     1.357255    21.922813
 H    17.406339    -0.493408    22.079211
 H    16.601807    -1.341719    20.748581
 C    19.442998    -1.915001    17.846000
 C    17.961758    -2.131631    18.143503
 S    17.208846    -3.420769    17.042100
 H    20.014828    -2.837396    17.981162
 H    17.824924    -2.458454    19.174122
 H    17.409765    -1.201996    18.004032
 H    19.593417    -1.570515    16.819317
 H    19.854630    -1.156484    18.520896
 C    13.733000    -7.099998    18.701998
 C    14.722699    -6.656922    17.629945
 S    14.078822    -5.278255    16.569835
 H    13.524296    -6.288793    19.402205
 H    15.665042    -6.335242    18.076008
 H    14.947615    -7.480352    16.947759
 H    12.784790    -7.412506    18.257469
 H    14.141946    -7.944741    19.268667
 C     7.455507    -3.646093    19.309052
 O     6.393881    -4.252598    19.470537
 N     8.330323    -3.371151    20.323877
 H     6.862894     0.654749    20.842238
 H     8.589545    -8.650979    13.942686
 C     8.899000    -8.791000    12.903000
 H     9.050572    -9.861140    12.733265
 C    10.180994    -7.996282    12.601247
 C    10.013979    -6.510686    12.737362
 N     9.120019    -5.807874    11.949307
 C    10.659648    -5.645844    13.589699
 C     9.230034    -4.549280    12.326894
 N    10.149882    -4.395267    13.314167
 H     8.081419    -8.452694    12.262083
 H    10.986542    -8.324760    13.265035
 H    10.506677    -8.225774    11.579246
 H    11.415400    -5.797588    14.343344
 H     8.674299    -3.716402    11.923342
 H    10.391741    -3.519864    13.779329
 O    12.500447    -0.666162    22.774377
 H    11.970648    -1.457954    22.584192
 H    12.595494    -0.235582    21.914699
 O    16.345537     0.925105    17.171187
 H    15.883494     0.941049    18.026529
 H    15.830474     0.278401    16.670928
 C    11.194001     2.102004    24.317001
 C     9.705908     1.871806    24.033338
 C     9.449177     1.497584    22.573153
 C     7.999183     1.256706    22.241580
 O     7.065505     1.460199    22.999812
 O     7.828378     0.790302    20.995681
 H    11.352797     2.359720    25.368126
 H    11.777860     1.208399    24.085249
 H    11.586480     2.925365    23.711227
 H     9.326248     1.072593    24.678132
 H     9.127043     2.766016    24.284714
 H     9.802542     2.286590    21.898059
 H    10.016817     0.606419    22.288413
 C     6.523843    -3.509639    22.140399
 O     5.873855    -4.286430    22.830470
 N     6.124100    -2.236792    21.885327
 C     4.873999    -1.683000    22.392000
 C     4.278485    -0.659116    21.437267
 O     5.125172     0.483437    21.240286
 H     6.725572    -1.656229    21.319297
 H     4.174854    -2.509996    22.529940
 H     5.028560    -1.221375    23.376826
 H     4.134003    -1.098976    20.449454
 H     3.303828    -0.335600    21.819419
 H     5.355235     0.876350    22.100643
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B3LYP BS34 S-OX_D^{5+}:

```
  101
Absolute Energy (Hartree): -5808.705205
Fe    11.513903    -2.241536    17.088720
Fe    13.834837    -1.533446    18.787723
Fe    15.095061    -3.734306    17.360701
Fe    10.273875    -2.971499    19.888348
 S    11.569261    -1.193492    19.339784
 S    13.884680    -1.949334    16.481358
 S    14.788068    -3.417479    19.606620
 C    10.010001     1.301992    15.409999
 C    10.889537     0.210796    14.807678
 S    10.288693    -1.490510    15.237904
 H    10.382240     2.293132    15.124833
 H    10.897088     0.277796    13.717177
 H    11.918150     0.319893    15.151523
 H     8.975637     1.211596    15.067293
 H    10.008385     1.239962    16.500617
 C     7.846006    -3.160987    17.912007
 C     8.722163    -4.182863    17.187466
 S    10.437689    -4.284141    17.892723
 H     6.898808    -3.064614    17.375394
 H     8.294655    -5.184181    17.262676
 H     8.821039    -3.931151    16.132736
 H     8.338792    -2.186239    17.911526
 C     8.042236    -3.725537    21.678064
 C     9.018445    -3.053984    22.645237
 S    10.744708    -3.286604    22.068691
 H     8.106974    -4.812777    21.788049
 H     8.831492    -1.980627    22.671541
 H     8.921108    -3.471383    23.649332
 C    16.815990    -0.358002    21.164998
 C    15.503102     0.386754    20.940582
 S    14.991826     0.443462    19.157112
 H    17.633046     0.103244    20.603587
 H    14.703718    -0.078150    21.515787
 H    15.588733     1.428597    21.258136
 H    17.077939    -0.340464    22.229368
 H    16.730162    -1.399460    20.852384
 C    19.442997    -1.915002    17.846000
 C    17.978521    -2.284090    18.069839
 S    17.374745    -3.554237    16.858510
 H    20.092945    -2.788823    17.948018
 H    17.836730    -2.693916    19.070152
