Understanding polyoxometalates as water oxidation catalysts through iron *vs* cobalt reactivity

Khalid Azmani,[a,b] Maria Besora,[b] Joaquín Soriano-López,[c]* Meriem Landolsi,[b,≠] Anne-Lucie Teillout,[d] Pedro de Oliveira,[d] Israël-Martyr Mbomekallé,[d] Josep M. Poblet,[b]* and José-Ramón Galán-Mascarós,[a,e]*

[a]Institute of Chemical Research of Catalonia (ICIQ), The Barcelona Institute of Science and Technology (BIST), Av. Països Catalans, 16. Tarragona, E-43007, Spain.

[b]Departament de Química Física i Inorgànica, Universitat Rovira i Virgili, Marcel·lí Domingo 1, E-43007 Tarragona, Spain.

[c] School of Chemistry & AMBER Center, Trinity College, University of Dublin, Dublin, D02 PN40, Ireland.

[d]Equipe d'Electrochimie et de Photo-électrochimie, Institut de Chimie Physique, UMR 8000, CNRS, Université Paris Saclay, Orsay, F-91405, France

[e]ICREA, Pg. Lluís Companys 23, 08010 Barcelona, Spain

[≠] Permanent address: Laboratory of Chemical Materials (LR13ES08), Faculty of Sciences of Bizerte, Carthage University, 7021 Zarzouna, Tunisia

1. Synthetic details

*Synthesis of $K_6[Fe_4(H_2O)_2(PW_9O_{34})_2]\cdot 20H_2O$ (**K[Fe$_4$-WS]**):*

About 1.43 of $FeSO_4.7H_2O$ (Fluka puriss. p.a. > 99.5%, 278.02 g.mol^{-1}, 5.1 mmol) was dissolved in 25 mL of water. Then 6.0 g of $Na_9PW_9O_{34}.11H_2O$ (A-β isomer, M.W. 2634.59 g.mol^{-1}, 2.3 mmol) are added in small portions under stirring and heating (60°C). After 20 minutes of evolution, the dark brown solution is hot-filtered and the clear filtrate treated with 7.5 g of solid KCl. A light brown precipitate starts to appear after a few minutes. The preparation is kept in the refrigerator overnight. After about 12 hours of this stay at 4°C, the light brown solid is collected and dissolved in 30 mL and then heat for about 4 hours at 80°C under stirring. After filtration and cooling at room temperature, the dark yellow solution is transferred into the refrigerator, in order to promote precipitation of the compound of interest. The yellow crystalline powder that forms is recovered by filtration after a few days and dried in the open air. We obtain 4.21 g of $K_6[Fe_4(PW_9O_{34})_2].20H_2O$.

Ba[Fe$_4$-WS] salts were obtained by metathesis of a **KFe$_4$-WS** aqueous solution upon addition of an excess of $BaCl_2$, which immediately yields the desired precipitate. The **BaFe$_4$-WS** precipitate was filtered, cleaned with water and acetone and dried in air.
$K_6[Fe_4(H_2O)_2(PW_9O_{34})_2]\cdot 20H_2O$ **K[Fe$_4$-WS]** M_w=5492.29 g/mol. Elemental analysis (%) calculated: K, 6 ; found: K, 6.3; $Ba_3[Fe_4(H_2O)_2(PW_9O_{34})_2]\cdot 39H_2O$ **Ba[Fe$_4$-WS]** M_w=5838.54 g/mol. Elemental analysis (%) calculated: Ba, 3 ; found: Ba, 3.4.

*Synthesis of $TBA_4[Fe(H_2O)(PW_{11}O_{39})]\cdot 3H_2O$ (**TBA[Fe-K]**):*
Solid $Fe(NO_3)_3\cdot 9H_2O$ (230 mg) was added to 6 mL of a hot (90°C) distillated water solution containing 1.73 g of $K_7PW_{11}O_{39}\cdot H_2O$ under continuous stirring and kept at that temperature for 10 minutes. Then, the solution was filtered using a Nylon membrane filter. To the cooled filtrated solution, 10 ml of a Tetra-n-butylammonium bromide (260 mg) aqueous solution were gradually added under stirring. The **TBA[Fe-K]** salt precipitates immediately, which did not contain any potassium cations.
Ba[Fe-K] salts were obtained by metathesis of a **TBA[Fe-K]** acetonitrile solution upon addition of an excess of $BaCl_2$, which immediately yields the desired precipitate. The **Ba[Fe-K]** precipitate was filtered, cleaned with water and acetone and dried in air.
$TBA_4[Fe(H_2O)(PW_{11}O_{39})]\cdot 3H_2O$ (**TBA[Fe-K]**) M_w=3784.49 g/mol.$Ba_2[Fe(H_2O)(PW_{11}O_{39})]\cdot 7H_2O$ **Ba[Fe-K**] M_w=3566.32 g/mol. Elemental analysis (%) calculated: Ba, 2; found: Ba, 2.1
The resulting products were characterized by Thermogravimetric analysis (TGA) (Figure S2–S3), Infrared spectroscopy (Figure S4-S5), Raman spectroscopy (Figure S6-S7) and Energy dispersive X-ray spectroscopy (EDX) (Table S1).

2. Pictures of the electrocatalytic electrodes

Figure S1. Images of the electrode preparative for long-term electrocatalytic experiments to avoid the expulsion of the blend out of the electrode pocket.

3. Thermogravimetric analysis of fresh compounds

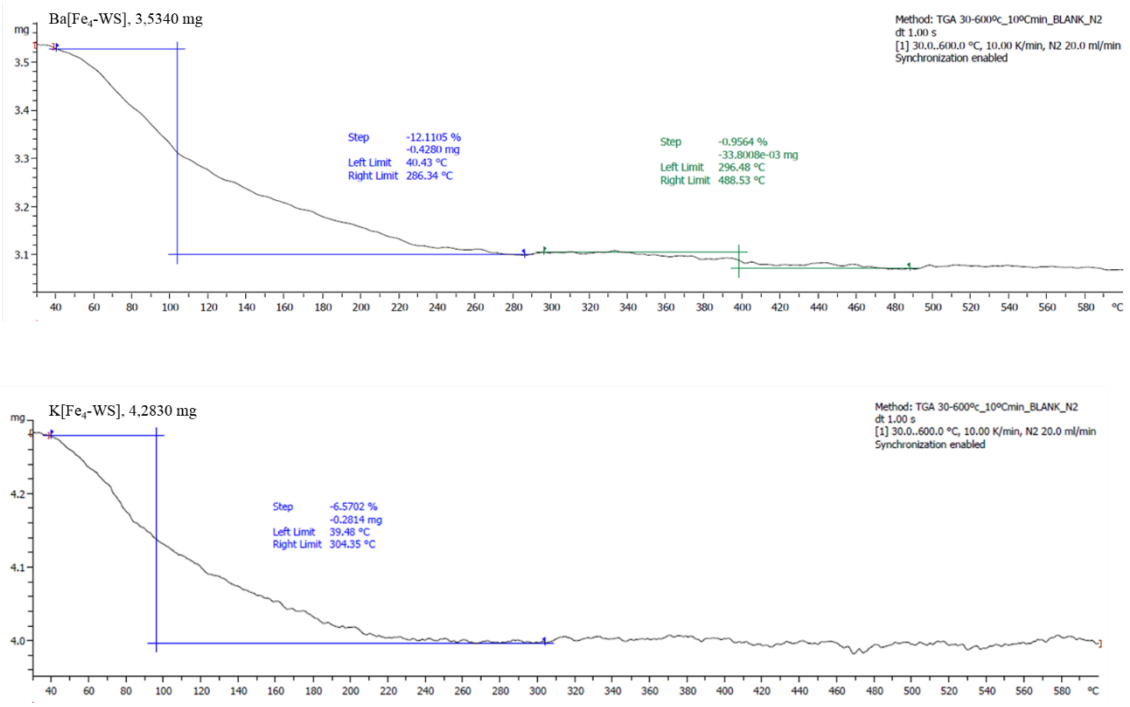

Figure S2. Thermogravimetric analysis for **Ba[Fe$_4$-WS]** (top) and **K[Fe$_4$-WS]** (bottom).

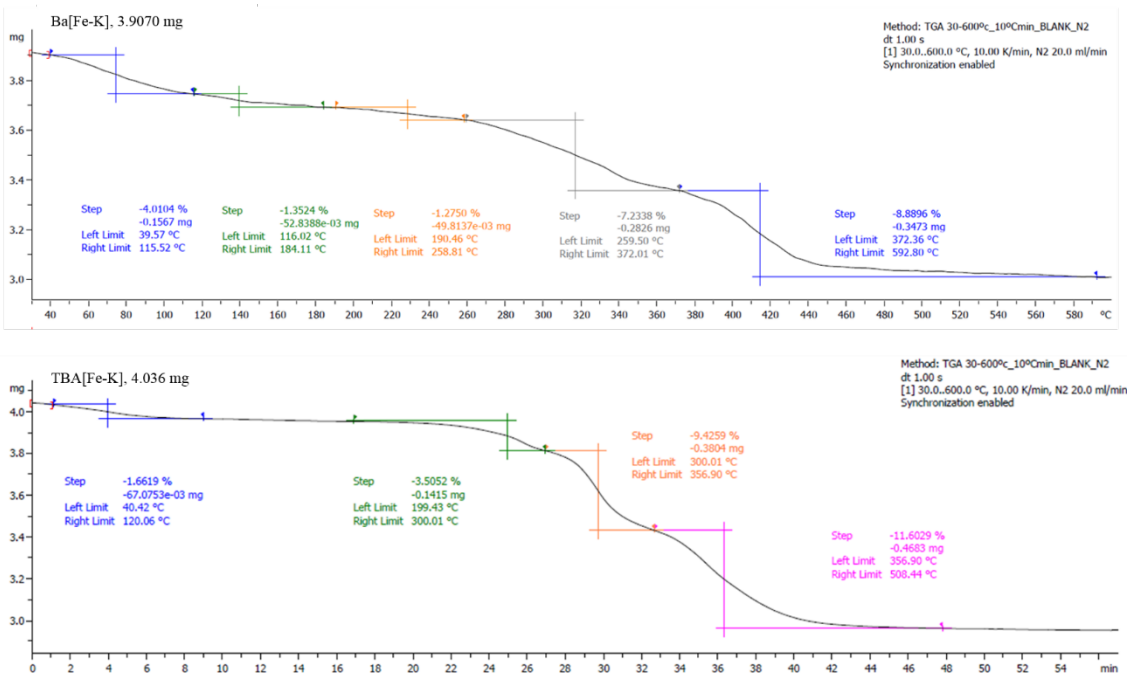

Figure S3. Thermogravimetric analysis for **Ba[Fe-K]** (top) and **TBA[Fe-K]** (bottom).

4. Infrared spectra of fresh compounds

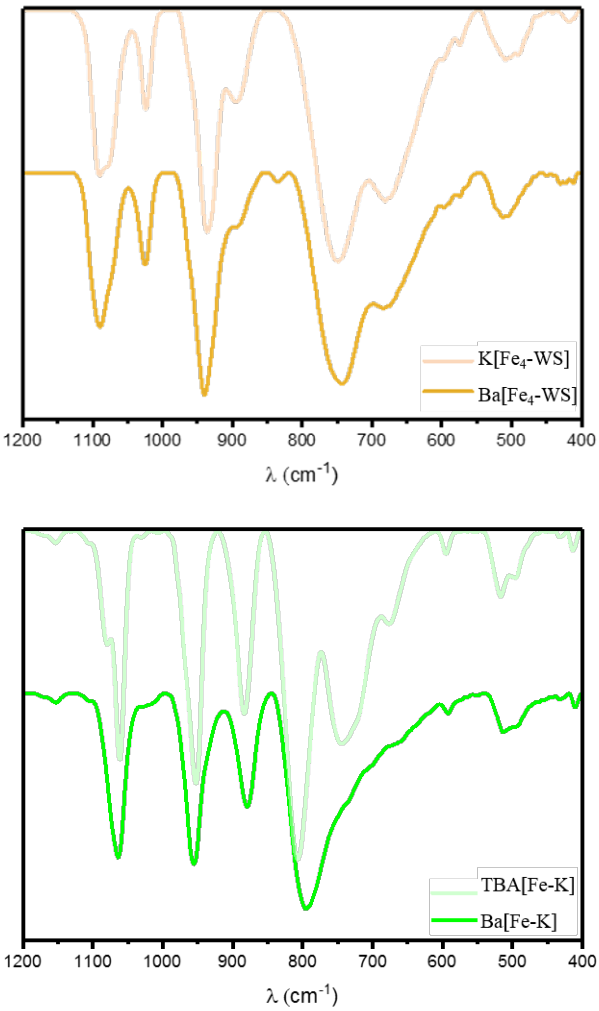

Figure S4. (Top) FT-IR spectra of $[Fe_4(H_2O)_2(PW_9O_{34})_2]^{6-}$ (**Fe_4-WS**) with different countercations: K^+ (**K[Fe_4-WS]**) (light) and Ba^{2+} (**Ba[Fe_4-WS]**) (bold). (Bottom) FT-IR spectra of $[Fe(H_2O)(PW_{11}O_{39})]^{4-}$ (Fe-K) with different countercations: TBA^+ (**TBA[Fe-K]**) (light) and Ba^{2+} (**Ba[Fe-K]**) (bold).

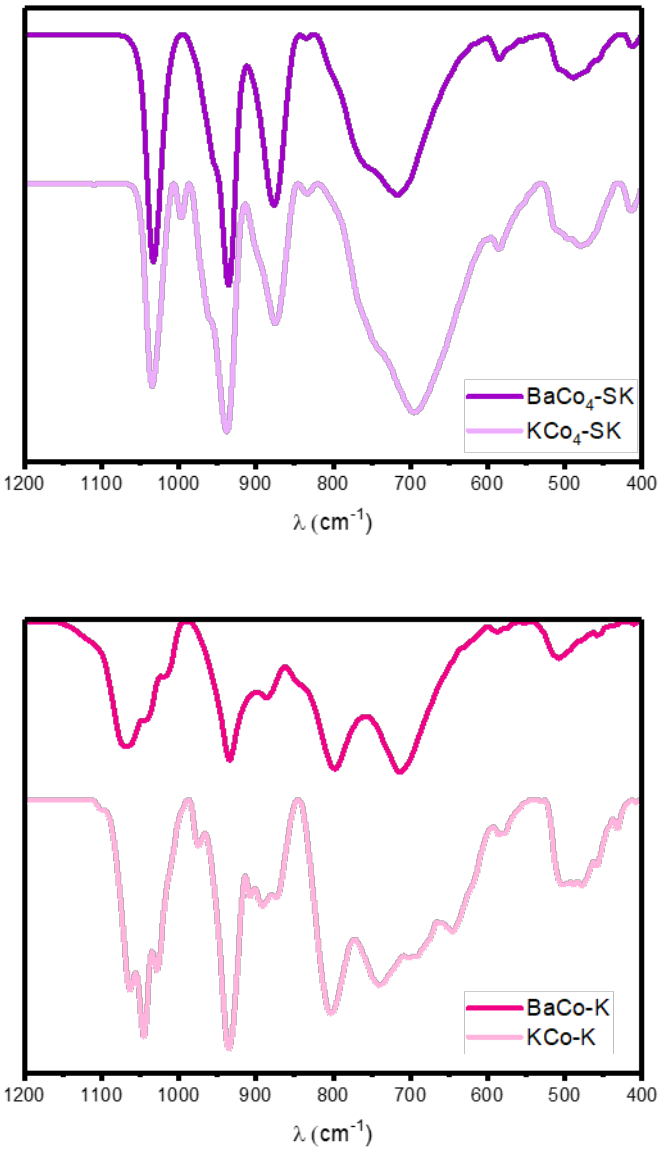

Figure S5. (Top) FT-IR spectra of $[Fe_4(H_2O)_2(PW_9O_{34})_2]^{6-}$ (**Co_4-WS**) with different countercations: K^+ (**K[Co_4-WS]**) (light) and Ba^{2+} (**Ba[Co_4-WS]**) (bold). (Bottom) FT-IR spectra of $[Fe(H_2O)(PW_{11}O_{39})]^{4-}$ (Fe-K) with different countercations: TBA^+ (**K[Co-K]**) (light) and Ba^{2+} (**Ba[Co-K]**) (bold).

5. Raman spectra of fresh compounds

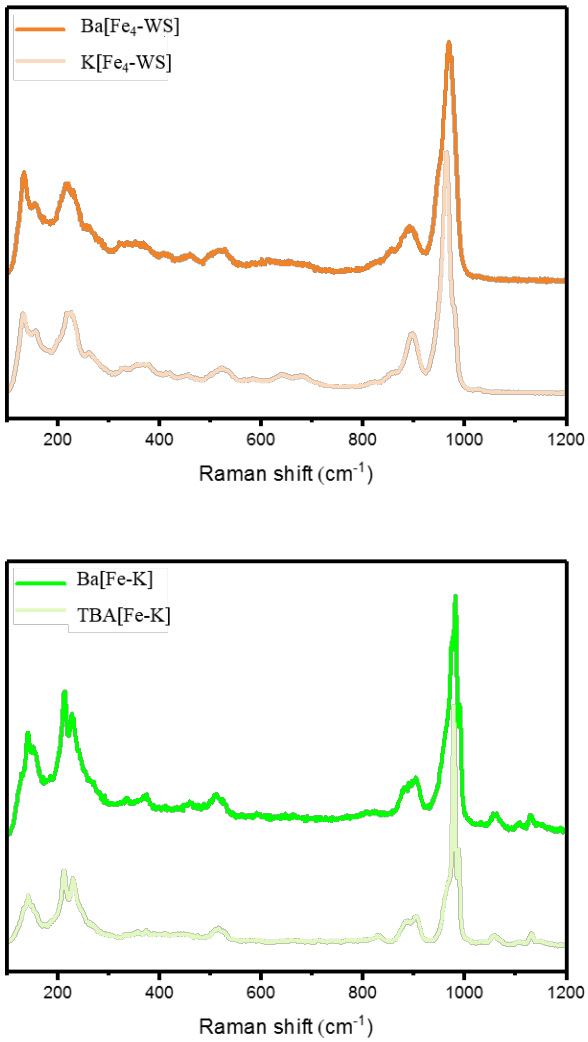

Figure S6. (Top) Raman spectra of $[Fe_4(H_2O)_2(PW_9O_{34})_2]^{6-}$ (**Fe_4-WS**) with different countercations: K^+ (**K[Fe_4-WS]**) (light) and Ba^{2+} (**Ba[Fe_4-WS]**) (bold). (Bottom) Raman spectra of $[Fe(H_2O)(PW_{11}O_{39})]^{4-}$ (Fe-K) with different countercations: TBA^+ (**TBA[Fe-K]**) (light) and Ba^{2+} (**Ba[Fe-K]**) (bold).