 H    17.339571    -1.403709    17.987919
 H    19.597795    -1.493602    16.849073
 H    19.759961    -1.168149    18.582412
 C    13.733001    -7.100000    18.701999
 C    14.759470    -6.995157    17.579408
 S    14.351074    -5.674487    16.343415
 H    13.687647    -6.173320    19.276771
 H    15.756634    -6.796774    17.977957
 H    14.811297    -7.928723    17.013398
 H    12.733945    -7.293725    18.303217
 H    13.995846    -7.916940    19.384621
 C     7.497475    -3.613505    19.331378
 O     6.428326    -4.196142    19.535565
 N     8.410939    -3.334917    20.304051
 H     8.584475    -8.650337    13.940947
 C     8.899002    -8.790998    12.903000
 H     9.036036    -9.862696    12.729825
 C    10.195007    -8.014198    12.613665
 C    10.053469    -6.526716    12.758725
 N     9.181628    -5.800594    11.966726
 C    10.707691    -5.681444    13.623931
 C     9.312613    -4.547204    12.355556
 N    10.225737    -4.419130    13.352735
 H     8.090749    -8.438194    12.257987
 H    10.990928    -8.360015    13.280213
 H    10.523343    -8.242669    11.592138
 H    11.452134    -5.854888    14.383874
 H     8.777283    -3.700037    11.954329
 H    10.478106    -3.551352    13.826109
 O    13.822095    -2.123450    22.682558
 H    12.856359    -2.139299    22.601027
 H    14.121733    -2.569734    21.877501
 O    14.490299     1.380565    15.863216
 H    14.459644     1.581031    16.807534
 H    14.459052     0.412270    15.851577
 C    11.193995     2.101997    24.316997
 C     9.838437     1.494818    23.951172
 C     9.512388     1.598891    22.453949
 C     8.136228     0.990885    22.137331
 O     7.142372     1.568835    22.658664
 O     8.102327    -0.042206    21.417403
 H    11.401075     2.007586    25.388074
 H    12.006049     1.606629    23.776139
 H    11.230578     3.167077    24.063101
 H     9.823776     0.438523    24.245612
 H     9.039391     1.985239    24.515810
 H     9.497924     2.656766    22.164118
 H    10.278758     1.092479    21.862317
 C     6.603012    -3.379550    22.130838
 O     5.913470    -4.241408    22.680429
 N     6.210450    -2.097682    21.981706
 C     4.874009    -1.683001    22.392000
 C     4.374378    -0.424901    21.664272
 O     4.619504     0.788190    22.342450
 H     6.872255    -1.376024    21.659511
 H     4.206368    -2.525337    22.193086
 H     4.827576    -1.487777    23.472034
 H     4.785030    -0.421084    20.643304
 H     3.285326    -0.506218    21.572889
 H     5.593071     0.984340    22.381484
```

B3LYP BS34 S-OX_P^{5+}:

```
  101
Absolute Energy (Hartree): -5808.711956
Fe    11.656974    -2.023089    17.106767
Fe    13.929706    -1.431413    18.685478
Fe    15.106035    -3.706334    17.290277
Fe     9.969643    -2.138436    20.005173
 S    11.755086    -0.789848    19.243396
 S    13.988995    -1.884561    16.366423
 S    14.715657    -3.388813    19.518353
 C    10.009999     1.302002    15.409998
 C    10.882655     0.247900    14.739199
 S    10.358881    -1.464474    15.211917
 H    10.332377     2.310655    15.124451
 H    10.815900     0.321147    13.650935
 H    11.928072     0.387717    15.016945
 H     8.960474     1.183428    15.126700
 H    10.074271     1.218152    16.497441
 C     7.845997    -3.161002    17.912000
 C     8.953569    -4.036840    17.327981
 S    10.548449    -3.815639    18.238010
 H     6.933767    -3.288001    17.323083
 H     8.686114    -5.092360    17.405254
 H     9.118136    -3.797604    16.278831
 H     8.140475    -2.109432    17.855805
 C     8.052000    -3.707281    21.666276
 C     9.086359    -3.200794    22.685966
 S    10.774569    -3.126796    21.958280
 H     8.085977    -4.800297    21.622547
 H     8.816148    -2.198245    23.022156
 H     9.097279    -3.858391    23.556958
 C    16.816003    -0.358000    21.165001
 C    15.614736     0.504383    20.792370
 S    15.261081     0.471532    18.973058
 H    17.721438    -0.019841    20.653675
 H    14.729343     0.169726    21.333179
 H    15.791310     1.551493    21.050652
 H    16.994049    -0.310458    22.246139
 H    16.640360    -1.400182    20.895584
 C    19.443000    -1.915000    17.846000
 C    18.002649    -2.344390    18.099220
 S    17.409414    -3.589249    16.859216
 H    20.128680    -2.766504    17.891262
 H    17.904327    -2.794884    19.088126
 H    17.336264    -1.482884    18.065958
 H    19.549038    -1.449064    16.862652
 H    19.758429    -1.185739    18.600901
 C    13.733000    -7.100000    18.702001
 C    14.857361    -6.908632    17.692145
 S    14.413429    -5.711264    16.346407
 H    13.452298    -6.148786    19.157924
 H    15.764794    -6.549639    18.181205
 H    15.102890    -7.851627    17.196776
 H    12.842651    -7.516284    18.223372
 H    14.045428    -7.786220    19.498397