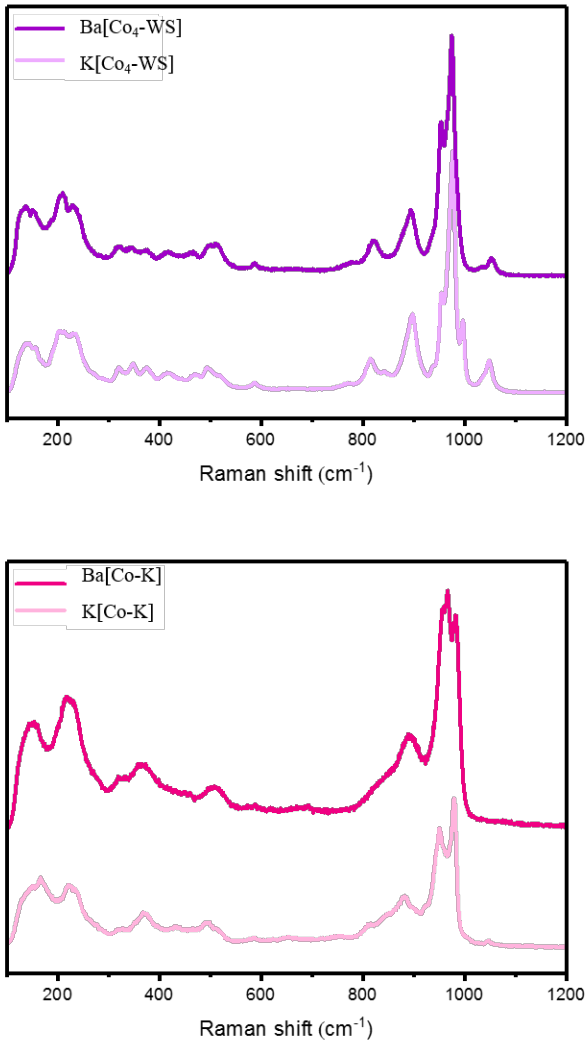

Figure S7. (Top) Raman spectra of $[Co_4(H_2O)_2(PW_9O_{34})_2]^{10-}$ (**Co_4-WS**) with different countercations: K^+ (**K[Co_4-WS]**) (light) and Ba^{2+} (**Ba[Co_4-WS]**) (bold). (Bottom) Raman spectra of $[Co(H_2O)(PW_{11}O_{39})]^{5-}$ (**Co-K**) with different countercations: TBA^+ (**K[Co-K]**) (light) and Ba^{2+} (**Ba[Co-K]**) (bold).

6. Energy dispersive X-ray spectroscopy measurements of fresh compounds

Table S1. P, Co and W elemental composition estimated from EDX analyses for the fresh catalysts. The data were normalized to the W content to facilitate comparison. The theoretical values are extracted from the POM formula.

	P	Fe or Co	W
Fe_4-WS (theoretical)	2	4	18
K[Fe_4-WS] (experimental)	2.5	4.4	18
Ba[Fe_4-WS] (experimental)	2.4	4.8	18
Fe-K (theoretical)	1	1	11
TBA[Fe-K] (experimental)	1.7	1.1	11
Ba[Fe-K] (experimental)	1.6	1.1	11
Co_4-WS (theoretical)	2	4	18
K[Co_4-WS] (experimental)	1.9	4.3	18
Ba[Co_4-WS] (experimental)	2.2	4.1	18
Co-K (theoretical)	1	1	11
K[Co-K] (experimental)	1.1	1.2	18
Ba[Co-K] (experimental)	1.5	1.3	11

7. Electrocatalytic activity of 20% POM/CP blends: Reproducibility of linear sweep voltammetry measurements

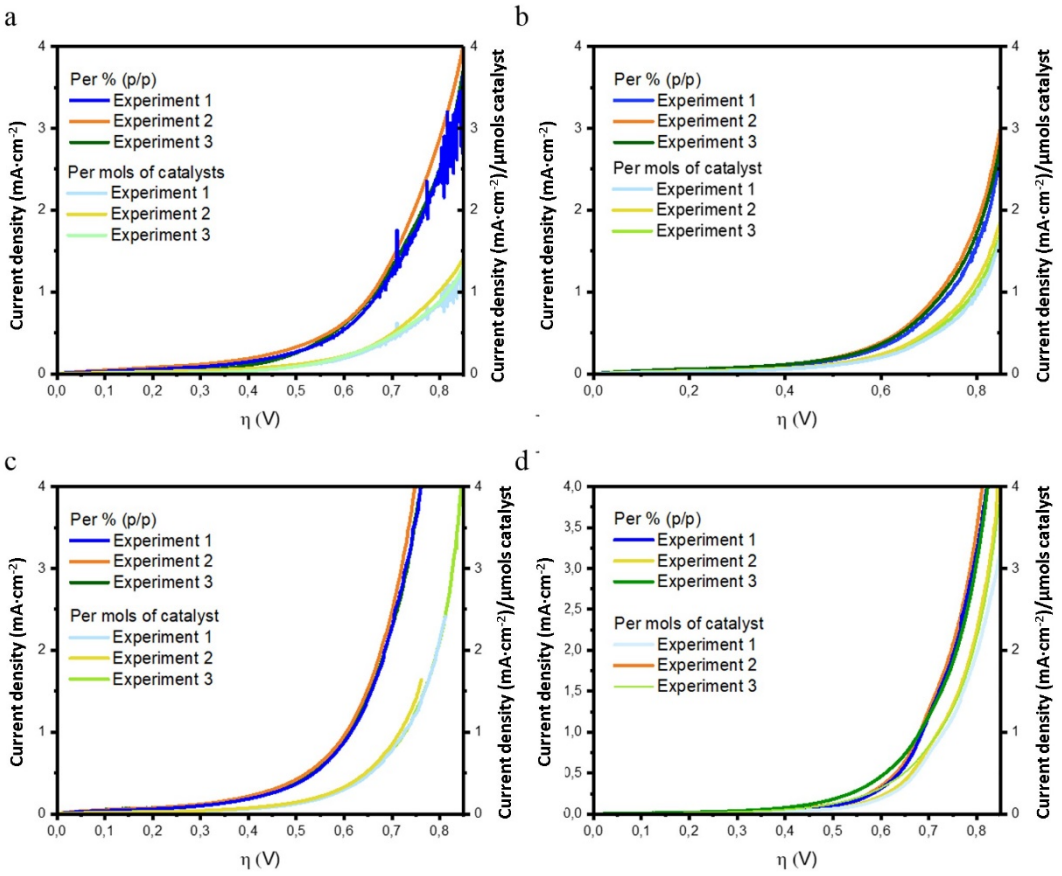

Figure S8. Linear sweep voltammetry of the 20% **Ba[POM]**/CP working electrodes and linear sweep voltammetry normalized by the total number of moles of (a) **Ba[Fe-K]** (b) **Ba[Fe$_4$-WS]** (c) **Ba[Co-K]** and (d) **Ba[Co$_4$-WS]** used in each blend. All the measurements where done in an aqueous potassium phosphate (50 mM) buffer solution at pH = 6.9 with KNO_3 (1 M) as the electrolyte.

8. Long-term stability test of Fe_4-WS

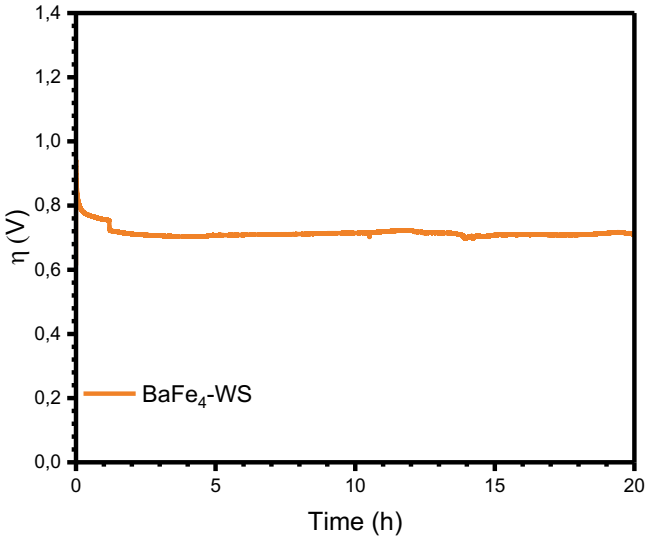

Figure S9. Chronopotentiometry at a constant current density of 1 mA/cm^2 using 20% **Ba[Fe_4-WS]**/CP . All the measurements where done in an aqueous potassium phosphate (50 mM) buffer solution at pH = 6.9 with KNO_3 (1 M) as the electrolyte.

9. Oxygen evolution

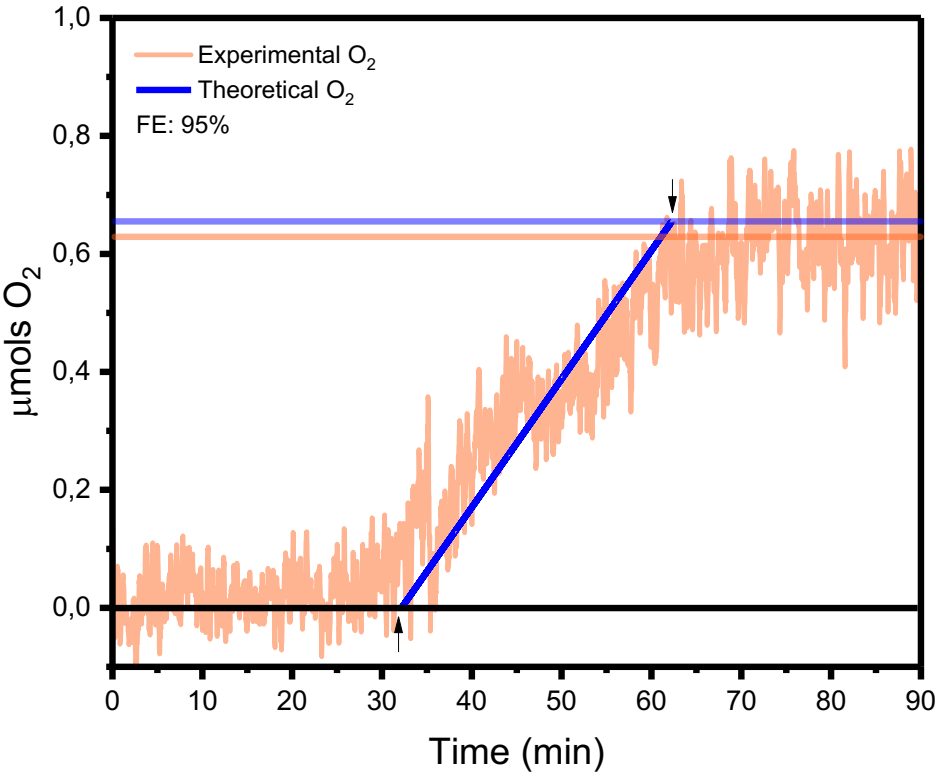

Figure S10. Oxygen evolution detection (orange) of the 20% **$BaFe_4$**/CP during water electrolysis (at a constant current of 1 mA · cm^{-2}) in an aqueous potassium phosphate (50 mM) buffer solution at pH = 6.9 with KNO_3 (1 M) as the electrolyte. Theoretical oxygen evolution (blue) taking into account a constant current of 1 mA · cm^{-2}. The arrows indicate initial and final electrolysis times.

10. Post-catalytic characterization

10.1. Raman and IR spectra of the recovered Ba[Fe_4-WS]

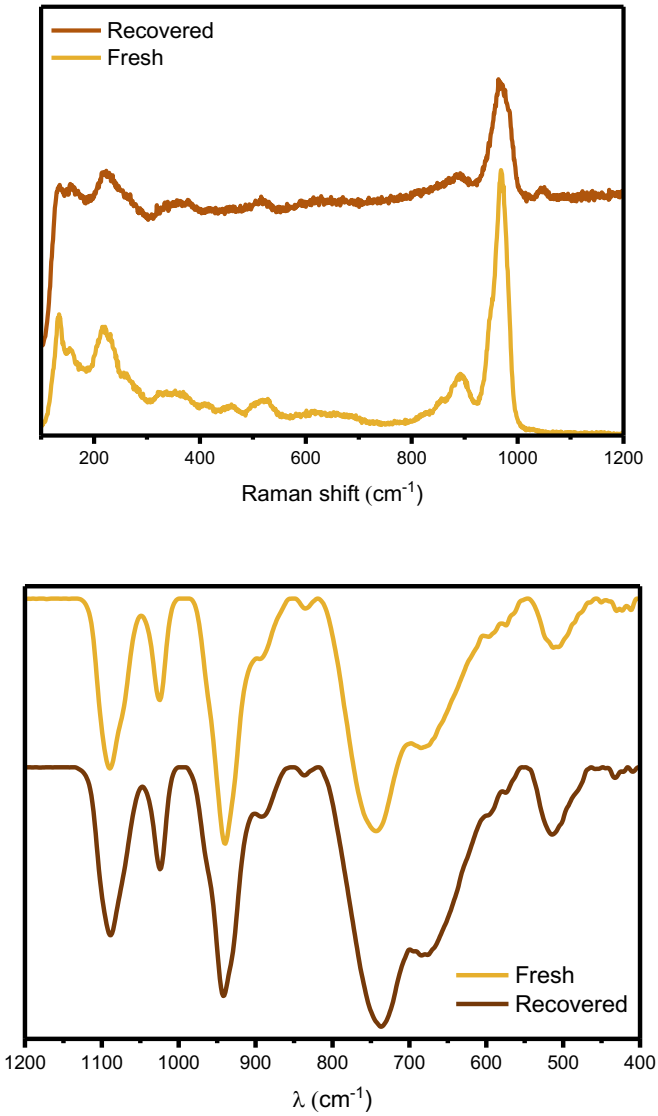

Figure S11. (**Top)** Raman spectra and **(Bottom)** IR spectra of **Ba[Fe_4-WS]** before and after 2 h of electrocatalytic bulk water electrolysis at a constant current density of 1 mA/cm^2 in a pH = 6.9 potassium phosphate (50 mM) buffer solution with KNO_3 (1 M) as the electrolyte.

10.2. Inductively coupled plasma mass spectrometry measurements of the buffer solutions after bulk water electrolysis experiments

Table S2. Fe, Ba and W elemental composition estimated from ICP analyses for the buffer solutions after 2 h of electrocatalytic bulk water electrolysis at a constant current density of 1 mA/cm^2 in a pH = 6.9 potassium phosphate (50 mM) buffer solution with KNO_3 (1 M) as the electrolyt.

Solution	Fe	Ba	W
Blank (KP_i 50mM; KNO_3 1M)	<1ppm	-	-
Ba[Fe-K]	< 1ppm	<1 ppm	<1 ppm
Ba[Fe_4-WS]	< 1ppm	<1 ppm	<1 ppm

11. Electrocatalytic activity of 20% POM/CP blends: Double layer capacitance measurements

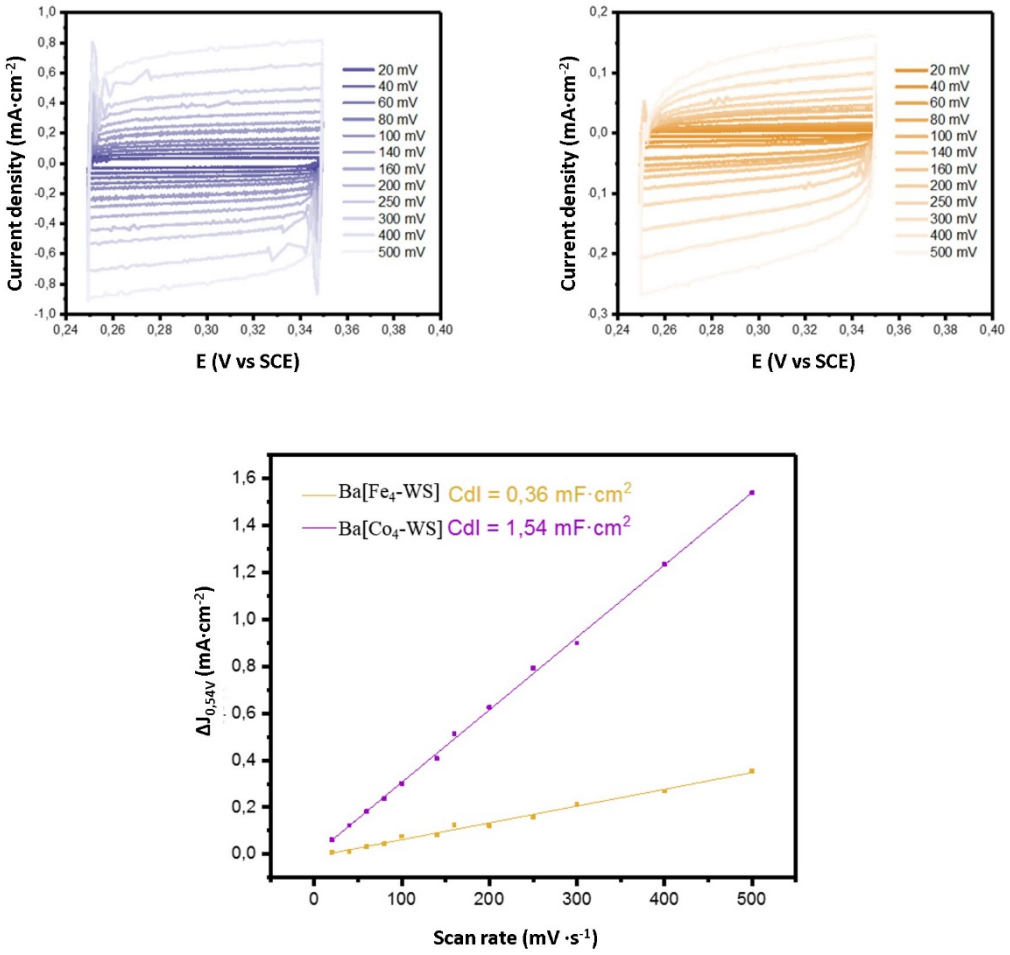

Figure S12. Double-layer capacitance (C_{dl}) measurements in a potassium phosphate (50 mM) buffer solution at pH = 6.9 with KNO_3 (1 M) as the electrolyte for 20% **Ba[Fe_4-WS]**/CP (orange) and 20% **Ba[Co_4-WS]**/CP (purple) electrodes. (Top) Cyclic voltammograms in the non-Faradaic region with increasing scan rates between 20 and 500 mV. (Bottom) Plot of Δj (j_a-j_c) versus the scan rate where the slope is twice the C_{dl}. Within the measured potential range, the current response does not arise from any redox or catalytic process, so it is attributed to the charging of the double layer.