 C     7.508463    -3.586049    19.345575
 O     6.536480    -4.330222    19.543149
 N     8.325895    -3.149910    20.335399
 H     8.565719    -8.647900    13.934705
 C     8.899000    -8.790999    12.903000
 H     9.027851    -9.863984    12.731362
 C    10.209556    -8.029004    12.639866
 C    10.087221    -6.539878    12.788381
 N     9.228066    -5.799924    11.995126
 C    10.753097    -5.704967    13.655068
 C     9.378264    -4.548867    12.384844
 N    10.291652    -4.435380    13.383233
 H     8.107162    -8.429301    12.242838
 H    10.989341    -8.388115    13.318373
 H    10.552641    -8.258468    11.623296
 H    11.495822    -5.889756    14.414156
 H     8.857024    -3.693175    11.983188
 H    10.555390    -3.570481    13.855781
 O    13.769961    -1.883873    22.604778
 H    12.811910    -2.041809    22.583907
 H    14.079848    -2.323500    21.800865
 O    14.492741     1.465967    15.827890
 H    14.489760     1.598945    16.786018
 H    14.492335     0.500023    15.753806
 C    11.193999     2.102000    24.317000
 C     9.930752     1.728173    23.519521
 C    10.168946     0.771471    22.340963
 C     8.906520     0.447274    21.527205
 O     7.856682     1.078869    21.756413
 O     8.974044    -0.459546    20.619787
 H    10.946146     2.776353    25.142256
 H    11.677154     1.215578    24.739790
 H    11.930592     2.604080    23.681665
 H     9.197577     1.276518    24.196642
 H     9.456900     2.638155    23.140254
 H    10.902573     1.187516    21.640097
 H    10.607321    -0.175201    22.674978
 C     6.652483    -3.377520    22.224424
 O     6.073018    -4.159984    22.975475
 N     6.172955    -2.148729    21.923116
 C     4.874003    -1.683000    22.391999
 C     4.760069    -0.161012    22.340201
 O     5.634077     0.497898    23.238181
 H     6.702934    -1.583684    21.269984
 H     4.067936    -2.121770    21.786615
 H     4.737544    -2.030386    23.418181
 H     4.922397     0.185987    21.310425
 H     3.731837     0.103144    22.613863
 H     6.463623     0.690251    22.758257
```

B3LYP-D3 BS12 RED_P^{5+}:

```
  102
Absolute Energy (Hartree): -5809.236246
Fe    11.882324    -1.640679    16.823760
Fe    14.144110    -0.809507    18.695955
Fe    15.009701    -3.365496    17.677784
Fe    10.559004    -1.588959    19.817641
 S    11.918614    -0.078446    18.819589
 S    14.315211    -1.493961    16.479384
 S    14.431938    -2.736571    19.807210
 C    10.010000     1.302000    15.409999
 C    11.100005     0.564019    14.642067
 S    10.887666    -1.278455    14.776124
 H    10.150202     2.386433    15.333217
 H    11.084738     0.821416    13.580385
 H    12.081452     0.824117    15.040244
 H     9.015997     1.052487    15.029475
 H    10.048716     1.025084    16.467044
 C     7.846003    -3.160999    17.912003
 C     9.097121    -3.547072    17.117152
 S    10.686980    -3.315878    18.057178
 H     6.960539    -3.495176    17.362711
 H     9.072681    -4.608642    16.869618
 H     9.162435    -2.959533    16.203955
 H     7.799898    -2.073033    18.022619
 C     8.165842    -3.485110    21.705312
 C     9.257218    -2.780386    22.535227
 S    10.948716    -2.800179    21.770981
 H     8.362203    -4.555161    21.673883
 H     8.989115    -1.748245    22.752230
 H     9.344322    -3.298861    23.492247
 C    16.815999    -0.358001    21.165000
 C    15.777200     0.728040    20.936187
 S    15.473551     1.001781    19.125913
 H    17.769188    -0.093043    20.700446
 H    14.829132     0.469454    21.409224
 H    16.106635     1.686831    21.342294
 H    16.983887    -0.502613    22.238884
 H    16.480747    -1.301810    20.738425
 C    19.442999    -1.915001    17.846000
 C    18.035530    -2.234096    18.352476
 S    17.297447    -3.680652    17.456164
 H    20.114823    -2.767597    17.981816
 H    18.052542    -2.478228    19.415386
 H    17.367390    -1.380509    18.224926
 H    19.427651    -1.659266    16.783284
 H    19.854550    -1.062546    18.397572
 C    13.733000    -7.099999    18.701999
 C    14.762018    -6.552337    17.724620
 S    14.060377    -5.190316    16.679724
 H    13.385608    -6.310610    19.373511
 H    15.634959    -6.164201    18.252555
 H    15.111321    -7.326072    17.037327
 H    12.860415    -7.496941    18.176551
 H    14.169065    -7.904394    19.306121
 C     7.864530    -3.858369    19.265295
 O     7.764442    -5.070515    19.373615
 N     8.118240    -3.020259    20.320479
 H     7.957261    -2.028896    20.185885
 H     8.128523    -8.379824    13.560288
 C     8.899000    -8.791000    12.903000
 H     8.883849    -9.879917    12.995284
 C    10.285740    -8.227267    13.263253
 C    10.428274    -6.741000    13.082766
 N    10.091952    -6.111670    11.893556