12. Experimental pK_a determination

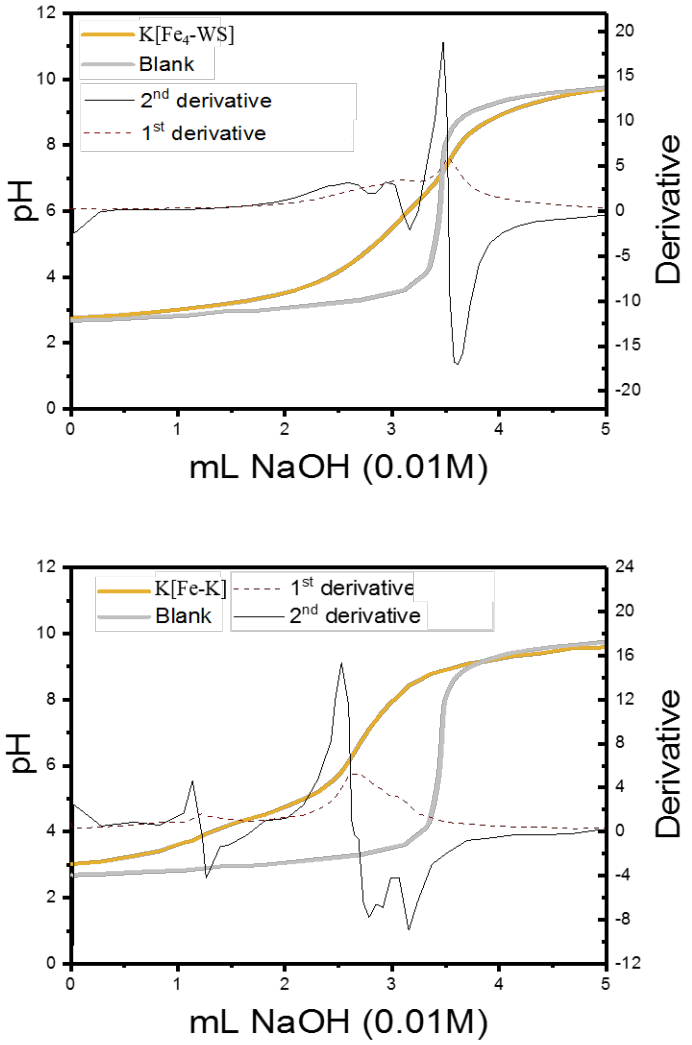

Figure S13. Acid-base titration of **K[Fe$_4$-WS]** (top) and **K[Fe-K]** (bottom) in a 0.010 mM $HClO_4$:$NaClO_4$ solution with the addition of a 0.010 mM NaOH solution. (Top) K[Fe4-SW], (Bottom) K[Fe-K].

13. Computational details of some Fe_4 intermediates -WS

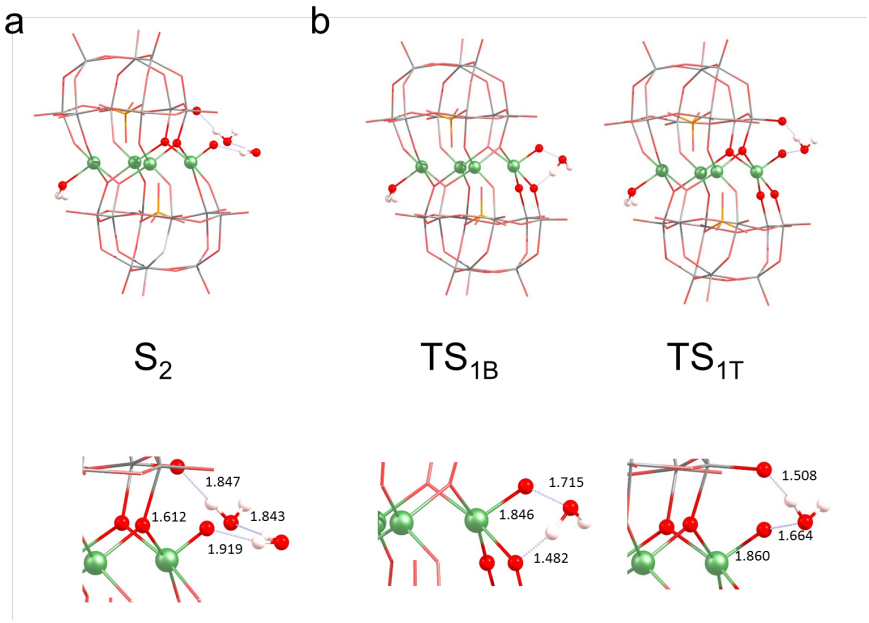

Figure S14. Ball and stick representations of (a) **S_2** species and (b) **TS_{1B}**, **TS_{1T}** species.

14. Computational comparison of TS of Fe- and Co-monosubstituted Keggin POMs

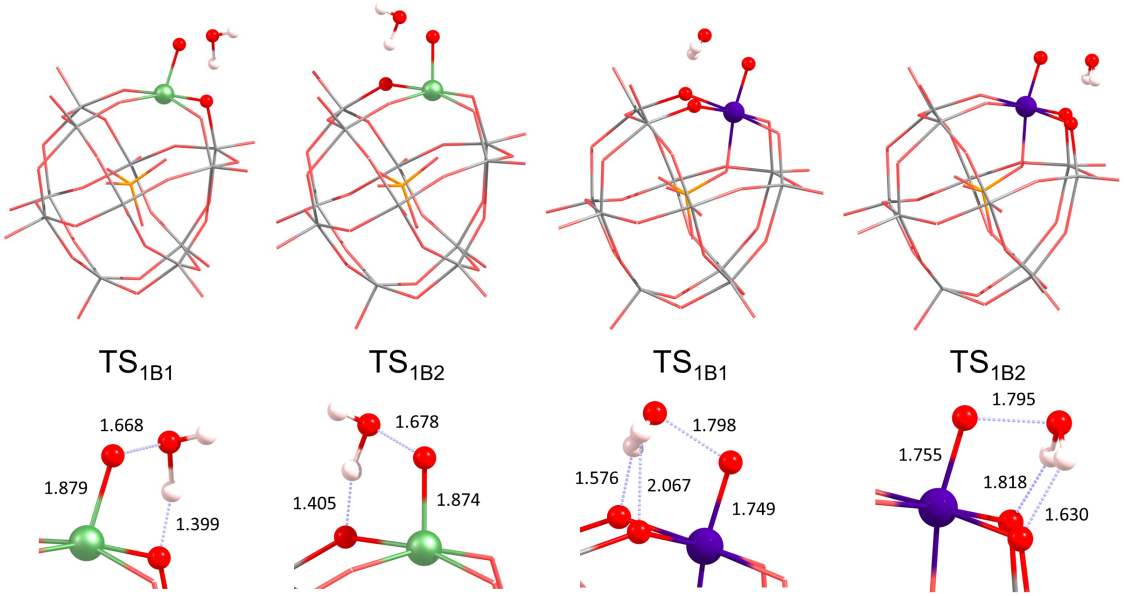

Figure S15. Structures of the computed transition states for **Fe-K** and **Co-K** using one molecule of water and the BS2 level of theory. Selected distances are given in Å.

Table S3. Comparison of free activation energy barriers for O-O bond formation using Fe and Co monosubstituted Keggin anions as catalysts.

POM	Basis Set	TS_{1B1}	TS_{1B2}
Fe-K	BS2	27.3 [(a)]	27.3 [(a)]
	BS1	25.5	25.1
Co-K	BS2	25.5 [(a)]	25.2 [(a)]
	BS1	24.0	23.2

(a) Transitions states are represented in Figure S13

15. Discussion on the Water Nucleophilic Attack

In this section, we present a discussion on the nature of the reaction that forms de O-O bond. The active species **S_2** (Fe^{IV}=O) reacts with water through **TS2** and leads to the formation of an intermediate species **Int** (Fe^{II}–OOH_2), where the O-O bond is already formed.

As shown in Figures 5 and 6 of the main text, the attack of a water molecule induces a significant electronic reorganization at the iron centre: the Fe–O bond elongates from 1.609 Å in **S_2** to 1.818 Å in **TS2** and then to 2.001 Å in **Int**. The formation of the new O–O bond causes the formal reduction of the active iron centre from IV to II.

The spin states of iron in these three key species is 3.125 e in **S_2**, 3.769 e in **TS2** and 3.744 e in **Int**, while for the oxygen bonded to it is 0.563 e in **S_2**, 0.139 e in **TS2** and 0.094 e in **Int**. The half unpaired electron on the oxygen of **S_2** can be explained by the fact that **S_2** is a combination of the two resonance forms $\mathrm{Fe^{IV}} = \overline{\underline{\mathrm{O}}} \leftrightarrow \mathrm{Fe^{III}} - \underline{\dot{\mathrm{O}}}\,|$, being actually closer to first species than to the second one. Importantly, the latter resonance form gives a partial radical character on the oxygen that we believe contributes to its electrophilic character. Note that in the case of an oxygen radical, it would have a full electron. In the transition state, this partial radical character has disappeared.

The electrophilic character of **S_2** can also be appreciated in the LUMO of the intermediate (Figure 7a), where we can clearly see that this orbital is able to take a pair of electrons from water.

16. Effect of Grimme's dispersion corrections

Table S4. Comparison of relative energies given upon inclusion of Grimme's dispersion energies. Values at pH=0. Energies in eV or V.

	S_0 Fe_4-SK Fe^{III}-OH_2	S_0' Fe_4-SK Fe^{III}-OH	S_1 Fe_4-SK Fe^{IV}=O	$HOFeFe_2(PW_9O_{34})_2FeOH$
B3LYP BS1	0.0	0.12	2.1	0.4
B3LYP BS2	0.0	0.36	2.3	0.9
B3LYP-D3[1] BS2	0.0	0.46	2.5	1.1
B3LYP-D2[2] BS2	0.0	0.51	2.5	1.2
B3LYP-D3bj[3] BS2	0.0	0.45	2.5	1.1

BS1: we used the 6-31G(d,p) basis set for all the H and O atoms directly bonded to either the iron or the cobalt atoms, and the 6-31G basis set for the rest of the oxygens.[4,5] The LANL2DZ effective core potential (ECP) and associated basis sets were used for the P, W, Co and Fe atoms.[6]

BS2: the 6-31G(d,p) basis set was used for all the oxygens instead, and was used to re-optimize all relevant structures.

All structures were optimized using the IEF-PCM approach to model implicitly the solvent effects of water (UFF radii).[7]

1 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
2 S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787–1799.
3 S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456–1465.
4 M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. DeFrees and J. A. Pople, *J. Chem. Phys.*, 1982, **77**, 3654–3665.
5 W. J. Hehre, K. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257–2261.
6 P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270–283.
7 E. Cancès, B. Mennucci and J. Tomasi, *J. Chem. Phys.*, 1997, **107**, 3032–3041.

17. Potential energies (in Hartrees) and atomic coordinates (Å) of the most relevant species studied

Fe_4-SK species.

Fe_4-SK species. Large basis sets BS2

Fe4-SK-7_20

Energy (POTENTIAL) = -6924.61431573 Eh

	Atom	X	Y	Z
1	Fe	-0.0266	-1.8024	0.0682
2	Fe	0.0031	1.7735	-0.0252
3	Fe	0.8619	0.0133	-2.4879
4	Fe	-0.8808	0.1154	2.6212
5	H	0.3190	-0.7030	4.8760
6	H	0.3738	0.8674	4.8725
7	O	1.3788	3.1371	-0.5222
8	O	-1.3460	-2.9996	0.6006
9	O	-0.5536	-1.4023	-1.8532
10	O	0.5757	1.4281	2.0263
11	O	5.5311	-0.0184	2.3033
12	O	-5.4933	-0.0985	-2.3737
13	O	2.3399	3.5057	1.8912
14	O	-2.2248	-3.5122	-1.7905
15	O	3.0576	5.3290	-0.2423
16	O	-2.9509	-5.2954	0.3254
17	O	3.2032	1.3116	0.8006
18	O	-3.1870	-1.3055	-0.8114
19	O	1.3490	-0.0007	-0.4989
20	O	-1.3397	0.0178	0.5262
21	O	3.2106	-1.2824	0.8321
22	O	-3.1750	1.2795	-0.8764
23	O	3.8355	-0.0176	-1.3225
24	O	-3.8614	0.0347	1.2770
25	O	2.4192	0.0279	3.2534
26	O	-2.3102	-0.0975	-3.3471
27	O	2.2481	-3.4447	1.9234
28	O	-2.3061	3.4293	-2.0330
29	O	3.7296	-2.9570	-1.5619
30	O	-3.8561	2.9840	1.4296
31	O	4.0911	-0.0369	-3.9509
32	O	-4.1471	0.1086	3.8840
33	O	6.1574	1.2329	0.1421
34	O	-6.1449	-1.3449	-0.1940
35	O	6.8649	2.4899	2.6016
36	O	-6.7644	-2.6079	-2.6644
37	O	4.7832	3.3852	0.9322
38	O	-4.6966	-3.4455	-0.9187
39	O	4.1253	2.0633	3.1525
40	O	-4.0078	-2.1784	-3.1495
41	O	1.4691	-2.3050	4.4329
42	O	-1.5488	2.3675	-4.5270
43	O	0.5700	-1.3254	1.9443
44	O	-0.5600	1.3484	-2.0622
45	O	4.0649	-2.0732	3.1859
46	O	-4.0685	1.9290	-3.2804
47	O	6.8065	-2.5230	2.6574
48	O	-6.8170	2.3977	-2.7910
49	O	6.1328	-1.3465	0.1578
50	O	-6.1661	1.2343	-0.2743
51	O	5.7240	-1.3983	-2.4761
52	O	-5.8195	1.3818	2.3636
53	O	8.0391	-0.0876	-1.5394
54	O	-8.0758	-0.0199	1.4237
55	O	5.7713	1.2857	-2.4938
56	O	-5.7832	-1.2976	2.4471
57	O	4.1649	2.7381	-4.3969
58	O	-4.1692	-2.6591	4.4074
59	O	2.0917	1.3850	-3.0266
60	O	-2.1000	-1.3191	3.0371
61	O	-1.4298	-2.5799	-4.3195
62	O	1.5806	2.4182	4.4402
63	O	2.9200	-5.2982	-0.1706
64	O	-3.0559	5.3325	0.0046
65	O	4.6960	-3.4157	0.9795
66	O	-4.7627	3.3477	-1.1289
67	O	1.3220	-3.0003	-0.4487
68	O	-1.3759	3.1682	0.4164
69	O	2.0387	-1.4085	-3.0543
70	O	-2.1372	1.5119	2.9383
71	O	-0.2033	0.1009	4.6781
72	O	4.0917	-2.8205	-4.3767
73	O	-4.2391	2.8980	4.2284
74	O	3.8259	2.9302	-1.5954
75	O	-3.7914	-2.9005	1.6078
76	P	2.9045	0.0048	-0.0392
77	P	-2.8829	0.0093	0.0239
78	W	3.0232	3.6258	0.0063
79	W	-3.0035	-3.6053	0.0107
80	W	3.8612	-1.7325	-3.0667
81	W	-3.9772	1.7936	2.9365
82	W	2.1416	-1.8319	2.9091
83	W	-2.1319	1.8158	-3.0061
84	W	5.4340	-1.8619	1.8653
85	W	-5.4367	1.8080	-1.9547
86	W	2.9920	-3.5985	0.0783
87	W	-3.0044	3.6199	-0.1771
88	W	2.1726	1.9188	2.8912
89	W	-2.0926	-1.9348	-2.8697
90	W	6.3424	-0.0630	-1.2755
91	W	-6.3745	-0.0095	1.1883
92	W	5.4657	1.8717	1.8201
93	W	-5.4086	-1.9215	-1.8642
94	W	3.9246	1.6819	-3.0625
95	W	-3.9220	-1.6216	3.0580

Fe4-SK-O_-6_21

Energy (POTENTIAL) = -6999.51735036 Eh

	Atom	X	Y	Z
1	Fe	-0.0039	-0.0560	1.7982
2	Fe	-0.0038	-0.0473	-1.7982
3	Fe	0.7935	-2.6687	-0.0062
4	Fe	-0.8742	2.6094	0.0063
5	H	0.3135	4.8915	0.7991
6	H	0.3140	4.8955	-0.7772
7	O	1.3701	-0.5049	-3.0284
8	O	-1.3305	0.4698	2.9925
9	O	-0.5449	-1.9456	1.3986
10	O	0.5787	1.8901	-1.3749
11	O	5.4868	2.2690	0.0055
12	O	-5.5145	-2.3221	-0.0052
13	O	2.2591	1.9194	-3.4932
14	O	-2.2727	-1.9009	3.4639
15	O	2.9161	-0.1279	-5.3522
16	O	-2.9429	0.1900	5.2893
17	O	3.1834	0.8027	-1.2951
18	O	-3.1970	-0.8230	1.2896
19	O	1.3433	-0.5870	-0.0016
20	O	-1.3246	0.5025	0.0012
21	O	3.1829	0.7969	1.2988
22	O	-3.1969	-0.8174	-1.2932
23	O	3.8782	-1.3116	-0.0029
24	O	-3.8305	1.3148	0.0030
25	O	2.3676	3.2420	0.0078
26	O	-2.3680	-3.2720	-0.0072
27	O	2.2581	1.9024	3.5025
28	O	-2.2719	-1.8857	-3.4721
29	O	3.8428	-1.5373	3.0473
30	O	-3.7730	1.5627	-2.9389
31	O	4.0841	-3.9444	-0.0095
32	O	-4.0798	3.9311	0.0085
33	O	6.1230	0.1397	-1.3052
34	O	-6.1380	-0.1687	1.2886
35	O	6.7902	2.6517	-2.4863
36	O	-6.8167	-2.6456	2.5001
37	O	4.7134	0.9915	-3.4208
38	O	-4.7198	-0.9765	3.4024
39	O	4.0467	3.1683	-2.0588
40	O	-4.0733	-3.1784	2.0626
41	O	1.4477	4.3886	2.3595
42	O	-1.5634	-4.4117	-2.4873
43	O	0.5783	1.8834	1.3837
44	O	-0.5445	-1.9392	-1.4071
45	O	4.0462	3.1582	2.0742
46	O	-4.0727	-3.1693	-2.0766
47	O	6.7900	2.6394	2.4996
48	O	-6.8163	-2.6352	-2.5119
49	O	6.1231	0.1335	1.3062
50	O	-6.1380	-0.1632	-1.2901
51	O	5.7691	-2.5211	1.3184
52	O	-5.7526	2.4727	-1.3374
53	O	8.0431	-1.4862	-0.0036
54	O	-8.0405	1.5177	0.0030
55	O	5.7693	-2.5148	-1.3304
56	O	-5.7528	2.4668	1.3481
57	O	4.2040	-4.3136	-2.8815
58	O	-4.1328	4.3607	2.7898
59	O	2.1888	-3.0162	-1.4405
60	O	-2.0699	2.9899	1.4263
61	O	-1.5637	-4.4221	2.4685
62	O	1.4482	4.3999	-2.3389
63	O	2.9157	-0.1543	5.3515
64	O	-2.9421	0.2127	-5.2884
65	O	4.7129	0.9752	3.4258
66	O	-4.7195	-0.9620	-3.4071
67	O	1.3697	-0.5201	3.0262
68	O	-1.3302	0.4835	-2.9904
69	O	2.1884	-3.0220	1.4262
70	O	-2.0696	2.9959	-1.4128
71	O	0.2886	-4.1946	-0.0098
72	O	-0.2168	4.6608	0.0102
73	O	4.2034	-4.3271	2.8609
74	O	-4.1320	4.3726	-2.7712
75	O	3.8430	-1.5229	-3.0549
76	O	-3.7734	1.5499	2.9457
77	P	2.8832	-0.0742	-0.0001
78	P	-2.8821	0.0423	0.0001
79	W	2.9848	0.1103	-3.6563
80	W	-3.0073	-0.0722	3.5945
81	W	3.9506	-2.9747	1.8327
82	W	-3.9038	3.0501	-1.7021
83	W	2.1211	2.8752	1.8734
84	W	-2.1527	-2.9205	-1.8847
85	W	5.4104	1.8414	1.8752
86	W	-5.4404	-1.8459	-1.8642
87	W	2.9844	0.0927	3.6568
88	W	-3.0068	-0.0567	-3.5948
89	W	2.1215	2.8844	-1.8594
90	W	-2.1531	-2.9285	1.8720
91	W	6.3483	-1.2397	-0.0030