 C    10.950617    -5.820452    13.963312
 C    10.411427    -4.840682    12.061177
 N    10.937291    -4.614326    13.292365
 H     8.637040    -8.526226    11.876939
 H    10.533472    -8.477157    14.299376
 H    11.038082    -8.726292    12.639463
 H    11.340928    -5.913518    14.965320
 H    10.284550    -4.049882    11.335604
 H    11.266502    -3.718490    13.633879
 O    13.657898    -1.126219    22.937946
 H    12.774179    -1.461494    22.718136
 H    14.227400    -1.624101    22.335359
 O    14.010063     2.031346    16.176101
 H    13.749150     2.040067    17.106973
 H    14.441607     1.172353    16.069437
 C    11.193999     2.101999    24.316999
 C     9.990827     1.415274    23.626950
 C    10.218123     0.978290    22.164998
 C     8.974863     0.378794    21.500378
 O     7.845281     0.601934    21.951792
 O     9.133450    -0.389820    20.452536
 H    10.941290     2.359436    25.348977
 H    12.068864     1.444520    24.330756
 H    11.475847     3.020993    23.793274
 H     9.706797     0.530843    24.208550
 H     9.123618     2.080099    23.653253
 H    10.518342     1.829930    21.540565
 H    11.032821     0.253579    22.082094
 C     6.738831    -3.313425    22.286852
 O     6.049909    -4.283285    22.584090
 N     6.289175    -2.032982    22.312597
 C     4.874001    -1.683000    22.392000
 C     4.480660    -0.704803    21.283595
 O     4.987080     0.612140    21.484165
 H     6.933967    -1.264649    22.159376
 H     4.304625    -2.609483    22.298744
 H     4.638627    -1.234914    23.364258
 H     4.796122    -1.114238    20.313460
 H     3.391102    -0.615114    21.270245
 H     5.957616     0.598928    21.437512
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B3LYP-D3 BS12 RED_D^{5+}:

```
  102
Absolute Energy (Hartree): -5809.234017
Fe    11.390631    -1.960533    16.844909
Fe    13.510074    -0.967101    18.838282
Fe    14.768564    -3.315018    17.541792
Fe    11.367689    -2.872653    19.689561
 S    11.191794    -0.692975    19.006606
 S    13.804229    -1.469959    16.569320
 S    13.804144    -3.063633    19.752778
 C    10.010001     1.302001    15.410001
 C    10.870921     0.329922    14.615789
 S    10.351548    -1.435794    14.884857
 H    10.348619     2.330253    15.245697
 H    10.805651     0.517047    13.541957
 H    11.914662     0.425347    14.911832
 H     8.957592     1.227690    15.123920
 H    10.085519     1.086155    16.479133
 C     7.846000    -3.161000    17.912000
 C     8.839998    -4.048124    17.147213
 S    10.639550    -4.077750    17.706297
 H     6.864139    -3.272815    17.443409
 H     8.526231    -5.090140    17.209761
 H     8.883905    -3.752353    16.100034
 H     8.157076    -2.114274    17.856851
 C     8.273926    -3.292898    21.692017
 C     9.432351    -2.659906    22.456196
 S    11.053331    -3.360745    21.902016
 H     8.379469    -4.376471    21.707686
 H     9.442978    -1.581669    22.312379
 H     9.350377    -2.886102    23.520559
 C    16.815997    -0.357999    21.165000
 C    15.525747     0.455378    21.139417
 S    14.882668     0.736976    19.415349
 H    17.589955     0.089937    20.536176
 H    14.736832    -0.026769    21.712771
 H    15.681921     1.457364    21.545580
 H    17.192284    -0.418142    22.192789
 H    16.625302    -1.372608    20.811886
 C    19.443000    -1.915000    17.846000
 C    17.972243    -2.029981    18.286830
 S    17.086113    -3.452050    17.473199
 H    19.994873    -2.829444    18.080115
 H    17.921376    -2.204941    19.359923
 H    17.419500    -1.114594    18.069638
 H    19.521778    -1.730965    16.771451
 H    19.914221    -1.081339    18.375553
 C    13.733000    -7.100000    18.702001
 C    14.785152    -6.489253    17.783837
 S    14.058369    -5.252235    16.598289
 H    13.247079    -6.323290    19.296260
 H    15.564741    -5.989611    18.359810
 H    15.267095    -7.250902    17.169371
 H    12.960436    -7.617763    18.129217
 H    14.203352    -7.817338    19.382845
 C     7.756306    -3.663945    19.338506
 O     7.287669    -4.770818    19.583744
 N     8.325563    -2.873995    20.295716
 H     8.463817    -1.879491    20.124449
 H     8.414854    -8.558277    13.856477
 C     8.899000    -8.791000    12.903000
 H     9.018862    -9.876101    12.834853
 C    10.258065    -8.077731    12.791693
 C    10.170139    -6.578096    12.780451
 N     9.466418    -5.897895    11.797522
 C    10.765529    -5.676426    13.631800
 C     9.643616    -4.614735    12.056981
 N    10.424162    -4.427993    13.151426
 H     8.231702    -8.463913    12.100871
 H    10.910308    -8.385972    13.614963
 H    10.751866    -8.401500    11.867448
 H    11.386758    -5.805179    14.504073
 H     9.235131    -3.788299    11.492990