92W -6.3459 1.2627 0.0025
93W 5.4106 1.8505 -1.8662
94W -5.4406 -1.8539 1.8557
95W 3.9509 -2.9661 -1.8471
96W -3.9043 3.0426 1.7153
Fe4-SK-O_-7_20
Energy (POTENTIAL) = -6999.75496445 Eh
Atom X Y Z
1 Fe -0.0084 -0.0546 -1.8072
2 Fe -0.0093 -0.0445 1.8076
3 Fe -0.8125 -2.6737 0.0074
4 Fe 0.8586 2.5752 -0.0070
5 H -0.3303 4.8422 -0.8005
6 H -0.3309 4.8465 0.7753
7 O -1.3672 -0.5162 3.0190
8 O 1.3450 0.4608 -3.0080
9 O 0.5730 -1.9442 -1.3955
10O -0.5538 1.8681 1.3753
11O -5.4806 2.3727 -0.0068
12O 5.5331 -2.3213 0.0066
13O -2.2496 1.8848 3.4724
14O 2.2959 -1.9102 -3.4675
15O -2.9814 -0.1987 5.3033
16O 2.9625 0.1839 -5.2940
17O -3.1856 0.7987 1.2901
18O 3.2164 -0.8273 -1.2897
19O -1.3383 -0.5889 0.0018
20O 1.3440 0.4951 -0.0007
21O -3.1853 0.7918 -1.2946
22O 3.2174 -0.8208 1.2943
23O -3.8783 -1.3151 0.0033
24O 3.8461 1.3122 -0.0033
25O -2.3296 3.2154 -0.0087
26O 2.3914 -3.2836 0.0091
27O -2.2485 1.8657 -3.4824
28O 2.2952 -1.8909 3.4779
29O -3.8515 -1.5515 -2.9645
30O 3.7880 1.5625 2.9402
31O -4.1726 -3.9267 0.0105
32O 4.0895 3.9315 -0.0108
33O -6.1522 0.2285 1.2849
34O 6.1523 -0.1686 -1.2889
35O -6.7855 2.7116 2.4943
36O 6.8312 -2.6485 -2.4993
37O -4.7160 1.0165 3.4044
38O 4.7391 -0.9772 -3.4024
39O -4.0224 3.1874 2.0540
40O 4.0908 -3.1804 -2.0599
41O -1.4226 4.3647 -2.3756
42O 1.5724 -4.4087 2.4881
43O -0.5530 1.8602 -1.3849
44O 0.5724 -1.9362 1.4058
45O -4.0215 3.1760 -2.0716
46O 4.0902 -3.1688 2.0775
47O -6.7846 2.6981 -2.5102
48O 6.8305 -2.6347 2.5146
49O -6.1518 0.2215 -1.2870
50O 6.1521 -0.1615 1.2903
51O -5.8211 -2.4247 -1.3397
52O 5.7622 2.4739 1.3363
53O -8.0856 -1.4433 0.0031
54O 8.0504 1.5212 -0.0037
55O -5.8215 -2.4174 1.3520
56O 5.7625 2.4666 -1.3494
57O -4.2039 -4.3462 2.7997
58O 4.1335 4.3562 -2.7929
59O -2.1524 -2.9738 1.4627
60O 2.0796 2.9818 -1.4254
61O 1.5729 -4.4226 -2.4639
62O -1.4237 4.3778 2.3523
63O -2.9800 -0.2276 -5.3022
64O 2.9618 0.2132 5.2930
65O -4.7149 0.9978 -3.4103
66O 4.7383 -0.9583 3.4079
67O -1.3662 -0.5327 -3.0160
68O 1.3441 0.4773 3.0057
69O -2.1518 -2.9818 -1.4462
70O 2.0793 2.9901 1.4091
71O -0.3091 -4.2014 0.0118
72O 0.2137 4.6398 -0.0119
73O -4.2030 -4.3615 -2.7762
74O 4.1333 4.3719 2.7689
75O -3.8526 -1.5351 2.9726
76O 3.7886 1.5460 -2.9485
77P -2.8800 -0.0804 0.0001
78P 2.8964 0.0382 0.0003
79W -3.0346 0.0448 3.6021
80W 3.0161 -0.0765 -3.5959
81W -3.9426 -3.0469 -1.6949
82W 3.9058 3.0469 1.6987
83W -2.1178 2.8556 -1.8877
84W 2.1583 -2.9148 1.8817
85W -5.4259 1.8747 -1.8616
86W 5.4506 -1.8465 1.8671
87W -3.0335 0.0250 -3.6024
88W 3.0153 -0.0563 3.5963
89W -2.1187 2.8661 1.8724
90W 2.1588 -2.9254 -1.8656
91W -6.3806 -1.2349 0.0028
92W 6.3537 1.2629 -0.0032
93W -5.4266 1.8847 1.8507
94W 5.4511 -1.8569 -1.8566
95W -3.9431 -3.0375 1.7113
96W 3.9061 3.0372 -1.7153
Fe4-SK-O_-8_19
Energy (POTENTIAL) = -6999.93878351 Eh
Atom X Y Z
1 Fe -0.0015 -0.0302 1.8040
2 Fe -0.0202 -0.0146 -1.7786
3 Fe 0.8032 -2.6612 0.0018
4 Fe -0.8087 2.6577 0.0154
5 H 0.4235 4.9477 0.7820
6 H 0.3784 4.9638 -0.7789
7 O 1.3577 -0.4877 -3.0033
8 O -1.3570 0.4857 2.9999
9 O -0.5581 -1.9316 1.4066
10O 0.5939 1.8799 -1.3866
11O 5.5332 2.3298 0.0062
12O -5.5264 -2.3792 -0.0078
13O 2.2909 1.8964 -3.4716
14O -2.2901 -1.8830 3.4636
15O 2.9679 -0.2034 -5.2922
16O -2.9908 0.2142 5.2745
17O 3.2088 0.7904 -1.2814
18O -3.2302 -0.8075 1.2868
19O 1.3537 -0.5854 0.0114
20O -1.3319 0.4799 0.0048
21O 3.2228 0.7776 1.3022
22O -3.2301 -0.8090 -1.2930
23O 3.8869 -1.3340 -0.0027
24O -3.8297 1.3451 -0.0117
25O 2.3698 3.2261 0.0227
26O -2.3747 -3.2669 -0.0031
27O 2.3347 1.8687 3.5165
28O -2.2799 -1.8736 -3.4679
29O 3.8581 -1.5696 2.9593
30O -3.8390 1.5608 -2.9581
31O 4.1581 -3.9470 -0.0130
32O -4.2131 3.9477 -0.0108
33O 6.1732 0.1853 -1.2963
34O -6.1709 -0.2170 1.2712
35O 6.8171 2.6712 -2.5029
36O -6.8254 -2.6761 2.5015
37O 4.7342 0.9870 -3.4002
38O -4.7447 -0.9850 3.3995
39O 4.0663 3.1676 -2.0413
40O -4.0749 -3.1810 2.0626
41O 1.4949 4.3637 2.4134
42O -1.5530 -4.3935 -2.4888
43O 0.6270 1.8465 1.4553
44O -0.5622 -1.9204 -1.4012
45O 4.0869 3.1467 2.0739
46O -4.0693 -3.1798 -2.0757
47O 6.8383 2.6488 2.5118
48O -6.8200 -2.6803 -2.5175
49O 6.1874 0.1763 1.2779
50O -6.1773 -0.2174 -1.2883
51O 5.8261 -2.4627 1.3300
52O -5.8399 2.4196 -1.3528
53O 8.0965 -1.4989 -0.0213
54O -8.1053 1.4704 -0.0016
55O 5.8148 -2.4518 -1.3604
56O -5.8254 2.4138 1.3452
57O 4.1805 -4.3603 -2.8051
58O -4.2621 4.3684 2.7835
59O 2.1416 -2.9810 -1.4566
60O -2.1505 3.1065 1.4685
61O -1.5637 -4.4025 2.4819
62O 1.4825 4.3880 -2.3568
63O 3.0097 -0.2485 5.3071
64O -2.9729 0.2159 -5.2804
65O 4.7708 0.9496 3.4086
66O -4.7396 -0.9856 -3.4107
67O 1.3768 -0.5131 3.0317
68O -1.3671 0.5049 -2.9823
69O 2.1516 -2.9928 1.4515
70O -2.1651 3.1461 -1.5270
71O 0.2966 -4.1891 -0.0024
72O -0.1651 4.8082 0.0167
73O 4.2010 -4.3787 2.7769
74O -4.2934 4.3752 -2.8226
75O 3.8381 -1.5477 -2.9672
76O -3.8219 1.5586 2.9357
77P 2.8966 -0.0899 0.0079
78P -2.8865 0.0622 -0.0036
79W 3.0252 0.0446 -3.5887
80W -3.0431 -0.0437 3.5719
81W 3.9415 -3.0599 1.6956
82W -3.9345 3.0881 -1.7282
83W 2.1549 2.8456 1.8988
84W -2.1509 -2.9013 -1.8798
85W 5.4651 1.8384 1.8689
86W -5.4550 -1.8677 -1.8586
87W 3.0478 0.0199 3.6062
88W -3.0418 -0.0395 -3.5780
89W 2.1436 2.8660 -1.8570
90W -2.1542 -2.9067 1.8747
91W 6.3915 -1.2693 -0.0119
92W -6.3958 1.2624 -0.0111
93W 5.4511 1.8552 -1.8522
94W -5.4568 -1.8659 1.8466
95W 3.9305 -3.0506 -1.7107
96W -3.9362 3.0748 1.6896
Fe4-SK-OH2_-5_22
Energy (POTENTIAL) = -7000.64039006 Eh
Atom X Y Z
1 Fe 0.0004 0.0056 1.7982

2 Fe	0.0008	0.0055	-1.7987
3 Fe	2.6492	0.8850	-0.0005
4 Fe	-2.6134	-0.8253	0.0008
5 H	-4.9091	0.3056	0.7870
6 H	4.9346	-0.3048	-0.7876
7 H	4.9345	-0.3043	0.7884
8 H	-4.9076	0.3051	-0.7895
9 O	0.5001	1.3380	-2.9922
10O	-0.4739	-1.3532	3.0257
11O	1.9319	-0.5829	1.3842
12O	-1.9134	0.5239	-1.3858
13O	-2.3476	5.4752	0.0007
14O	2.2351	-5.5037	-0.0003
15O	-1.8880	2.2356	-3.4713
16O	1.9374	-2.2720	3.5003
17O	0.2093	2.9428	-5.2927
18O	-0.1258	-2.9005	5.3549
19O	-0.8171	3.1757	-1.2930
20O	0.8227	-3.1909	1.2984
21O	0.5273	1.3168	-0.0001
22O	-0.5170	-1.3362	-0.0002
23O	-0.8180	3.1756	1.2926
24O	0.8224	-3.1914	-1.2988
25O	1.3081	3.8318	0.0006
26O	-1.3075	-3.8376	0.0002
27O	-3.2261	2.3206	-0.0003
28O	3.2609	-2.3923	-0.0000
29O	-1.8882	2.2344	3.4708
30O	1.9372	-2.2715	-3.5003
31O	1.5547	3.7859	2.9485
32O	-1.5374	-3.7855	-3.0382
33O	3.9242	4.1066	0.0005
34O	-3.9481	-4.0153	-0.0003
35O	-0.1964	6.1241	-1.2879
36O	0.0956	-6.1010	1.3088
37O	-2.6744	6.7834	-2.5024
38O	2.6067	-6.8063	2.4929
39O	-0.9922	4.6953	-3.4040
40O	0.9634	-4.7138	3.4238
41O	-3.1863	4.0271	-2.0663
42O	3.1631	-4.0733	2.0701
43O	-4.4052	1.4490	2.3717
44O	4.4282	-1.4831	-2.3480
45O	-1.9140	0.5233	1.3856
46O	1.9313	-0.5829	-1.3842
47O	-3.1860	4.0270	2.0675
48O	3.1632	-4.0730	-2.0705
49O	-2.6736	6.7835	2.5035
50O	2.6072	-6.8062	-2.4933
51O	-0.1960	6.1246	1.2892
52O	0.0958	-6.1018	-1.3098
53O	2.4457	5.7641	1.3425
54O	-2.5567	-5.7016	-1.3226
55O	1.4760	8.0430	-0.0000
56O	-1.5440	-7.9960	-0.0003
57O	2.4458	5.7643	-1.3426
58O	-2.5570	-5.7016	1.3220
59O	4.3650	4.1601	-2.7760
60O	-4.3283	-4.1225	2.8676
61O	3.0022	2.0866	-1.4186
62O	-3.0218	-2.1113	1.4071
63O	4.4284	-1.4832	2.3478
64O	-4.4041	1.4481	-2.3732
65O	0.2072	2.9402	5.2934
66O	-0.1258	-2.9004	-5.3550
67O	-0.9918	4.6946	3.4047
68O	0.9634	-4.7135	-3.4240
69O	0.5010	1.3377	2.9913
70O	-0.4738	-1.3535	-3.0254
71O	3.0023	2.0868	1.4183
72O	-3.0222	-2.1113	-1.4069
73O	4.6862	0.2183	0.0002
74O	-4.6656	-0.2214	-0.0008
75O	4.3628	4.1598	2.7782
76O	-4.3286	-4.1223	-2.8676
77O	1.5557	3.7864	-2.9476
78O	-1.5372	-3.7856	3.0380
79P	0.0485	2.8696	0.0001
80P	-0.0394	-2.8839	-0.0001
81W	-0.0494	3.0090	-3.5998
82W	0.1253	-2.9706	3.6633
83W	3.0442	3.9226	1.7100
84W	-2.9739	-3.9000	-1.8436
85W	-2.8962	2.1293	1.8851
86W	2.9086	-2.1378	-1.8664
87W	-1.8684	5.4192	1.8574
88W	1.8319	-5.4144	-1.8736
89W	-0.0522	3.0070	3.6006
90W	0.1254	-2.9709	-3.6635
91W	-2.8950	2.1284	-1.8870
92W	2.9086	-2.1375	1.8661
93W	1.2388	6.3480	-0.0001
94W	-1.2601	-6.3096	-0.0006
95W	-1.8693	5.4186	-1.8570
96W	1.8317	-5.4141	1.8737
97W	3.0469	3.9233	-1.7072
98W	-2.9737	-3.9006	1.8434

Fe4-SK-OH2_-6_21

Energy (POTENTIAL) = -7000.88531594 Eh

Atom	X	Y	Z
1 Fe	-0.0000	-0.0000	1.8049
2 Fe	0.0000	0.0000	-1.8049
3 Fe	2.6178	0.8713	-0.0000
4 Fe	-2.6178	-0.8713	0.0000
5 H	-4.8835	0.3267	0.7878
6 H	4.8835	-0.3267	-0.7878
7 H	4.8834	-0.3267	0.7878
8 H	-4.8834	0.3267	-0.7878
9 O	0.4928	1.3511	-3.0090
10O	-0.4928	-1.3511	3.0090
11O	1.9071	-0.5567	1.3833
12O	-1.9071	0.5567	-1.3833
13O	-2.3434	5.4965	0.0000
14O	2.3434	-5.4965	-0.0000
15O	-1.8938	2.2616	-3.4773
16O	1.8938	-2.2616	3.4773
17O	0.2072	2.9622	-5.2989
18O	-0.2072	-2.9622	5.2989
19O	-0.8177	3.1972	-1.2938
20O	0.8177	-3.1973	1.2938
21O	0.5223	1.3375	-0.0000
22O	-0.5223	-1.3375	0.0000
23O	-0.8176	3.1975	1.2934
24O	0.8176	-3.1974	-1.2935
25O	1.3083	3.8489	-0.0003
26O	-1.3083	-3.8489	0.0002
27O	-3.2347	2.3540	0.0000
28O	3.2347	-2.3540	-0.0000
29O	-1.8938	2.2616	3.4773
30O	1.8938	-2.2616	-3.4773
31O	1.5563	3.7988	2.9507
32O	-1.5563	-3.7988	-2.9507
33O	3.9265	4.1150	0.0000
34O	-3.9265	-4.1150	-0.0000
35O	-0.1926	6.1388	-1.2890
36O	0.1926	-6.1388	1.2890
37O	-2.6736	6.7976	-2.5048
38O	2.6736	-6.7976	2.5048
39O	-0.9850	4.7164	-3.4057
40O	0.9850	-4.7164	3.4057
41O	-3.1820	4.0459	-2.0685
42O	3.1820	-4.0459	2.0685
43O	-4.4008	1.4553	2.3643
44O	4.4008	-1.4553	-2.3643
45O	-1.9071	0.5567	1.3833
46O	1.9071	-0.5567	-1.3833
47O	-3.1820	4.0459	2.0685
48O	3.1820	-4.0459	-2.0685
49O	-2.6736	6.7976	2.5049
50O	2.6736	-6.7976	-2.5049
51O	-0.1926	6.1388	1.2891
52O	0.1926	-6.1388	-1.2891
53O	2.4488	5.7731	1.3429
54O	-2.4488	-5.7731	-1.3429
55O	1.4811	8.0520	0.0000
56O	-1.4811	-8.0520	-0.0000
57O	2.4488	5.7731	-1.3429
58O	-2.4488	-5.7731	1.3429
59O	4.3638	4.1613	-2.7775
60O	-4.3638	-4.1613	2.7775
61O	2.9981	2.0956	-1.4161
62O	-2.9981	-2.0956	1.4161
63O	4.4008	-1.4553	2.3643
64O	-4.4008	1.4553	-2.3642
65O	0.2072	2.9622	5.2989
66O	-0.2072	-2.9622	-5.2989
67O	-0.9850	4.7164	3.4057
68O	0.9850	-4.7164	-3.4057
69O	0.4928	1.3510	3.0090
70O	-0.4928	-1.3510	-3.0090
71O	2.9981	2.0956	1.4161
72O	-2.9981	-2.0956	-1.4161
73O	4.6658	0.2120	0.0000
74O	-4.6658	-0.2120	0.0000
75O	4.3638	4.1612	2.7776
76O	-4.3638	-4.1612	-2.7775
77O	1.5563	3.7988	-2.9507
78O	-1.5563	-3.7988	2.9507
79P	0.0472	2.8860	-0.0002
80P	-0.0472	-2.8860	0.0001
81W	-0.0521	3.0179	-3.6031
82W	0.0521	-3.0179	3.6031
83W	3.0434	3.9248	1.7071
84W	-3.0434	-3.9248	-1.7071
85W	-2.8859	2.1319	1.8792
86W	2.8859	-2.1319	-1.8792
87W	-1.8695	5.4287	1.8599
88W	1.8695	-5.4287	-1.8599
89W	-0.0521	3.0179	3.6031
90W	0.0521	-3.0179	-3.6031
91W	-2.8859	2.1319	-1.8791
92W	2.8859	-2.1319	1.8791
93W	1.2398	6.3549	0.0000
94W	-1.2398	-6.3549	-0.0000
95W	-1.8695	5.4287	-1.8598
96W	1.8695	-5.4287	1.8598
97W	3.0434	3.9249	-1.7071
98W	-3.0434	-3.9249	1.7071

Fe4-SK-OH2_-7_20

Energy (POTENTIAL) = -7001.07571755 Eh

Atom	X	Y	Z
1 Fe	-0.0290	-0.0109	1.8040
2 Fe	-0.0384	-0.0290	-1.7801
3 Fe	2.5909	0.8532	0.0047
4 Fe	-2.6998	-0.8174	0.0152
5 H	-4.9917	0.4270	0.7698
6 H	4.8467	-0.3484	-0.7860
7 H	4.8484	-0.3493	0.7900

8 H	-5.0044	0.3701	-0.7901
9 O	0.4561	1.3401	-2.9962
10O	-0.5164	-1.3658	3.0029
11O	1.8897	-0.5440	1.3913
12O	-1.9261	0.5991	-1.3920
13O	-2.2918	5.5520	0.0025
14O	2.4065	-5.4847	-0.0023
15O	-1.9113	2.3054	-3.4739
16O	1.8711	-2.2542	3.4731
17O	0.2033	2.9484	-5.2899
18O	-0.2303	-2.9934	5.2806
19O	-0.8104	3.2219	-1.2851
20O	0.8012	-3.2109	1.2911
21O	0.5117	1.3517	0.0111
22O	-0.5122	-1.3299	0.0049
23O	-0.7997	3.2365	1.3019
24O	0.8062	-3.2115	-1.2925
25O	1.3300	3.8525	-0.0035
26O	-1.3375	-3.8403	-0.0120
27O	-3.2430	2.4028	0.0184
28O	3.2156	-2.3355	0.0028
29O	-1.8906	2.3516	3.5135
30O	1.8723	-2.2459	-3.4696
31O	1.5832	3.7993	2.9420
32O	-1.5556	-3.8553	-2.9655
33O	3.9526	4.0879	-0.0116
34O	-3.9415	-4.2523	-0.0149
35O	-0.1416	6.1584	-1.3018
36O	0.2496	-6.1612	1.2730
37O	-2.6259	6.8342	-2.5087
38O	2.7118	-6.7892	2.5050
39O	-0.9558	4.7356	-3.4014
40O	1.0011	-4.7222	3.4026
41O	-3.1621	4.0965	-2.0522
42O	3.1894	-4.0268	2.0699
43O	-4.3995	1.5437	2.4089
44O	4.3807	-1.4306	-2.3615
45O	-1.8975	0.6342	1.4567
46O	1.8826	-0.5487	-1.3792
47O	-3.1444	4.1202	2.0762
48O	3.1940	-4.0223	-2.0705
49O	-2.6045	6.8589	2.5093
50O	2.7233	-6.7852	-2.5083
51O	-0.1338	6.1742	1.2779
52O	0.2539	-6.1679	-1.2849
53O	2.4985	5.7687	1.3268
54O	-2.3893	-5.8570	-1.3554
55O	1.5552	8.0558	-0.0248
56O	-1.4226	-8.1117	-0.0018
57O	2.4910	5.7568	-1.3589
58O	-2.3882	-5.8431	1.3445
59O	4.3793	4.1193	-2.7934
60O	-4.3700	-4.2974	2.7762
61O	3.0001	2.0747	-1.4185
62O	-3.1195	-2.1788	1.4609
63O	4.3826	-1.4396	2.3705
64O	-4.4169	1.5251	-2.3625
65O	0.2387	2.9907	5.3024
66O	-0.2157	-2.9783	-5.2849
67O	-0.9234	4.7738	3.4044
68O	1.0114	-4.7191	-3.4075
69O	0.4748	1.3595	3.0237
70O	-0.5260	-1.3774	-2.9858
71O	3.0084	2.0860	1.4142
72O	-3.1523	-2.1926	-1.5232
73O	4.6536	0.1999	0.0027
74O	-4.8273	-0.1604	0.0092
75O	4.3906	4.1426	2.7689
76O	-4.3678	-4.3261	-2.8239
77O	1.5674	3.7789	-2.9510
78O	-1.5625	-3.8382	2.9419
79P	0.0564	2.9029	0.0068
80P	-0.0712	-2.8793	-0.0024
81W	-0.0562	3.0096	-3.5914
82W	0.0236	-3.0479	3.5799
83W	3.0641	3.9123	1.7000
84W	-3.0854	-3.9612	-1.7295
85W	-2.8748	2.1791	1.8946
86W	2.8677	-2.1251	-1.8799
87W	-1.8190	5.4730	1.8693
88W	1.8926	-5.4331	-1.8519
89W	-0.0393	3.0321	3.6062
90W	0.0306	-3.0481	-3.5837
91W	-2.8896	2.1633	-1.8607
92W	2.8677	-2.1272	1.8858
93W	1.2878	6.3599	-0.0152
94W	-1.2338	-6.4021	-0.0106
95W	-1.8353	5.4562	-1.8586
96W	1.8856	-5.4338	1.8493
97W	3.0600	3.8987	-1.7137
98W	-3.0785	-3.9635	1.6859

Fe4-SK-O-H2O_addTS2-7_20

Energy (POTENTIAL) = -7152.63919292 Eh

	Atom	X	Y	Z
1	Fe	-0.0017	0.4284	-1.7271
2	Fe	0.0027	-0.4657	1.7801
3	Fe	0.8232	2.5099	0.7002
4	Fe	-0.8816	-2.5497	-0.6183
5	H	0.2841	-4.5560	-1.9561
6	H	0.2887	-4.9496	-0.4297
7	O	1.3577	-0.3209	3.0741
8	O	-1.3563	0.2288	-3.0188
9	O	-0.5772	2.1606	-0.8653
10	O	0.5349	-2.2155	0.8873
11	O	5.4538	-2.3878	-0.5725
12	O	-5.5184	2.2229	0.5933
13	O	2.2220	-2.7686	2.9154
14	O	-2.2880	2.6468	-2.8802
15	O	2.9586	-1.2176	5.2101
16	O	-2.9720	1.0667	-5.1645
17	O	3.1696	-1.1808	1.0734
18	O	-3.2156	1.0786	-1.0304
19	O	1.3324	0.4955	0.1710
20	O	-1.3540	-0.5310	-0.1055
21	O	3.1707	-0.5291	-1.4290
22	O	-3.2169	0.4429	1.4752
23	O	3.8766	1.1812	0.3563
24	O	-3.8637	-1.3033	-0.3013
25	O	2.3033	-3.1907	-0.7883
26	O	-2.3780	3.1327	0.8208
27	O	2.2328	-1.0198	-3.8161
28	O	-2.2824	0.9440	3.8495
29	O	3.8450	2.1535	-2.4546
30	O	-3.8118	-2.2641	2.4960
31	O	4.1769	3.7062	1.0181
32	O	-4.1206	-3.8422	-0.9440
33	O	6.1416	-0.6396	1.2111
34	O	-6.1610	0.4581	-1.1837
35	O	6.7571	-3.3507	1.7611
36	O	-6.8166	3.1643	-1.7519
37	O	4.6959	-1.9264	3.0695
38	O	-4.7387	1.7464	-3.0415
39	O	3.9920	-3.6862	1.2190
40	O	-4.0704	3.5501	-1.2037
41	O	1.3894	-3.7120	-3.3665
42	O	-1.5525	3.6260	3.4968
43	O	0.5337	-1.5285	-1.7830
44	O	-0.5648	1.4752	1.8461
45	O	3.9967	-2.6493	-2.7764
46	O	-4.0733	2.5369	2.8076
47	O	6.7609	-2.0931	-3.0783
48	O	-6.8177	1.9305	3.1043
49	O	6.1389	0.0091	-1.2806
50	O	-6.1577	-0.1774	1.3177
51	O	5.8172	2.5871	-0.6695
52	O	-5.7850	-2.7468	0.7181
53	O	8.0798	1.2911	0.3772
54	O	-8.0673	-1.4844	-0.3437
55	O	5.8240	1.9068	1.9338
56	O	-5.7867	-2.0865	-1.8840
57	O	4.2197	3.4167	3.8252
58	O	-4.1679	-3.5815	-3.7449
59	O	2.1604	2.4279	2.1922
60	O	-2.1068	-2.5832	-2.0903
61	O	-1.5337	4.8344	-1.2985
62	O	1.3838	-4.8981	1.2050
63	O	2.9821	1.4609	-5.0541
64	O	-2.9676	-1.5335	5.1029
65	O	4.7024	-0.2087	-3.5285
66	O	-4.7348	0.0769	3.5644
67	O	1.3578	1.1892	-2.7731
68	O	-1.3578	-1.2512	2.8141
69	O	2.1487	3.1558	-0.6186
70	O	-2.1062	-3.2823	0.6600
71	O	0.3140	3.9865	1.0969
72	O	-0.2554	-4.5493	-1.1389
73	O	4.2069	4.8222	-1.5704
74	O	-4.1671	-4.9442	1.6467
75	O	3.8522	0.6524	3.2904
76	O	-3.8105	-0.8178	-3.2178
77	P	2.8714	-0.0066	0.0429
78	P	-2.9026	-0.0776	0.0105
79	W	3.0163	-1.0283	3.5026
80	W	-3.0235	0.9034	-3.4545
81	W	3.9444	3.2823	-0.8489
82	W	-3.9320	-3.4006	0.9300
83	W	2.0941	-2.3755	-2.5207
84	W	-2.1488	2.3248	2.5526
85	W	5.4056	-1.4488	-2.2464
86	W	-5.4446	1.3115	2.2828
87	W	3.0282	0.7907	-3.4719
88	W	-3.0218	-0.8606	3.5226
89	W	2.0923	-3.3203	1.1189
90	W	-2.1445	3.2358	-1.0814
91	W	6.3746	1.0943	0.3305
92	W	-6.3694	-1.2435	-0.2851
93	W	5.4039	-2.3800	1.3488
94	W	-5.4442	2.2265	-1.3276
95	W	3.9511	2.4202	2.4471
96	W	-3.9333	-2.5644	-2.3802
97	O	1.5789	6.5309	0.7564
98	H	1.3469	6.5743	-0.1955
99	H	1.2915	5.6352	0.9991
100O		0.7414	6.3812	-1.9258
101H		0.4084	7.2204	-2.2705
102H		-0.0575	5.8446	-1.7573

Fe4-SK-OH_-5_21

Energy (POTENTIAL) = -6999.93848952 Eh

	Atom	X	Y	Z
1	Fe	0.1014	0.6397	-1.7406
2	Fe	-0.0998	-0.6399	1.6640
3	Fe	-0.9055	-2.4796	-0.9159
4	Fe	0.8444	2.4285	0.8984
5	H	-0.2689	4.8692	0.8724
6	H	-0.6809	-4.2441	-2.3607
7	H	-0.3175	4.3520	2.3619
8	O	-1.4457	-1.4663	2.6584
9	O	1.4674	1.5236	-2.6902

10O	0.6669	-1.2642	-2.0234
11O	-0.5827	1.3111	1.9073
12O	-5.4873	2.2073	0.6837
13O	5.5800	-2.1963	-0.6779
14O	-2.3102	0.6713	3.8777
15O	2.4818	-0.5566	-3.9130
16O	-3.0512	-1.8699	4.9479
17O	3.1711	2.0432	-4.8602
18O	-3.2137	0.3593	1.4537
19O	3.2769	-0.3173	-1.4713
20O	-1.3420	-0.5508	-0.1837
21O	1.3566	0.4831	0.1522
22O	-3.1454	1.1820	-0.9979
23O	3.1700	-1.2469	0.9318
24O	-3.8847	-1.2255	-0.4397
25O	3.8604	1.2205	0.4929
26O	-2.3348	3.0519	1.0157
27O	2.3997	-3.0718	-1.1282
28O	-2.2044	2.9128	-2.7043
29O	2.1982	-3.0021	2.5442
30O	-3.6724	-0.5489	-3.2735
31O	3.7145	0.3971	3.3239
32O	-4.0776	-3.6958	-1.2843
33O	4.1261	3.6457	1.4182
34O	-6.1999	-0.2151	1.2524
35O	6.2389	0.2518	-1.1215
36O	-6.8235	1.8135	3.1586
37O	6.9223	-1.6537	-3.1506
38O	-4.7777	-0.1098	3.5072
39O	4.9064	0.2795	-3.4282
40O	-4.0631	2.3775	2.9387
41O	4.1925	-2.2721	-2.9496
42O	-1.4203	4.9236	-0.8337
43O	1.4405	-5.0071	0.7275
44O	-0.5138	2.2464	-0.6951
45O	0.4604	-2.3197	0.5481
46O	-4.0100	3.6684	-0.9772
47O	4.0069	-3.8201	0.8635
48O	-6.7443	3.3336	-1.6128
49O	6.7144	-3.5408	1.5318
50O	-6.1047	0.5893	-1.2189
51O	6.1345	-0.6737	1.1871
52O	-5.7903	-1.8678	-2.1442
53O	5.7539	1.7242	2.1911
54O	-8.0807	-1.3482	-0.5292
55O	8.0873	1.4677	0.6487
56O	-5.8184	-2.7438	0.3829
57O	5.8408	2.8312	-0.3145
58O	-4.2053	-5.0149	1.2379
59O	4.1476	5.0792	-1.0189
60O	-2.1685	-3.2562	0.4602
61O	2.1073	3.3057	-0.2787
62O	1.6242	-3.2264	-3.8480
63O	-1.4596	3.3831	3.6384
64O	-2.8753	1.4773	-5.1106
65O	2.8457	-1.6974	5.0058
66O	-4.6453	2.0018	-2.9609
67O	4.6807	-2.1113	2.8613
68O	-1.2397	0.5369	-3.0374
69O	1.2688	-0.6163	2.9483
70O	-2.0215	-2.3180	-2.2122
71O	2.0600	2.3036	2.3691
72O	-0.2912	-4.0342	-1.4939
73O	0.2293	4.3712	1.5499
74O	-4.1539	-3.2168	-4.0208
75O	4.1029	3.0710	4.1613
76O	-3.9382	-2.3980	2.3135
77O	3.9065	2.4832	-2.1541
78P	-2.8888	-0.0552	-0.0430
79P	2.9114	0.0333	0.0309
80W	-3.1005	-1.0948	3.4215
81W	3.1530	1.2057	-3.3665
82W	-4.0186	-2.3190	-2.5703
83W	3.8765	2.2242	2.6898
84W	-2.0953	3.3380	-0.8711
85W	2.0466	-3.4111	0.7120
86W	-5.3851	2.3651	-1.2394
87W	5.3504	-2.5827	1.1540
88W	-2.9224	1.2006	-3.4204
89W	2.9253	-1.3214	3.3360
90W	-2.1564	2.1231	2.6873
91W	2.2112	-2.0458	-2.7552
92W	-6.3890	-1.1330	-0.4005
93W	6.3975	1.2633	0.4786
94W	-5.4575	1.2248	2.3163
95W	5.5260	-1.1138	-2.3255
96W	-3.9527	-3.4146	0.6723
97W	3.9153	3.4645	-0.4983

Fe4-SK-OH_-6_20

Energy (POTENTIAL) = -7000.19016215 Eh

Atom	X	Y	Z
1 Fe	-0.0930	-0.5244	-1.6849
2 Fe	0.0954	0.5179	1.7970
3 Fe	-0.8510	-2.5372	0.7125
4 Fe	0.8658	2.4958	-0.7097
5 H	-0.3361	4.4870	-2.0431
6 H	0.1165	-4.6107	0.3741
7 H	-0.2905	4.9101	-0.5255
8 O	-1.2603	0.3408	3.0842
9 O	1.2611	-0.3969	-2.9528
10O	0.4588	-2.2643	-0.6670
11O	-0.5311	2.2018	0.8548
12O	-5.5017	2.2488	-0.5367
13O	5.5033	-2.2581	0.5878
14O	-2.2329	2.7243	2.9009
15O	2.1292	-2.8145	-2.7077
16O	-2.9131	1.1254	5.2035
17O	2.7820	-1.3743	-5.1099
18O	-3.1564	1.1057	1.0751
19O	3.1601	-1.1793	-0.9947
20O	-1.3438	-0.5590	0.1423
21O	1.3374	0.4932	-0.1044
22O	-3.2166	0.4583	-1.4299
23O	3.2476	-0.4032	1.4695
24O	-3.8816	-1.2600	0.3411
25O	3.8449	1.2359	-0.4193
26O	-2.3531	3.1237	-0.7980
27O	2.3652	-3.1088	0.9696
28O	-2.3102	0.9453	-3.8266
29O	2.4059	-0.7795	3.9073
30O	-3.9379	-2.2337	-2.4993
31O	3.8898	2.3441	2.3311
32O	-4.0742	-3.7908	0.9947
33O	4.0940	3.7405	-1.1889
34O	-6.1111	0.4989	1.2513
35O	6.1154	-0.5808	-1.3042
36O	-6.7671	3.2070	1.8273
37O	6.7577	-3.2988	-1.7344
38O	-4.6697	1.7895	3.0867
39O	4.5990	-1.9774	-3.0184
40O	-4.0303	3.5913	1.2263
41O	4.0128	-3.6833	-1.0844
42O	-1.4651	3.6324	-3.3838
43O	1.5903	-3.4567	3.6890
44O	-0.5973	1.4476	-1.8021
45O	0.6290	-1.3929	1.9607
46O	-4.0702	2.5678	-2.7632
47O	4.1297	-2.4436	2.8627
48O	-6.8314	2.0031	-3.0316
49O	6.8822	-1.8526	3.0475
50O	-6.1883	-0.1386	-1.2631
51O	6.1752	0.1631	1.1641
52O	-5.8160	-2.7165	-0.5961
53O	5.8057	2.7239	0.4729
54O	-8.0654	-1.4069	0.4497
55O	8.0470	1.4015	-0.5861
56O	-5.7560	-2.0242	1.9901
57O	5.7215	1.9265	-2.0903
58O	-4.0942	-3.5145	3.7586
59O	4.0578	3.3422	-3.9731
60O	-2.0221	-2.4658	2.0197
61O	2.0424	2.4428	-2.2105
62O	1.4528	-4.9274	-0.9513
63O	-1.4383	4.8588	1.1804
64O	-3.0340	-1.5199	-5.0783
65O	3.1454	1.7537	5.0007
66O	-4.7747	0.1286	-3.5177
67O	4.8458	0.0522	3.4794
68O	-1.4420	-1.2749	-2.7607
69O	1.4453	1.3604	2.7882
70O	-2.1679	-3.2173	-0.7249
71O	2.1236	3.2677	0.5047
72O	-0.3675	-4.1914	1.1192
73O	0.2204	4.4764	-1.2369
74O	-4.2016	-4.9219	-1.6170
75O	4.2163	4.9761	1.3361
76O	-3.6858	-0.7782	3.2347
77O	3.7077	0.6042	-3.3014
78P	-2.8894	-0.0602	0.0349
79P	2.8894	0.0366	-0.0103
80W	-2.9488	0.9557	3.4964
81W	2.9070	-1.1113	-3.4186
82W	-3.9459	-3.3668	-0.9302
83W	3.9574	3.4002	0.7096
84W	-2.1571	2.3016	-2.5242
85W	2.1823	-2.2044	2.6781
86W	-5.4599	1.3642	-2.2298
87W	5.4844	-1.2641	2.2503
88W	-3.0887	-0.8550	-3.4980
89W	3.1371	1.0017	3.4584
90W	-2.1053	3.2680	1.1035
91W	2.1522	-3.3500	-0.9039
92W	-6.3716	-1.1796	0.3328
93W	6.3530	1.1757	-0.4633
94W	-5.3999	2.2728	1.3891
95W	5.4103	-2.3301	-1.3115
96W	-3.9553	-2.5080	2.3784
97W	3.8629	2.3983	-2.5537