 H    10.701531    -3.525845    13.526232
 O    12.641350    -0.446242    22.287733
 H    12.317128    -1.360404    22.187763
 H    12.328000    -0.007120    21.486345
 O    13.382603     1.966122    16.546835
 H    12.982111     1.845016    17.419779
 H    13.796084     1.112155    16.358416
 C    11.193999     2.101998    24.316999
 C     9.832194     1.502592    23.925434
 C     9.598785     1.410402    22.407469
 C     8.195356     0.896044    22.037151
 O     7.229918     1.374945    22.686974
 O     8.098403     0.029476    21.113875
 H    11.307015     2.135378    25.407426
 H    12.009899     1.498085    23.902082
 H    11.295437     3.125270    23.932603
 H     9.745460     0.496398    24.354836
 H     9.016347     2.089767    24.357374
 H     9.699995     2.409407    21.961924
 H    10.348325     0.770318    21.939351
 C     6.891116    -3.047554    22.348824
 O     6.411018    -3.911970    23.089645
 N     6.265167    -1.906726    22.017405
 C     4.874004    -1.682999    22.392000
 C     4.308509    -0.386998    21.801406
 O     4.610946     0.774972    22.557458
 H     6.798841    -1.146100    21.573622
 H     4.287902    -2.541192    22.042398
 H     4.765390    -1.643299    23.482650
 H     4.639582    -0.290573    20.752756
 H     3.217965    -0.477411    21.788820
 H     5.586367     0.941833    22.529797
```

B3LYP-D3 BS12 TS^{5+}:

```
  102
Absolute Energy (Hartree): -5809.211230
Fe    11.500714    -2.436446    17.103586
Fe    13.794231    -1.516798    18.798153
Fe    15.032930    -3.672074    17.398389
Fe    10.430786    -3.192178    19.898627
 S    11.503726    -1.303195    19.286845
 S    13.811422    -1.908083    16.497452
 S    14.658744    -3.392844    19.633166
 C    10.010000     1.302000    15.409999
 C    10.958862     0.143287    15.124265
 S    10.168170    -1.503235    15.476212
 H    10.506833     2.253796    15.192883
 H    11.266060     0.136060    14.076909
 H    11.860966     0.232522    15.726361
 H     9.104137     1.236906    14.801218
 H     9.713107     1.302076    16.461648
 C     7.846005    -3.161000    17.912001
 C     8.681692    -4.273151    17.249353
 S    10.432053    -4.501814    17.887486
 H     6.909918    -3.066380    17.357501
 H     8.194180    -5.240216    17.376837
 H     8.782508    -4.070911    16.184562
 H     8.393449    -2.215222    17.850738
 C     8.058347    -3.713190    21.653074
 C     9.187041    -3.456006    22.654586
 S    10.817658    -4.064926    21.985044
 H     8.017562    -4.787918    21.468804
 H     9.285124    -2.399435    22.900989
 H     8.988151    -4.006149    23.575732
 C    16.815992    -0.358001    21.165001
 C    15.453612     0.315914    21.046650
 S    14.868644     0.447802    19.286757
 H    17.574070     0.171597    20.581822
 H    14.705200    -0.225027    21.623057
 H    15.489321     1.342010    21.420069
 H    17.132770    -0.378270    22.213932
 H    16.759082    -1.386002    20.802244
 C    19.442998    -1.915001    17.846000
 C    17.980682    -2.274767    18.142079
 S    17.313830    -3.542557    16.955788
 H    20.086898    -2.796428    17.914272
 H    17.879573    -2.689884    19.145624
 H    17.337119    -1.394960    18.089682
 H    19.548678    -1.490782    16.843794
 H    19.795401    -1.174183    18.571792
 C    13.733000    -7.099999    18.701999
 C    14.793464    -6.832755    17.643345
 S    14.224825    -5.573677    16.405724
 H    13.502707    -6.183727    19.250486
 H    15.718149    -6.468014    18.095152
 H    15.034876    -7.738886    17.082760
 H    12.806287    -7.460491    18.248045
 H    14.085509    -7.852180    19.417135
 C     7.505216    -3.520924    19.340218
 O     6.580692    -4.284174    19.571819
 N     8.352537    -3.034761    20.354749
 H     8.501132    -1.689559    20.581827
 H     8.327518    -8.694239    13.829849
 C     8.899000    -8.791000    12.903000
 H     9.052134    -9.855012    12.703837
 C    10.242973    -8.050526    13.007533
 C    10.120958    -6.564280    13.199416
 N     9.321337    -5.782993    12.378438
 C    10.779566    -5.762481    14.104112
 C     9.503824    -4.538853    12.785167
 N    10.377691    -4.473506    13.821891
 H     8.296816    -8.369801    12.096175
 H    10.834679    -8.462065    13.830557
 H    10.818296    -8.238967    12.092477
 H    11.487762    -5.977723    14.889183
 H     9.033998    -3.656804    12.374191
 H    10.672213    -3.613111    14.278308
 O    12.959183    -1.494231    22.602123
 H    12.761087    -2.432618    22.733284
 H    12.710706    -1.359612    21.676785
 O    13.918916     1.702873    16.279726
 H    13.790846     1.746971    17.235916
 H    14.217167     0.794359    16.139181
 C    11.194001     2.102001    24.317001
 C     9.908934     1.478217    23.753183
 C    10.097454     0.771545    22.403921
 C     8.854405     0.033787    21.935841
 O     7.815064     0.054727    22.607391
 O     8.979633    -0.632259    20.823203
 H    11.006510     2.574022    25.285353
 H    11.969348     1.341725    24.452105
 H    11.596200     2.864559    23.642274
 H     9.513932     0.752247    24.469695
 H     9.134758     2.244764    23.650334
 H    10.395823     1.469332    21.613177
 H    10.902638     0.029957    22.460880
 C     6.650069    -3.387240    22.218729
 O     6.003064    -4.260164    22.792462
 N     6.202542    -2.133522    22.000421
 C     4.874003    -1.683000    22.392000
 C     4.542367    -0.303994    21.825663
 O     5.093307     0.775919    22.578213
 H     6.885614    -1.392969    21.884478
 H     4.151410    -2.418653    22.025021
 H     4.771097    -1.646862    23.484322
 H     4.851780    -0.258214    20.771320
 H     3.458158    -0.171539    21.857852
 H     6.058079     0.671227    22.591241
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B3LYP-D3 BS12 S-OX_{D-H}^{5+}:

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  102
Absolute Energy (Hartree): -5809.248572
Fe    11.311330    -2.097945    17.200728
Fe    13.387616    -1.154210    19.185726
Fe    14.790178    -3.258104    17.715542
Fe    10.213953    -2.939226    19.937519
 S    11.026489    -0.901476    19.354386
 S    13.640893    -1.418477    16.865879
 S    14.247880    -3.068239    19.937519
 C    10.009994     1.302000    15.409996
 C    10.789616     0.143383    14.797813
 S    10.115334    -1.502867    15.321740
 H    10.426850     2.261125    15.082185
 H    10.743117     0.173270    13.706691
 H    11.840222     0.181443    15.088467
 H     8.956651     1.264684    15.118836
 H    10.059701     1.259142    16.501450
 C     7.846002    -3.161001    17.912001
 C     8.771423    -4.215527    17.279546
 S    10.517813    -4.266037    17.955299
 H     6.939351    -3.093916    17.305837
 H     8.364225    -5.217883    17.420582
 H     8.873041    -4.032326    16.210995
 H     8.342878    -2.186081    17.902668
 C     8.017908    -3.746658    21.649741
 C     9.115496    -3.288193    22.625022
 S    10.823071    -3.712324    22.017966
 H     8.011328    -4.840243    21.607374
 H     9.064402    -2.205149    22.756529
 H     8.973349    -3.766836    23.594161
 C    16.816008    -0.358005    21.165007
 C    15.429130     0.166193    21.526631
 S    14.422057     0.718358    20.058611
 H    17.391124     0.380848    20.600589
 H    14.844541    -0.590440    22.048085
 H    15.493568     1.045657    22.171387
 H    17.367784    -0.611851    22.076626
 H    16.716012    -1.257418    20.559312
 C    19.442998    -1.915000    17.846000
 C    17.981650    -2.083786    18.277110
 S    17.065506    -3.292141    17.206358
 H    19.983753    -2.864364    17.892075
 H    17.930972    -2.453591    19.301037
 H    17.455509    -1.131764    18.222345
 H    19.507962    -1.533360    16.823625
 H    19.942244    -1.201445    18.510060
 C    13.733001    -7.099998    18.701997
 C    14.761626    -6.456223    17.778655
 S    14.012036    -5.156813    16.683938
 H    13.282137    -6.346767    19.353352
 H    15.566679    -5.991926    18.351469
 H    15.217334    -7.196559    17.116777
 H    12.929657    -7.572266    18.130080
 H    14.209449    -7.862878    19.327914
 C     7.429165    -3.562867    19.322955
 O     6.400682    -4.218387    19.512363
 N     8.293504    -3.197416    20.315027
 H     6.694101     0.713874    21.013660
 H     8.295928    -8.631046    13.800489
 C     8.899000    -8.791000    12.903000
 H     9.012280    -9.868028    12.753471
 C    10.268769    -8.102429    13.034443
 C    10.196902    -6.606997    13.161991
 N     9.516668    -5.827332    12.238535
 C    10.786602    -5.798630    14.106962
 C     9.700669    -4.577501    12.627371
 N    10.463352    -4.507288    13.747146
 H     8.348991    -8.379476    12.054718
 H    10.807952    -8.502265    13.898396
 H    10.872530    -8.350636    12.152691
 H    11.398691    -6.011864    14.969153
 H     9.307677    -3.694621    12.144087
 H    10.729784    -3.643201    14.213183
 O    12.333240    -0.765062    22.692244
 H    12.006009    -1.631903    22.397365
 H    12.427934    -0.262738    21.872097
 O    16.288385     0.769864    17.200825
 H    15.762068     0.717014    18.016745
 H    15.868664     0.107174    16.636616
 C    11.193997     2.102004    24.316999
 C     9.704653     1.807943    24.094413
 C     9.400019     1.337253    22.669655
 C     7.926190     1.145903    22.400752
 O     7.041394     1.297968    23.226142
 O     7.673513     0.796458    21.128861
 H    11.379695     2.422750    25.345799
 H    11.796263     1.213055    24.114483