Fe4-SK-OH_-7_21

Energy (POTENTIAL) = -7000.42562932 Eh

Atom	X	Y	Z
1 Fe	0.0315	0.0591	-1.7805
2 Fe	0.0136	0.0860	1.7855
3 Fe	0.8016	2.8168	-0.0144
4 Fe	-0.8506	-2.5742	0.0151
5 H	0.3386	-4.8517	-0.7480
6 H	-0.2136	4.8416	-0.8877
7 H	0.3300	-4.8378	0.8284
8 O	1.3607	0.5534	3.0046
9 O	-1.3322	-0.4590	-2.9834
10O	-0.5816	1.9589	-1.3993
11O	0.5514	-1.8545	1.3986
12O	5.4800	-2.3843	0.0313
13O	-5.5479	2.3021	-0.0163
14O	2.2428	-1.8388	3.5005
15O	-2.2977	1.9023	-3.4766
16O	2.9725	0.2737	5.2946
17O	-2.9305	-0.2147	-5.2875

18O	3.1903	-0.7916	1.3043
19O	-3.2170	0.8202	-1.2942
20O	1.3318	0.5506	-0.0054
21O	-1.3402	-0.4879	0.0053
22O	3.1978	-0.8204	-1.2821
23O	-3.2230	0.8245	1.2887
24O	3.8671	1.3090	-0.0113
25O	-3.8395	-1.3175	-0.0019
26O	2.3326	-3.2193	0.0366
27O	-2.4118	3.2783	-0.0040
28O	2.2548	-1.9162	-3.4578
29O	-2.3208	1.9142	3.4748
30O	3.8649	1.5026	-2.9859
31O	-3.7866	-1.5577	2.9431
32O	4.1847	3.9186	-0.0462
33O	-4.0740	-3.9413	0.0045
34O	6.1491	-0.2209	1.2931
35O	-6.1536	0.1413	-1.3045
36O	6.7763	-2.6847	2.5409
37O	-6.8397	2.6112	-2.5288
38O	4.7107	-0.9676	3.4217
39O	-4.7309	0.9474	-3.4121
40O	4.0167	-3.1645	2.1067
41O	-4.1035	3.1631	-2.0795
42O	1.4251	-4.3994	-2.3136
43O	-1.6172	4.4317	2.4883
44O	0.5593	-1.8787	-1.3649
45O	-0.5793	1.9839	1.4063
46O	4.0245	-3.2117	-2.0293
47O	-4.1168	3.1709	2.0553
48O	6.7875	-2.7433	-2.4649
49O	-6.8507	2.6223	2.4905
50O	6.1583	-0.2509	-1.2767
51O	-6.1565	0.1478	1.2758
52O	5.8286	2.3926	-1.3659
53O	-5.7563	-2.4845	1.3393
54O	8.0874	1.4316	-0.0033
55O	-8.0455	-1.5488	-0.0113
56O	5.8188	2.4244	1.3256
57O	-5.7472	-2.4895	-1.3461
58O	4.2257	4.3848	2.7323
59O	-4.1076	-4.3786	-2.7768
60O	2.1461	3.0353	1.4162
61O	-2.0642	-2.9917	-1.4071
62O	-1.5609	4.4225	-2.4281
63O	1.4161	-4.3481	2.4101
64O	2.9847	0.1482	-5.3010
65O	-2.9609	-0.1967	5.2849
66O	4.7246	-1.0515	-3.3949
67O	-4.7516	0.9589	3.3937
68O	1.3807	0.4939	-3.0099
69O	-1.3465	-0.4415	2.9912
70O	2.1615	2.9686	-1.4964
71O	-2.0734	-2.9860	1.4282
72O	0.2784	4.5748	-0.0927
73O	-0.2105	-4.6423	0.0357
74O	4.2233	4.3135	-2.8394
75O	-4.1267	-4.3694	2.7870
76O	3.8357	1.5802	2.9429
77O	-3.7700	-1.5679	-2.9438
78P	2.8726	0.0682	0.0006
79P	-2.8954	-0.0399	0.0004
80W	3.0287	0.0011	3.5981
81W	-2.9992	0.0553	-3.5912
82W	3.9500	3.0137	-1.7430
83W	-3.9002	-3.0493	1.7103
84W	2.1212	-2.8836	-1.8459
85W	-2.1745	2.9288	1.8781
86W	5.4287	-1.9090	-1.8300
87W	-5.4629	1.8412	1.8507
88W	3.0428	-0.0847	-3.5985
89W	-3.0192	0.0682	3.5871
90W	2.1108	-2.8417	1.9125
91W	-2.1757	2.9098	-1.8731
92W	6.3823	1.2238	-0.0072
93W	-6.3500	-1.2815	-0.0073
94W	5.4190	-1.8678	1.8808
95W	-5.4585	1.8297	-1.8756
96W	3.9475	3.0629	1.6662
97W	-3.8886	-3.0539	-1.7041

Fe4-SK-OH_-8_20

Energy (POTENTIAL) = -7000.60902594 Eh

Atom	X	Y	Z
1 Fe	-0.0010	0.0261	-1.7536
2 Fe	-0.0082	-0.1155	1.7837
3 Fe	-0.8018	-2.7935	-0.0971
4 Fe	0.8158	2.6471	0.1101
5 H	-0.3519	4.9943	-0.5899
6 H	0.2257	-4.7852	-1.0148
7 H	-0.3949	4.9174	0.9689
8 O	-1.3767	-0.6247	3.0045
9 O	1.3610	0.5674	-2.9465
10O	0.5634	-1.9016	-1.4550
11O	-0.6172	1.7948	1.5291
12O	-5.5219	2.3666	0.0956
13O	5.5301	-2.3869	-0.0801
14O	-2.3267	1.7387	3.5877
15O	2.2806	-1.7910	-3.5212
16O	-3.0155	-0.4500	5.2820
17O	2.9560	0.3656	-5.2606
18O	-3.2248	0.7524	1.3295
19O	3.2270	-0.7872	-1.3118
20O	-1.3489	-0.5361	-0.0139
21O	1.3290	0.4626	0.0252
22O	-3.2143	0.8717	-1.2537
23O	3.2284	-0.8619	1.2664
24O	-3.8804	-1.3049	-0.0640
25O	3.8275	1.3282	0.0325
26O	-2.3543	3.2384	0.1498
27O	2.3743	-3.2741	-0.0959
28O	-2.2801	2.0536	-3.3990
29O	2.2964	-2.0073	3.4153
30O	-3.8509	-1.3977	-3.0402
31O	3.8237	1.4561	2.9901
32O	-4.1860	-3.9125	-0.1870
33O	4.2132	3.9325	0.1170
34O	-6.1849	0.1644	1.2766
35O	6.1807	-0.1885	-1.2964
36O	-6.8217	2.5846	2.6139
37O	6.8207	-2.6130	-2.5998
38O	-4.7681	0.8325	3.4385
39O	4.7340	-0.8940	-3.4342
40O	-4.0704	3.0863	2.2004
41O	4.0703	-3.1306	-2.1664
42O	-1.4557	4.4916	-2.1779
43O	1.5752	-4.4957	2.3674
44O	-0.5846	1.9385	-1.3199
45O	0.5519	-2.0150	1.3551
46O	-4.0474	3.2771	-1.9192
47O	4.0781	-3.2560	1.9643
48O	-6.7998	2.8190	-2.3970
49O	6.8244	-2.7634	2.4229
50O	-6.1762	0.2818	-1.2944
51O	6.1700	-0.2680	1.2644
52O	-5.8287	-2.3512	-1.4654
53O	5.8261	2.3580	1.4224
54O	-8.1037	-1.4447	-0.0880
55O	8.1061	1.4561	0.0479
56O	-5.8365	-2.4740	1.2216
57O	5.8383	2.4461	-1.2726
58O	-4.2472	-4.4645	2.5783
59O	4.2948	4.4450	-2.6820
60O	-2.1609	-3.0764	1.3145
61O	2.1655	3.1834	-1.4214
62O	1.5227	-4.3397	-2.5573
63O	-1.4706	4.2737	2.5838
64O	-2.9623	0.0378	-5.2999
65O	2.9792	0.0431	5.2788
66O	-4.7319	1.1572	-3.3664
67O	4.7443	-1.0996	3.3694
68O	-1.3694	-0.3587	-3.0108
69O	1.3557	0.3682	3.0015
70O	-2.1598	-2.9115	-1.5934
71O	2.1547	3.0412	1.5742
72O	-0.2961	-4.5599	-0.2258
73O	0.1923	4.8051	0.1982
74O	-4.2120	-4.2110	-2.9938
75O	4.2662	4.2689	2.9229
76O	-3.8532	-1.6702	2.8734
77O	3.8326	1.6353	-2.9008
78P	-2.8884	-0.0606	-0.0009
79P	2.8839	0.0468	0.0040
80W	-3.0484	-0.1059	3.5948
81W	3.0323	0.0565	-3.5673
82W	-3.9457	-2.9474	-1.8499
83W	3.9408	3.0084	1.7910
84W	-2.1259	2.9534	-1.7420
85W	2.1490	-2.9787	1.7992
86W	-5.4396	1.9675	-1.7799
87W	5.4538	-1.9359	1.7936
88W	-3.0277	0.2188	-3.5884
89W	3.0378	-0.1644	3.5691
90W	-2.1371	2.7801	2.0089
91W	2.1578	-2.8480	-1.9575
92W	-6.3975	-1.2239	-0.0722
93W	6.3968	1.2467	0.0319
94W	-5.4522	1.7958	1.9364
95W	5.4574	-1.8210	-1.9131
96W	-3.9627	-3.1060	1.5558
97W	3.9344	3.1266	-1.6259

Fe4-SK-OHiOH_-8_21

Energy (POTENTIAL) = -6999.95930590 Eh

Atom	X	Y	Z
1 Fe	0.0171	0.0261	1.7590
2 Fe	-0.0172	-0.0261	-1.7592
3 Fe	0.7819	-2.7816	0.0296
4 Fe	-0.7817	2.7815	-0.0292
5 H	-0.2309	-4.7941	0.9179
6 H	0.2313	4.7942	-0.9170
7 O	1.3415	-0.5184	-2.9797
8 O	-1.3416	0.5182	2.9796
9 O	-0.5757	-1.9085	1.4148
10O	0.5757	1.9084	-1.4151
11O	5.5345	2.3421	-0.0472
12O	-5.5346	-2.3421	0.0471
13O	2.2810	1.8474	-3.4996
14O	-2.2809	-1.8477	3.4993
15O	2.9420	-0.2822	-5.2828
16O	-2.9419	0.2816	5.2827
17O	3.2107	0.7936	-1.3046
18O	-3.2107	-0.7936	1.3044
19O	1.3332	-0.5155	0.0100
20O	-1.3331	0.5155	-0.0101
21O	3.2232	0.8264	1.2771
22O	-3.2231	-0.8261	-1.2774
23O	3.8566	-1.3195	0.0102
24O	-3.8565	1.3197	-0.0104
25O	2.3930	3.2631	-0.0412

26O	-2.3931	-3.2631	0.0408
27O	2.3140	1.9364	3.4546
28O	-2.3142	-1.9362	-3.4548
29O	3.8528	-1.5053	2.9789
30O	-3.8528	1.5056	-2.9787
31O	4.1446	-3.9332	0.0516
32O	-4.1444	3.9332	-0.0511
33O	6.1654	0.1685	-1.3079
34O	-6.1654	-0.1686	1.3079
35O	6.8209	2.6215	-2.5648
36O	-6.8209	-2.6217	2.5646
37O	4.7270	0.9290	-3.4277
38O	-4.7269	-0.9293	3.4277
39O	4.0768	3.1449	-2.1172
40O	-4.0768	-3.1450	2.1169
41O	1.5861	4.4323	2.4403
42O	-1.5865	-4.4322	-2.4408
43O	0.5804	1.9562	1.3870
44O	-0.5806	-1.9562	-1.3873
45O	4.0957	3.2002	2.0158
46O	-4.0959	-3.2000	-2.0162
47O	6.8406	2.6931	2.4520
48O	-6.8408	-2.6927	-2.4521
49O	6.1770	0.2058	1.2648
50O	-6.1770	-0.2056	-1.2647
51O	5.8131	-2.4289	1.3633
52O	-5.8129	2.4291	-1.3630
53O	8.0829	-1.4981	-0.0053
54O	-8.0828	1.4983	0.0055
55O	5.7947	-2.4650	-1.3264
56O	-5.7946	2.4650	1.3268
57O	4.1781	-4.3996	-2.7306
58O	-4.1779	4.3993	2.7311
59O	2.1153	-3.0336	-1.4072
60O	-2.1151	3.0333	1.4076
61O	-1.5232	-4.3700	2.4748
62O	1.5233	4.3698	-2.4754
63O	2.9827	-0.1378	5.2868
64O	-2.9829	0.1382	-5.2868
65O	4.7604	1.0249	3.3830
66O	-4.7605	-1.0245	-3.3831
67O	1.3754	-0.4435	2.9907
68O	-1.3755	0.4436	-2.9908
69O	2.1395	-2.9590	1.5086
70O	-2.1393	2.9592	-1.5083
71O	0.2634	-4.5463	0.1181
72O	-0.2631	4.5462	-0.1173
73O	4.1920	-4.3190	2.8492
74O	-4.1918	4.3193	-2.8487
75O	3.8071	-1.5924	-2.9338
76O	-3.8071	1.5921	2.9340
77P	2.8808	-0.0612	0.0001
78P	-2.8808	0.0612	-0.0003
79W	3.0103	0.0019	-3.5857
80W	-3.0103	-0.0023	3.5857
81W	3.9276	-3.0186	1.7475
82W	-3.9274	3.0187	-1.7471
83W	2.1615	2.9276	1.8436
84W	-2.1618	-2.9276	-1.8440
85W	5.4626	1.8816	1.8214
86W	-5.4627	-1.8814	-1.8215
87W	3.0434	0.1010	3.5822
88W	-3.0435	-0.1008	-3.5822
89W	2.1552	2.8655	-1.9062
90W	-2.1552	-2.8657	1.9058
91W	6.3790	-1.2637	0.0023
92W	-6.3789	1.2638	-0.0021
93W	5.4506	1.8277	-1.8965
94W	-5.4507	-1.8278	1.8963
95W	3.9148	-3.0731	-1.6625
96W	-3.9146	3.0729	1.6628

Fe4-SK-OO_-7_20

Energy (POTENTIAL) = -7074.91573860 Eh

Atom	X	Y	Z
1 Fe	-0.0839	-0.0810	-1.6595
2 Fe	0.0506	-0.0729	1.8612
3 Fe	0.8235	2.5159	0.0579
4 Fe	-0.8992	-2.6708	-0.0026
5 H	0.3033	-4.8873	-0.8557
6 H	0.3331	-4.9240	0.7207
7 O	1.4026	0.3597	3.0781
8 O	-1.3902	-0.5952	-3.0346
9 O	-0.5810	1.7622	-1.4488
10O	0.5331	-1.9901	1.4015
11O	5.4534	-2.4417	-0.1142
12O	-5.4851	2.2979	-0.0183
13O	2.2906	-2.0430	3.4518
14O	-2.2906	1.8122	-3.5173
15O	3.0729	-0.0049	5.3175
16O	-2.9755	-0.3041	-5.3217
17O	3.2291	-0.9160	1.2931
18O	-3.2184	0.7676	-1.3116
19O	1.3258	0.4155	0.0962
20O	-1.3528	-0.5736	-0.0412
21O	3.1756	-0.8321	-1.2912
22O	-3.1940	0.7768	1.2772
23O	3.8087	1.2775	0.0562
24O	-3.8702	-1.3485	-0.0057
25O	2.2875	-3.2611	-0.0667
26O	-2.2585	3.2247	-0.0173
27O	2.1524	-1.8447	-3.4922
28O	-2.2849	1.8472	3.4806
29O	3.7255	1.6064	-2.8687
30O	-3.8099	-1.5805	2.9382
31O	4.2047	3.8918	0.1292
32O	-4.1543	-3.9600	0.0090
33O	6.1484	-0.3344	1.2315
34O	-6.1677	0.1583	-1.2948
35O	6.7990	-2.8501	2.3487
36O	-6.7776	2.6513	-2.5271
37O	4.7601	-1.1707	3.3615
38O	-4.7392	0.9314	-3.4175
39O	4.0297	-3.3138	1.9613
40O	-4.0230	3.1304	-2.0692
41O	1.3671	-4.3742	-2.4421
42O	-1.4653	4.3346	2.4572
43O	0.4899	-1.8833	-1.3861
44O	-0.5548	1.8171	1.4505
45O	3.9659	-3.1914	-2.1647
46O	-4.0245	3.1444	2.0356
47O	6.7076	-2.6493	-2.6640
48O	-6.7809	2.6720	2.4797
49O	6.1027	-0.2425	-1.3294
50O	-6.1591	0.1683	1.2845
51O	5.7712	2.3907	-1.3004
52O	-5.8030	-2.4674	1.3522
53O	8.0639	1.3927	-0.0178
54O	-8.0863	-1.4942	0.0091
55O	5.8288	2.3098	1.3982
56O	-5.8175	-2.4909	-1.3271
57O	4.2954	4.2360	2.9447
58O	-4.2166	-4.4135	-2.7694
59O	2.1626	3.0412	1.6189
60O	-2.1373	-3.0562	-1.4205
61O	-1.4416	4.2825	-2.5020
62O	1.4446	-4.5142	2.2784
63O	2.7656	0.3543	-5.2116
64O	-2.9846	-0.2364	5.2972
65O	4.5966	-0.9408	-3.4491
66O	-4.7288	0.9532	3.3854
67O	1.2519	0.4926	-2.8550
68O	-1.3525	-0.5463	3.0248
69O	2.1035	3.1521	-1.3368
70O	-2.1236	-3.0381	1.4074
71O	0.9074	6.4035	0.3984
72O	-0.2308	-4.7126	-0.0529
73O	4.2182	4.4080	-2.6531
74O	-4.1976	-4.3824	2.7871
75O	3.8620	1.4142	3.0107
76O	-3.8602	-1.6137	-2.9515
77P	2.8720	-0.0047	0.0374
78P	-2.9061	-0.0886	-0.0166
79W	3.0978	-0.1997	3.6092
80W	-3.0064	-0.0255	-3.6232
81W	3.8925	3.0883	-1.5972
82W	-3.9583	-3.0668	1.7069
83W	2.0882	-2.8807	-1.9406
84W	-2.1012	2.8513	1.8638
85W	5.3650	-1.8519	-1.9495
86W	-5.4194	1.8446	1.8397
87W	2.8963	0.0379	-3.5245
88W	-3.0143	0.0310	3.5988
89W	2.1223	-2.9815	1.8369
90W	-2.1046	2.8094	-1.9101
91W	6.3560	1.1957	0.0124
92W	-6.3857	-1.2597	-0.0007
93W	5.4299	-2.0028	1.7515
94W	-5.4157	1.8210	-1.8909
95W	3.9340	2.9827	1.8175
96W	-3.9652	-3.0820	-1.7112
97O	1.0281	6.6173	-0.7907

Fe4-SK-OO_-7_22

Energy (POTENTIAL) = -7074.94686189 Eh

Atom	X	Y	Z
1 Fe	0.0166	0.0432	-1.7884
2 Fe	-0.0152	-0.1095	1.8103
3 Fe	0.8255	2.5533	0.1191
4 Fe	-0.8961	-2.6323	-0.1046
5 H	0.3030	-4.8592	-0.9804
6 H	0.2965	-4.9237	0.5934
7 O	1.3434	0.3286	3.0258
8 O	-1.3464	-0.3775	-3.0219
9 O	-0.5637	1.9303	-1.3240
10O	0.5154	-2.0106	1.3145
11O	5.4686	-2.4720	-0.0807
12O	-5.5104	2.3366	0.0848
13O	2.2247	-2.0754	3.4005
14O	-2.2657	2.0300	-3.3965
15O	2.9610	-0.0464	5.2960
16O	-2.9461	0.0185	-5.3030
17O	3.1953	-0.9247	1.2666
18O	-3.2041	0.8697	-1.2552
19O	1.3207	0.4283	0.0276
20O	-1.3615	-0.5453	-0.0145
21O	3.2033	-0.8276	-1.3173
22O	-3.2239	0.7513	1.3234
23O	3.8217	1.2665	0.0500
24O	-3.8761	-1.3144	-0.0693
25O	2.3146	-3.2793	-0.1209
26O	-2.3013	3.2879	0.1497
27O	2.2433	-1.8025	-3.5384
28O	-2.3318	1.7183	3.5810
29O	3.8423	1.6075	-2.8888
30O	-3.8375	-1.6836	2.8556
31O	4.2310	3.8723	0.1528
32O	-4.1560	-3.9243	-0.1864
33O	6.1325	-0.3659	1.2819
34O	-6.1541	0.2537	-1.3092

35O	6.7600	-2.8781	2.4169
36O	-6.7776	2.8007	-2.4099
37O	4.6938	-1.2018	3.3764
38O	-4.7139	1.1305	-3.3697
39O	3.9989	-3.3362	1.9527
40O	-4.0290	3.2639	-1.9212
41O	1.4141	-4.3492	-2.5319
42O	-1.4957	4.2487	2.6801
43O	0.5312	-1.8917	-1.4580
44O	-0.6078	1.7875	1.5414
45O	4.0098	-3.1777	-2.1840
46O	-4.0640	3.0742	2.1890
47O	6.7746	-2.6923	-2.5922
48O	-6.8162	2.5686	2.5979
49O	6.1500	-0.2696	-1.2760
50O	-6.1772	0.1381	1.2663
51O	5.8359	2.3764	-1.2412
52O	-5.8188	-2.5017	1.2068
53O	8.0849	1.3546	0.0817
54O	-8.0839	-1.4634	-0.1109
55O	5.8099	2.2679	1.4549
56O	-5.7975	-2.3827	-1.4753
57O	4.2589	4.1928	2.9544
58O	-4.1859	-4.2347	-2.9837
59O	2.1462	2.9955	1.5720
60O	-2.1182	-2.9572	-1.5464
61O	-1.4635	4.4741	-2.2705
62O	1.4072	-4.5396	2.1937
63O	2.9859	0.3573	-5.2688
64O	-3.0191	-0.4570	5.2835
65O	4.7159	-0.9429	-3.4329
66O	-4.7717	0.8131	3.4275
67O	1.3735	0.5722	-2.9696
68O	-1.3784	-0.6496	3.0080
69O	2.1734	3.1548	-1.3831
70O	-2.1395	-3.0816	1.2796
71O	1.0386	6.6226	-0.4671
72O	-0.2478	-4.6928	-0.1875
73O	4.3128	4.4124	-2.6358
74O	-4.2280	-4.4744	2.5755
75O	3.8039	1.3822	3.0101
76O	-3.8008	-1.4257	-3.0173
77P	2.8713	-0.0056	0.0064
78P	-2.9054	-0.0579	-0.0032
79W	3.0197	-0.2341	3.5871
80W	-3.0011	0.2136	-3.5954
81W	3.9451	3.0872	-1.5961
82W	-3.9702	-3.1097	1.5618
83W	2.1080	-2.8573	-1.9886
84W	-2.1284	2.7976	2.0075
85W	5.4189	-1.8892	-1.9096
86W	-5.4447	1.7811	1.9295
87W	3.0458	0.0425	-3.5788
88W	-3.0405	-0.1025	3.6008
89W	2.0959	-3.0065	1.7736
90W	-2.1025	2.9669	-1.7455
91W	6.3761	1.1634	0.0569
92W	-6.3833	-1.2279	-0.0855
93W	5.4060	-2.0277	1.7898
94W	-5.4180	1.9543	-1.7913
95W	3.9352	2.9422	1.8158
96W	-3.9440	-2.9654	-1.8496
97O	0.9721	6.4264	0.7294

Fe4-SK-OOH2_-7_20

Energy (POTENTIAL) = -7076.15912024 Eh

	Atom	X	Y	Z
1	Fe	-0.0130	-0.1664	1.7855
2	Fe	-0.0386	0.2718	-1.7555
3	Fe	-0.8235	2.7673	0.3457
4	Fe	0.8629	-2.5562	-0.3252
5	H	-0.2978	-4.9160	0.1712
6	H	-0.3076	-4.7143	-1.3929
7	O	-1.3951	0.8871	-2.8868
8	O	1.3631	-0.8379	2.9242
9	O	0.6239	1.7454	1.6955
10	O	-0.5343	-1.6893	-1.6049
11	O	-5.4492	-2.4560	-0.2928
12	O	5.5693	2.2605	0.2852
13	O	-2.2334	-1.4462	-3.6730
14	O	2.3701	1.4238	3.7253
15	O	-3.0004	0.8440	-5.2059
16	O	2.9952	-0.9255	5.2149
17	O	-3.1991	-0.6712	-1.3736
18	O	3.2438	0.6330	1.3922
19	O	-1.3322	0.5153	0.0758
20	O	1.3554	-0.4900	-0.0552
21	O	-3.1915	-0.9923	1.1894
22	O	3.2275	0.9842	-1.1691
23	O	-3.8713	1.2742	0.1704
24	O	3.8567	-1.3084	-0.1835
25	O	-2.2922	-3.2142	-0.3967
26	O	2.4283	3.2287	0.4307
27	O	-2.2167	-2.3186	3.2180
28	O	2.3263	2.3493	-3.1847
29	O	-3.8642	1.1246	3.1350
30	O	3.7771	-1.1664	-3.1344
31	O	-4.3122	3.8523	0.4932
32	O	4.0865	-3.9157	-0.5282
33	O	-6.1772	-0.1733	-1.2950
34	O	6.1819	-0.0408	1.2759
35	O	-6.7601	-2.4795	-2.8137
36	O	6.8750	2.2529	2.8141
37	O	-4.7185	-0.6414	-3.4986
38	O	4.7852	0.4765	3.4877
39	O	-3.9881	-2.9593	-2.4444
40	O	4.1435	2.8537	2.4537
41	O	-1.3695	-4.6549	1.8025
42	O	1.5569	4.7131	-1.8263
43	O	-0.5230	-2.0395	1.1423
44	O	0.6279	2.1059	-1.1467
45	O	-3.9750	-3.4750	1.6587
46	O	4.1102	3.3954	-1.6302
47	O	-6.7419	-3.1061	2.1556
48	O	6.8508	2.9226	-2.1616
49	O	-6.1664	-0.4965	1.2473
50	O	6.1811	0.3026	-1.2868
51	O	-5.8855	2.1193	1.6491
52	O	5.7577	-2.2953	-1.6745
53	O	-8.1418	1.2949	0.1988
54	O	8.0637	-1.5514	-0.2306
55	O	-5.9068	2.4576	-1.0278
56	O	5.7736	-2.6550	0.9839
57	O	-4.3953	4.6201	-2.2385
58	O	4.1450	-4.7109	2.1760
59	O	-2.2554	3.2466	-1.1098
60	O	2.0925	-3.1563	1.0170
61	O	1.6237	4.0372	3.0586
62	O	-1.3833	-4.0620	-2.8894
63	O	-2.9781	-0.4758	5.2746
64	O	2.9391	0.4962	-5.2726
65	O	-4.6992	-1.4874	3.2601
66	O	4.7460	1.3830	-3.2556
67	O	-1.3697	0.1295	3.0415
68	O	1.3382	-0.0511	-3.0260
69	O	-2.2294	2.8645	1.8597
70	O	2.0782	-2.7779	-1.7950
71	O	-0.2699	4.6864	0.6138
72	O	0.2433	-4.6171	-0.5885
73	O	-4.3543	3.9255	3.3200
74	O	4.1167	-3.9747	-3.3429
75	O	-3.9008	1.8569	-2.7413
76	O	3.8083	-1.9456	2.7024
77	P	-2.8740	0.0443	0.0168
78	P	2.9090	-0.0470	-0.0011
79	W	-3.0617	0.3815	-3.5497
80	W	3.0396	-0.4260	3.5694
81	W	-4.0038	2.7857	2.0739
82	W	3.9000	-2.8062	-2.1005
83	W	-2.0813	-3.1006	1.5161
84	W	2.1859	3.1100	-1.4536
85	W	-5.4034	-2.1782	1.6101
86	W	5.4760	2.0502	-1.6181
87	W	-3.0384	-0.5110	3.5553
88	W	3.0073	0.5273	-3.5547
89	W	-2.0994	-2.6321	-2.2200
90	W	2.1879	2.6234	2.2643
91	W	-6.4294	1.1346	0.1662
92	W	6.3692	-1.2782	-0.1853
93	W	-5.4188	-1.7130	-2.0632
94	W	5.4832	1.5630	2.0821
95	W	-4.0240	3.2125	-1.3115
96	W	3.9182	-3.2594	1.2830
97	O	-0.3899	5.5587	-0.6090
98	H	-0.2205	6.4470	-0.2457
99	H	0.4634	5.2641	-1.1874

Fe4-SK-OOH2-OH2_prodTS2-7_20

Energy (POTENTIAL) = -7152.61513293 Eh

	Atom	X	Y	Z
1	Fe	-0.0505	0.1045	1.7737
2	Fe	-0.0406	-0.0586	-1.7938
3	Fe	-0.8126	2.7751	-0.1371
4	Fe	0.8323	-2.6097	0.0940
5	H	-0.3439	-4.8508	0.9595
6	H	-0.3452	-4.9054	-0.6164
7	O	-1.3915	0.3752	-3.0124
8	O	1.3307	-0.3724	2.9997
9	O	0.5931	1.9850	1.3534
10	O	-0.5538	-1.9623	-1.3166
11	O	-5.4810	-2.4764	0.0889
12	O	5.5684	2.2268	-0.0865
13	O	-2.2522	-2.0437	-3.4002
14	O	2.3313	1.9899	3.4083
15	O	-3.0048	-0.0257	-5.2881
16	O	2.9407	-0.0727	5.2871
17	O	-3.2140	-0.8960	-1.2587
18	O	3.2155	0.8187	1.2570
19	O	-1.3420	0.4965	-0.0198
20	O	1.3363	-0.5346	0.0135
21	O	-3.2123	-0.8043	1.3230
22	O	3.2243	0.7222	-1.3233
23	O	-3.8732	1.2767	-0.0389
24	O	3.8350	-1.3692	0.0457
25	O	-2.3258	-3.2581	0.1188
26	O	2.3980	3.2317	-0.1193
27	O	-2.2499	-1.7883	3.5424
28	O	2.3428	1.7371	-3.5576
29	O	-3.8931	1.5969	2.9089
30	O	3.7761	-1.7254	-2.8928
31	O	-4.2852	3.8685	-0.1378
32	O	4.0558	-3.9994	0.1395
33	O	-6.1826	-0.3755	-1.2662
34	O	6.1575	0.1190	1.2832
35	O	-6.7871	-2.8866	-2.4024
36	O	6.8523	2.6376	2.4154
37	O	-4.7303	-1.2019	-3.3663
38	O	4.7442	1.0100	3.3605
39	O	-4.0178	-3.3234	-1.9484
40	O	4.1227	3.1739	1.9312

41	O	-1.4103	-4.3234	2.5236
42	O	1.5480	4.2775	-2.5824
43	O	-0.5563	-1.8505	1.4498
44	O	0.6381	1.8210	-1.5041
45	O	-4.0125	-3.1725	2.1845
46	O	4.1177	3.0244	-2.1678
47	O	-6.7807	-2.7134	2.6036
48	O	6.8550	2.4586	-2.6079
49	O	-6.1846	-0.2850	1.2918
50	O	6.1668	0.0269	-1.2988
51	O	-5.8975	2.3637	1.2651
52	O	5.7398	-2.6006	-1.2519
53	O	-8.1442	1.3285	-0.0484
54	O	8.0399	-1.6284	0.0593
55	O	-5.8860	2.2594	-1.4327
56	O	5.7383	-2.5045	1.4305
57	O	-4.3465	4.1922	-2.9454
58	O	4.0965	-4.3337	2.9345
59	O	-2.2240	2.9723	-1.6145
60	O	2.0570	-2.9834	1.5235
61	O	1.6448	4.4822	2.3242
62	O	-1.4228	-4.5043	-2.2024
63	O	-3.0058	0.3584	5.2770
64	O	2.9592	-0.4505	-5.2892
65	O	-4.7302	-0.9542	3.4425
66	O	4.7543	0.7631	-3.4352
67	O	-1.3958	0.5981	2.9763
68	O	1.3370	-0.6026	-2.9991
69	O	-2.2302	3.1256	1.4197
70	O	2.0594	-3.0788	-1.3111
71	O	-0.5510	4.7517	0.0298
72	O	0.2031	-4.6824	0.1645
73	O	-4.3662	4.4025	2.6510
74	O	4.0944	-4.5302	-2.6251
75	O	-3.8876	1.3792	-3.0129
76	O	3.7681	-1.5159	2.9986
77	P	-2.8856	0.0303	0.0005
78	P	2.8899	-0.0934	-0.0008
79	W	-3.0651	-0.2126	-3.5786
80	W	3.0044	0.1305	3.5806
81	W	-3.9955	3.0781	1.6075
82	W	3.8804	-3.1680	-1.5984
83	W	-2.1184	-2.8346	1.9876
84	W	2.1818	2.7668	-1.9764
85	W	-5.4356	-1.8938	1.9188
86	W	5.4723	1.6981	-1.9322
87	W	-3.0681	0.0492	3.5855
88	W	3.0116	-0.1276	-3.6012
89	W	-2.1276	-2.9792	-1.7750
90	W	2.1749	2.9277	1.7758
91	W	-6.4324	1.1568	-0.0345
92	W	6.3460	-1.3487	0.0462
93	W	-5.4404	-2.0213	-1.7794
94	W	5.4666	1.8359	1.7944
95	W	-4.0036	2.9421	-1.8082
96	W	3.8801	-3.0496	1.8123
97	O	0.1083	5.6701	-0.9568
98	H	0.7856	6.1598	-0.3169
99	H	0.6377	5.1049	-1.6110
100	O	1.5863	6.7049	0.7546
101	H	2.4947	6.9190	0.4990
102	H	1.6452	5.9603	1.3997

Fe4-SK-O-OH2_TS2-7_20

Energy (POTENTIAL) = -7152.61042869 Eh

	Atom	X	Y	Z
1	Fe	-0.0433	0.1063	1.7821
2	Fe	-0.0363	-0.0419	-1.7852
3	Fe	-0.8016	2.7851	-0.1213
4	Fe	0.8301	-2.6084	0.0958
5	H	-0.3466	-4.8543	0.9548
6	H	-0.3440	-4.9048	-0.6214
7	O	-1.3889	0.3852	-3.0057
8	O	1.3345	-0.3734	3.0044
9	O	0.6020	1.9841	1.3589
10	O	-0.5567	-1.9518	-1.3136
11	O	-5.4797	-2.4661	0.0853
12	O	5.5771	2.2148	-0.0869
13	O	-2.2495	-2.0334	-3.4036
14	O	2.3429	1.9881	3.4092
15	O	-2.9972	-0.0116	-5.2866
16	O	2.9481	-0.0723	5.2897
17	O	-3.2088	-0.8935	-1.2583
18	O	3.2238	0.8125	1.2603
19	O	-1.3432	0.5065	-0.0118
20	O	1.3363	-0.5315	0.0183
21	O	-3.2096	-0.8057	1.3243
22	O	3.2261	0.7161	-1.3206
23	O	-3.8811	1.2695	-0.0411
24	O	3.8323	-1.3771	0.0481
25	O	-2.3258	-3.2578	0.1144
26	O	2.4260	3.2208	-0.1173
27	O	-2.2504	-1.7970	3.5433
28	O	2.3394	1.7311	-3.5473
29	O	-3.8912	1.5854	2.9164
30	O	3.7707	-1.7346	-2.8899
31	O	-4.2672	3.8699	-0.1286
32	O	4.0465	-4.0070	0.1433
33	O	-6.1797	-0.3640	-1.2674
34	O	6.1616	0.1051	1.2821
35	O	-6.7835	-2.8764	-2.4065
36	O	6.8664	2.6209	2.4136
37	O	-4.7267	-1.1886	-3.3658
38	O	4.7548	0.9996	3.3621
39	O	-4.0162	-3.3148	-1.9542
40	O	4.1387	3.1664	1.9370
41	O	-1.4120	-4.3283	2.5165
42	O	1.5993	4.2830	-2.6019
43	O	-0.5584	-1.8500	1.4507
44	O	0.6254	1.8516	-1.4889
45	O	-4.0139	-3.1739	2.1790
46	O	4.1326	3.0155	-2.1709
47	O	-6.7815	-2.7106	2.5988
48	O	6.8661	2.4370	-2.6087
49	O	-6.1787	-0.2780	1.2942
50	O	6.1665	0.0106	-1.2995
51	O	-5.8825	2.3691	1.2713
52	O	5.7341	-2.6143	-1.2505
53	O	-8.1350	1.3369	-0.0420
54	O	8.0379	-1.6483	0.0586
55	O	-5.8804	2.2750	-1.4246
56	O	5.7345	-2.5174	1.4320
57	O	-4.3325	4.2026	-2.9385
58	O	4.0870	-4.3391	2.9388
59	O	-2.2182	2.9722	-1.6000
60	O	2.0513	-2.9844	1.5269
61	O	1.6649	4.4818	2.3251
62	O	-1.4175	-4.4936	-2.2095
63	O	-3.0021	0.3459	5.2855
64	O	2.9493	-0.4558	-5.2813
65	O	-4.7287	-0.9603	3.4452
66	O	4.7527	0.7528	-3.4346
67	O	-1.3923	0.5935	2.9863
68	O	1.3347	-0.6012	-2.9836
69	O	-2.2166	3.0516	1.3917
70	O	2.0525	-3.0814	-1.3090
71	O	-0.3942	4.5481	0.0559
72	O	0.2016	-4.6825	0.1613
73	O	-4.3132	4.3885	2.6534
74	O	4.0835	-4.5408	-2.6209
75	O	-3.8844	1.3894	-3.0102
76	O	3.7676	-1.5207	3.0007
77	P	-2.8846	0.0301	0.0032
78	P	2.8928	-0.0972	0.0028
79	W	-3.0596	-0.2028	-3.5780
80	W	3.0108	0.1305	3.5832
81	W	-3.9886	3.0564	1.6059
82	W	3.8738	-3.1777	-1.5946
83	W	-2.1185	-2.8381	1.9831
84	W	2.1965	2.7740	-1.9746
85	W	-5.4336	-1.8915	1.9195
86	W	5.4801	1.6842	-1.9311
87	W	-3.0618	0.0392	3.5936
88	W	3.0105	-0.1339	-3.5934
89	W	-2.1232	-2.9703	-1.7785
90	W	2.1891	2.9292	1.7744
91	W	-6.4244	1.1589	-0.0345
92	W	6.3448	-1.3643	0.0475
93	W	-5.4359	-2.0143	-1.7819
94	W	5.4767	1.8247	1.7950
95	W	-3.9972	2.9474	-1.8049
96	W	3.8743	-3.0547	1.8164
97	O	0.0391	5.7432	-1.0734
98	H	0.6589	6.2258	-0.4142
99	H	0.6217	5.2189	-1.6948
100	O	1.4692	6.7729	0.7719
101	H	2.3782	7.0234	0.5567
102	H	1.5374	5.9918	1.3651