 H    11.540036     2.897458    23.648390
 H     9.367433     1.040867    24.798855
 H     9.107031     2.699693    24.309450
 H     9.770979     2.052013    21.925247
 H     9.919862     0.398428    22.445947
 C     6.655079    -3.365008    22.252511
 O     6.091793    -4.118011    23.044550
 N     6.174492    -2.145912    21.923718
 C     4.874001    -1.683000    22.392000
 C     4.237324    -0.689086    21.433202
 O     4.961221     0.552573    21.338308
 H     6.709989    -1.584001    21.276595
 H     4.222895    -2.554812    22.494323
 H     4.963952    -1.227291    23.386967
 H     4.207514    -1.099109    20.421390
 H     3.208469    -0.492605    21.755164
 H     5.059226     0.932471    22.227187
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B3LYP-D3 BS12 S-OX_D^{5+}:

```
  101
Absolute Energy (Hartree): -5808.725303
Fe    11.415066    -2.102019    17.029576
Fe    13.521720    -1.062158    18.919866
Fe    14.843411    -3.332042    17.640502
Fe    10.259758    -2.580925    19.850515
 S    11.186351    -0.663272    19.022188
 S    13.782988    -1.539561    16.626848
 S    14.257582    -2.991364    19.828094
 C    10.010000     1.302000    15.410000
 C    10.934388     0.228320    14.850042
 S    10.263314    -1.486165    15.127184
 H    10.447812     2.294094    15.254538
 H    11.088630     0.350232    13.775653
 H    11.904235     0.296702    15.339870
 H     9.025924     1.272973    14.933373
 H     9.871292     1.155163    16.484327
 C     7.846001    -3.160999    17.912001
 C     8.828778    -4.173618    17.299719
 S    10.570589    -4.141971    17.996718
 H     6.914117    -3.198995    17.343353
 H     8.469206    -5.192643    17.451002
 H     8.929662    -3.996577    16.229628
 H     8.266594    -2.153599    17.827948
 C     8.185878    -3.432797    21.677333
 C     9.228008    -2.739448    22.563944
 S    10.961099    -3.102660    21.985248
 H     8.317542    -4.517070    21.750752
 H     9.082242    -1.659748    22.519558
 H     9.135042    -3.079313    23.596032
 C    16.815994    -0.358001    21.164999
 C    15.465656     0.353003    21.222969
 S    14.781953     0.761418    19.541937
 H    17.551864     0.224728    20.603177
 H    14.740194    -0.259606    21.758106
 H    15.548129     1.309868    21.744988
 H    17.194611    -0.520241    22.181016
 H    16.698660    -1.328697    20.681056
 C    19.442999    -1.915000    17.846000
 C    17.990870    -2.142846    18.280813
 S    17.147110    -3.424033    17.239177
 H    20.024306    -2.839008    17.916587
 H    17.955003    -2.484255    19.315741
 H    17.412476    -1.219564    18.220433
 H    19.491643    -1.560260    16.812732
 H    19.911896    -1.163272    18.490293
 C    13.733000    -7.100000    18.702000
 C    14.795048    -6.524447    17.773929
 S    14.093036    -5.250863    16.622770
 H    13.286863    -6.307365    19.307881
 H    15.602568    -6.059599    18.342723
 H    15.241204    -7.302582    17.149874
 H    12.929334    -7.576964    18.134482
 H    14.174174    -7.846003    19.373310
 C     7.521622    -3.502193    19.361777
 O     6.559345    -4.230152    19.629210
 N     8.392468    -3.009106    20.283313
 H     8.172443    -8.518135    13.672184
 C     8.899002    -8.790998    12.903000
 H     8.958187    -9.881699    12.857833
 C    10.275949    -8.174107    13.207497
 C    10.301518    -6.671153    13.201350
 N     9.855047    -5.938453    12.112143
 C    10.793237    -5.818088    14.163466
 C    10.077574    -4.672530    12.422521
 N    10.646542    -4.548192    13.647129
 H     8.523974    -8.424378    11.946106
 H    10.637191    -8.525390    14.178134
 H    10.994104    -8.538545    12.462808
 H    11.237444    -5.989578    15.130892
 H     9.846751    -3.815090    11.807712
 H    10.894587    -3.663958    14.085894
 O    13.916547    -1.999216    23.222651
 H    12.980954    -1.941629    22.980252
 H    14.285969    -2.502768    22.486467
 O    13.275764     2.044388    16.720150
 H    12.807950     1.861794    17.543946
 H    13.791045     1.242866    16.561406
 C    11.193997     2.101998    24.316998
 C     9.877763     1.372587    24.023328
 C     9.429019     1.467304    22.559826
 C     7.989548     0.969146    22.324763
 O     7.136619     1.272990    23.209037
 O     7.761721     0.310986    21.275021
 H    11.482108     1.998480    25.367583
 H    12.011563     1.706688    23.705631
 H    11.104417     3.170790    24.096189
 H     9.974827     0.314841    24.295240
 H     9.078066     1.776702    24.648216
 H     9.452875     2.518410    22.241095
 H    10.103709     0.917904    21.897928
 C     6.774802    -3.172515    22.238546
 O     6.204279    -4.047087    22.902461
 N     6.248415    -1.962313    22.002035
 C     4.874006    -1.683001    22.391999
 C     4.356826    -0.332615    21.880961
 O     4.555965     0.744299    22.781134
 H     6.805592    -1.206576    21.579178
 H     4.247579    -2.492861    22.001115
 H     4.765250    -1.699529    23.482828
 H     4.796786    -0.126020    20.894724
 H     3.274545    -0.423389    21.741894
 H     5.532719     0.902482    22.882739
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B3LYP-D3 BS12 S-OX_P^{5+}:

```
  101
Absolute Energy (Hartree): -5808.734856
Fe    11.516501    -1.896920    17.083364
Fe    13.587397    -0.922038    18.909992
Fe    14.844796    -3.256743    17.684574
Fe     9.912307    -1.936663    20.095904
 S    11.331269    -0.373154    19.028069
 S    13.895034    -1.433712    16.622478
 S    14.271292    -2.858649    19.856521
 C    10.009999     1.302001    15.409999
 C    10.933751     0.283687    14.755274
 S    10.374273    -1.453227    15.099276
 H    10.367058     2.320719    15.220492
 H    10.969596     0.415050    13.671240
 H    11.944537     0.399400    15.145286
 H     8.987332     1.211530    15.033007
 H     9.989309     1.143550    16.491050
 C     7.845998    -3.161001    17.912001
 C     9.006295    -3.991076    17.346403
 S    10.604786    -3.731778    18.260377
 H     6.962568    -3.300629    17.283668
 H     8.773493    -5.055839    17.412892
 H     9.171750    -3.742044    16.299245
 H     8.123131    -2.101478    17.897141
 C     8.054873    -3.654913    21.645033
 C     9.056647    -3.049103    22.658199
 S    10.789003    -2.930257    22.006702
 H     8.164844    -4.743705    21.626681
 H     8.738784    -2.040503    22.922418
 H     9.066512    -3.657388    23.563453
 C    16.816002    -0.358000    21.165000
 C    15.504306     0.418013    21.221976
 S    14.881050     0.897972    19.539253
 H    17.588883     0.202778    20.632511
 H    14.733842    -0.168083    21.722666
 H    15.624556     1.352263    21.775486
 H    17.172705    -0.571007    22.179577
 H    16.656877    -1.304411    20.650074
 C    19.443000    -1.915000    17.846000
 C    18.005436    -2.155676    18.315450
 S    17.153607    -3.452972    17.303839
 H    20.035775    -2.831701    17.909857
 H    17.997079    -2.486666    19.354257
 H    17.414920    -1.240282    18.260249
 H    19.463450    -1.569429    16.809178
 H    19.920511    -1.153079    18.471803
 C    13.733000    -7.100000    18.702001
 C    14.781132    -6.460094    17.801077
 S    14.050296    -5.175771    16.679346
 H    13.252585    -6.341187    19.323518
 H    15.566640    -5.986331    18.392025
 H    15.260620    -7.205236    17.162157
 H    12.953011    -7.589212    18.112840
 H    14.194094    -7.848845    19.356594
 C     7.499748    -3.632692    19.324820
 O     6.613036    -4.489852    19.493759
 N     8.259521    -3.106558    20.304485
 H     8.182897    -8.517560    13.683059
 C     8.899001    -8.790999    12.903000
 H     8.943527    -9.882071    12.844462
 C    10.287742    -8.196029    13.200884
 C    10.333220    -6.693305    13.218085
 N     9.873106    -5.933956    12.152223
 C    10.857315    -5.865141    14.185000
 C    10.120913    -4.677068    12.481507
 N    10.718318    -4.584286    13.695440
 H     8.519006    -8.407302    11.953553
 H    10.654172    -8.566997    14.163236
 H    10.994009    -8.558681    12.442862
 H    11.319859    -6.059488    15.140103
 H     9.888931    -3.804031    11.888709
 H    10.995614    -3.714294    14.144331
 O    13.800242    -1.949380    23.256622
 H    12.851027    -2.019676    23.067826
 H    14.197335    -2.398026    22.495756
 O    13.235627     2.065441    16.747114
 H    12.727459     1.828569    17.535690
 H    13.792194     1.289630    16.592386
 C    11.193998     2.102000    24.317000
 C     9.874571     1.707110    23.635725
 C    10.043402     0.847914    22.376834
 C     8.723642     0.538978    21.668794
 O     7.711862     1.226032    21.912357
 O     8.698969    -0.438467    20.832919
 H    11.008594     2.701865    25.213105
 H    11.767281     1.217542    24.614013
 H    11.825996     2.687421    23.640734
 H     9.244738     1.162987    24.348692
 H     9.310443     2.604258    23.368127
 H    10.681916     1.347989    21.638271
 H    10.545131    -0.099983    22.591997
 C     6.655971    -3.375815    22.225358
 O     6.113962    -4.162539    23.005278
 N     6.148247    -2.170735    21.892802
 C     4.874003    -1.683000    22.391999
 C     4.873447    -0.171476    22.602181
 O     5.786022     0.242180    23.614232
 H     6.687920    -1.602104    21.247122
 H     4.063400    -1.942425    21.696034
 H     4.671190    -2.191954    23.336501
 H     5.104230     0.336206    21.657942
 H     3.859790     0.124084    22.899301
 H     6.560359     0.600998    23.141796
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