Fe4-SK-OOH_-7_21

Energy (POTENTIAL) = -7075.55886203 Eh

	Atom	X	Y	Z
1	Fe	-0.0203	-0.1181	1.7853
2	Fe	0.0180	0.1968	-1.7998
3	Fe	-0.7997	2.6662	0.2490
4	Fe	0.8750	-2.5774	-0.2375
5	H	-0.3006	-4.9146	0.3333
6	H	-0.2958	-4.7698	-1.2368
7	O	-1.3506	0.7796	-2.9491
8	O	1.3331	-0.7274	2.9482
9	O	0.5702	1.8212	1.5732
10	O	-0.5267	-1.7556	-1.5604
11	O	-5.4576	-2.4324	-0.2385
12	O	5.5545	2.2922	0.2233
13	O	-2.2270	-1.5626	-3.6447
14	O	2.2941	1.5873	3.6324
15	O	-2.9715	0.6987	-5.2436
16	O	2.9380	-0.6703	5.2582
17	O	-3.1841	-0.7112	-1.3692
18	O	3.2179	0.7035	1.3634
19	O	-1.3342	0.5219	0.0435
20	O	1.3548	-0.4985	-0.0494
21	O	-3.1954	-0.9588	1.2027
22	O	3.2394	0.9230	-1.2110
23	O	-3.8628	1.2774	0.1227
24	O	3.8607	-1.3140	-0.1029
25	O	-2.3043	-3.2316	-0.3135
26	O	2.3678	3.2754	0.2868
27	O	-2.2358	-2.2262	3.2749
28	O	2.3546	2.1866	-3.3116
29	O	-3.8808	1.2116	3.0971
30	O	3.8224	-1.3027	-3.0588
31	O	-4.2610	3.8647	0.3780
32	O	4.1030	-3.9254	-0.3305
33	O	-6.1498	-0.1767	-1.3056
34	O	6.1642	0.0351	1.3305
35	O	-6.7523	-2.5207	-2.7686
36	O	6.8300	2.4007	2.7573
37	O	-4.6987	-0.7121	-3.4907
38	O	4.7290	0.6598	3.4900

39O	-3.9902	-3.0151	-2.3719
40O	4.0923	2.9755	2.3376
41O	-1.3866	-4.6019	1.9302
42O	1.6029	4.5946	-2.1104
43O	-0.5395	-2.0051	1.1950
44O	0.6076	2.0402	-1.2708
45O	-3.9932	-3.4186	1.7440
46O	4.1195	3.3250	-1.7616
47O	-6.7592	-3.0246	2.2167
48O	6.8623	2.8373	-2.2395
49O	-6.1694	-0.4320	1.2489
50O	6.1847	0.2617	-1.2412
51O	-5.8654	2.2002	1.5587
52O	5.7874	-2.3570	-1.5279
53O	-8.1151	1.3342	0.1280
54O	8.0680	-1.5333	-0.0926
55O	-5.8531	2.4509	-1.1236
56O	5.7675	-2.5903	1.1464
57O	-4.3380	4.5546	-2.3486
58O	4.1279	-4.5952	2.4066
59O	-2.1905	3.2162	-1.1492
60O	2.0848	-3.1049	1.1490
61O	1.5772	4.1793	2.8548
62O	-1.3882	-4.1568	-2.7745
63O	-2.9876	-0.3279	5.2808
64O	3.0147	0.2455	-5.2909
65O	-4.7149	-1.3854	3.2850
66O	4.7850	1.2415	-3.2911
67O	-1.3872	0.2214	3.0256
68O	1.3759	-0.2111	-3.0483
69O	-2.2053	2.8758	1.7746
70O	2.1052	-2.8547	-1.6750
71O	-0.3179	4.5684	0.3454
72O	0.2457	-4.6383	-0.4317
73O	-4.3073	4.0228	3.2069
74O	4.1688	-4.1139	-3.1388
75O	-3.8276	1.7912	-2.7809
76O	3.7804	-1.8089	2.8034
77P	-2.8740	0.0385	0.0019
78P	2.9087	-0.0460	0.0001
79W	-3.0184	0.2737	-3.5784
80W	3.0012	-0.2532	3.5915
81W	-3.9789	2.8373	1.9998
82W	3.9337	-2.8895	-1.9558
83W	-2.0942	-3.0568	1.5940
84W	2.1800	3.0547	-1.6215
85W	-5.4125	-2.1213	1.6548
86W	5.4789	1.9910	-1.6773
87W	-3.0469	-0.4140	3.5646
88W	3.0507	0.3698	-3.5767
89W	-2.0891	-2.7018	-2.1496
90W	2.1650	2.7411	2.1263
91W	-6.4074	1.1477	0.1222
92W	6.3718	-1.2708	-0.0818
93W	-5.4040	-1.7505	-2.0370
94W	5.4564	1.6683	2.0347
95W	-4.0104	3.1595	-1.3982
96W	3.9087	-3.1874	1.4453
97O	-1.0257	5.4454	-0.4422
98H	-1.6128	4.8235	-0.9566

Fe4-SK-OOH-OH2_-7_21

Energy (POTENTIAL) = -7152.00153996 Eh

	Atom	X	Y	Z
1	Fe	0.0024	0.0979	1.7679
2	Fe	0.0113	-0.0777	-1.8178
3	Fe	-0.7544	2.6885	-0.1655
4	Fe	0.8444	-2.6306	0.0992
5	H	-0.3608	-4.8547	0.9783
6	H	-0.3592	-4.9189	-0.5970
7	O	-1.3490	0.3552	-3.0341
8	O	1.3657	-0.3797	2.9900
9	O	0.6377	1.9729	1.3016
10	O	-0.5475	-1.9745	-1.3156
11	O	-5.4778	-2.4029	0.0979
12	O	5.6127	2.1690	-0.1305
13	O	-2.2503	-2.0509	-3.4026
14	O	2.3741	1.9848	3.3595
15	O	-2.9753	-0.0288	-5.3003
16	O	2.9837	-0.0498	5.2687
17	O	-3.1873	-0.8804	-1.2641
18	O	3.2590	0.7891	1.2273
19	O	-1.3103	0.5090	-0.0339
20	O	1.3626	-0.5566	-0.0009
21	O	-3.1838	-0.7722	1.3179
22	O	3.2595	0.6627	-1.3543
23	O	-3.8349	1.2997	-0.0601
24	O	3.8535	-1.4171	0.0404
25	O	-2.3337	-3.2448	0.1270
26	O	2.4646	3.1905	-0.1715
27	O	-2.2324	-1.7537	3.5423
28	O	2.3723	1.6564	-3.5943
29	O	-3.8249	1.6475	2.8888
30	O	3.7896	-1.7985	-2.8921
31	O	-4.1898	3.9081	-0.1685
32	O	4.0513	-4.0423	0.1600
33	O	-6.1460	-0.3049	-1.2719
34	O	6.1914	0.0684	1.2609
35	O	-6.7875	-2.8212	-2.3899
36	O	6.9108	2.5911	2.3605
37	O	-4.7123	-1.1637	-3.3643
38	O	4.7885	0.9961	3.3306
39	O	-4.0277	-3.2921	-1.9371
40	O	4.1824	3.1488	1.8852
41	O	-1.4279	-4.3051	2.5363
42	O	1.6803	4.2186	-2.7077
43	O	-0.5452	-1.8474	1.4467
44	O	0.6445	1.8175	-1.5350
45	O	-4.0167	-3.1177	2.1950
46	O	4.1775	2.9563	-2.2286
47	O	-6.7762	-2.6136	2.6161
48	O	6.9057	2.3558	-2.6532
49	O	-6.1436	-0.1970	1.2911
50	O	6.1898	-0.0512	-1.3186
51	O	-5.8104	2.4444	1.2419
52	O	5.7488	-2.6764	-1.2475
53	O	-8.0758	1.4282	-0.0624
54	O	8.0563	-1.7072	0.0496
55	O	-5.8067	2.3272	-1.4538
56	O	5.7501	-2.5507	1.4339
57	O	-4.2251	4.2203	-2.9702
58	O	4.0915	-4.3475	2.9576
59	O	-2.1351	2.9678	-1.5914
60	O	2.0614	-2.9948	1.5339
61	O	1.7092	4.4726	2.2579
62	O	-1.4436	-4.5106	-2.1880
63	O	-2.9488	0.4133	5.2692
64	O	2.9829	-0.5441	-5.3033
65	O	-4.6986	-0.8818	3.4423
66	O	4.7869	0.6761	-3.4676
67	O	-1.3446	0.6209	2.9628
68	O	1.3595	-0.6681	-3.0097
69	O	-2.1411	3.0849	1.3291
70	O	2.0608	-3.1221	-1.2991
71	O	-0.0923	4.4727	-0.1156
72	O	0.1880	-4.6930	0.1833
73	O	-4.2125	4.4523	2.6099
74	O	4.0844	-4.6030	-2.5994
75	O	-3.8188	1.4060	-3.0229
76	O	3.7916	-1.5264	2.9919
77	P	-2.8576	0.0467	-0.0102
78	P	2.9234	-0.1303	-0.0222
79	W	-3.0281	-0.2094	-3.5909
80	W	3.0456	0.1345	3.5604
81	W	-3.9150	3.1064	1.5745
82	W	3.8829	-3.2278	-1.5878
83	W	-2.1156	-2.8115	1.9900
84	W	2.2357	2.7397	-2.0366
85	W	-5.4183	-1.8199	1.9279
86	W	5.5126	1.6200	-1.9718
87	W	-3.0155	0.0913	3.5811
88	W	3.0387	-0.1982	-3.6200
89	W	-2.1248	-2.9737	-1.7686
90	W	2.2427	2.9218	1.7163
91	W	-6.3694	1.2224	-0.0509
92	W	6.3645	-1.4164	0.0363
93	W	-5.4263	-1.9743	-1.7755
94	W	5.5180	1.7940	1.7510
95	W	-3.9273	2.9655	-1.8292
96	W	3.8858	-3.0734	1.8223
97	O	-0.7957	5.6275	-0.3743
98	H	-0.1912	6.2890	0.0903
99	O	0.9327	6.9256	1.0960
100	H	1.6951	7.2690	0.6103
101	H	1.2505	6.1031	1.5250

H2O

Energy (POTENTIAL) = -76.4251273544 Eh

	Atom	X	Y	Z
1	O	0.0175	0.0000	0.0123
2	H	0.0734	0.0000	0.9766
3	H	0.9428	0.0000	-0.2651

O2

Energy (POTENTIAL) = -150.316691773 Eh

	Atom	X	Y	Z
1	O	0.0000	0.0000	0.2931
2	O	0.0000	0.0000	1.5069

Fe4-SK-O-OH2_TS1T-7_20

Energy (POTENTIAL) = -7076.15647586 Eh

	Atom	X	Y	Z
1	Fe	-0.0182	-0.1509	1.7879
2	Fe	-0.0325	0.2653	-1.7572
3	Fe	-0.8109	2.7789	0.3423
4	Fe	0.8568	-2.5593	-0.3056
5	H	-0.3088	-4.9139	0.2038
6	H	-0.3132	-4.7227	-1.3619
7	O	-1.3873	0.8697	-2.8992
8	O	1.3535	-0.8139	2.9291
9	O	0.6121	1.7666	1.6740
10	O	-0.5374	-1.6980	-1.5932
11	O	-5.4537	-2.4435	-0.2845
12	O	5.5702	2.2574	0.2713
13	O	-2.2320	-1.4667	-3.6690
14	O	2.3577	1.4563	3.7060
15	O	-2.9914	0.8178	-5.2169
16	O	2.9809	-0.8773	5.2234
17	O	-3.1946	-0.6764	-1.3733
18	O	3.2382	0.6429	1.3869
19	O	-1.3331	0.5218	0.0746
20	O	1.3513	-0.4913	-0.0516
21	O	-3.1935	-0.9839	1.1928
22	O	3.2287	0.9676	-1.1774
23	O	-3.8747	1.2729	0.1591
24	O	3.8516	-1.3159	-0.1679
25	O	-2.2993	-3.2153	-0.3808
26	O	2.4289	3.2346	0.4030
27	O	-2.2260	-2.3013	3.2306
28	O	2.3278	2.3162	-3.2073

29O	-3.8731	1.1383	3.1317
30O	3.7777	-1.1999	-3.1210
31O	-4.2825	3.8555	0.4715
32O	4.0780	-3.9250	-0.4896
33O	-6.1717	-0.1652	-1.3014
34O	6.1766	-0.0375	1.2845
35O	-6.7603	-2.4811	-2.8068
36O	6.8715	2.2685	2.8009
37O	-4.7143	-0.6527	-3.5004
38O	4.7749	0.5046	3.4880
39O	-3.9907	-2.9665	-2.4316
40O	4.1409	2.8711	2.4311
41O	-1.3801	-4.6441	1.8255
42O	1.5724	4.6906	-1.8743
43O	-0.5323	-2.0306	1.1549
44O	0.6202	2.0992	-1.1611
45O	-3.9851	-3.4599	1.6734
46O	4.1161	3.3764	-1.6584
47O	-6.7525	-3.0798	2.1630
48O	6.8539	2.8935	-2.1810
49O	-6.1663	-0.4746	1.2445
50O	6.1770	0.2832	-1.2810
51O	-5.8767	2.1430	1.6313
52O	5.7541	-2.3186	-1.6483
53O	-8.1311	1.3163	0.1787
54O	8.0575	-1.5629	-0.2086
55O	-5.8892	2.4694	-1.0453
56O	5.7647	-2.6526	1.0140
57O	-4.3544	4.6123	-2.2617
58O	4.1308	-4.6942	2.2222
59O	-2.2315	3.2156	-1.1222
60O	2.0825	-3.1483	1.0445
61O	1.6384	4.0726	3.0197
62O	-1.3850	-4.0772	-2.8654
63O	-2.9842	-0.4496	5.2797
64O	2.9437	0.4431	-5.2745
65O	-4.7072	-1.4660	3.2657
66O	4.7492	1.3477	-3.2647
67O	-1.3760	0.1485	3.0439
68O	1.3399	-0.0814	-3.0238
69O	-2.2179	2.8318	1.8401
70O	2.0733	-2.7956	-1.7712
71O	-0.2858	4.5397	0.6321
72O	0.2353	-4.6210	-0.5564
73O	-4.3271	3.9432	3.2947
74O	4.1124	-4.0104	-3.3036
75O	-3.8896	1.8452	-2.7557
76O	3.7971	-1.9236	2.7223
77P	-2.8733	0.0450	0.0146
78P	2.9059	-0.0505	-0.0005
79W	-3.0528	0.3637	-3.5587
80W	3.0300	-0.3944	3.5733
81W	-3.9966	2.7892	2.0566
82W	3.8955	-2.8299	-2.0728
83W	-2.0901	-3.0904	1.5307
84W	2.1860	3.0992	-1.4853
85W	-5.4094	-2.1588	1.6175
86W	5.4754	2.0306	-1.6315
87W	-3.0425	-0.4936	3.5607
88W	3.0102	0.4919	-3.5569
89W	-2.0994	-2.6418	-2.2065
90W	2.1892	2.6482	2.2363
91W	-6.4199	1.1473	0.1505
92W	6.3631	-1.2881	-0.1684
93W	-5.4166	-1.7149	-2.0605
94W	5.4807	1.5741	2.0716
95W	-4.0034	3.2030	-1.3305
96W	3.9077	-3.2511	1.3148
97O	-0.3736	5.6679	-0.5881
98H	-0.0666	6.4442	-0.0874
99H	0.4190	5.3460	-1.1574

Fe4-SK-O-OH2_TS1B-7_20

Energy (POTENTIAL) = -7076.15567806 Eh

Atom	X	Y	Z
1 Fe	0.0053	-0.1945	1.7890
2 Fe	-0.0003	0.3203	-1.7525
3 Fe	-0.7982	2.7220	0.4206
4 Fe	0.8844	-2.5524	-0.3685
5 H	-0.2862	-4.9208	0.0833
6 H	-0.2881	-4.6921	-1.4773
7 O	-1.3783	0.9490	-2.8741
8 O	1.3622	-0.8794	2.9142
9 O	0.6169	1.7189	1.7184
10O	-0.5260	-1.6565	-1.6364
11O	-5.4425	-2.4396	-0.3468
12O	5.5767	2.2641	0.3259
13O	-2.2246	-1.3689	-3.7074
14O	2.3607	1.3849	3.7296
15O	-2.9787	0.9539	-5.1887
16O	2.9886	-0.9650	5.2108
17O	-3.1809	-0.6426	-1.3908
18O	3.2464	0.6254	1.3985
19O	-1.3239	0.5266	0.0840
20O	1.3643	-0.4874	-0.0635
21O	-3.1815	-1.0142	1.1640
22O	3.2399	0.9922	-1.1595
23O	-3.8623	1.2712	0.1838
24O	3.8661	-1.3071	-0.1869
25O	-2.2876	-3.2093	-0.4640
26O	2.4049	3.2538	0.4743
27O	-2.2160	-2.3880	3.1686
28O	2.3371	2.3749	-3.1730
29O	-3.8743	1.0525	3.1518
30O	3.7951	-1.1315	-3.1356
31O	-4.3014	3.8318	0.5652
32O	4.0981	-3.9035	-0.5620
33O	-6.1655	-0.1395	-1.2976
34O	6.1903	-0.0497	1.2954
35O	-6.7433	-2.4115	-2.8753
36O	6.8739	2.2304	2.8542
37O	-4.7057	-0.5495	-3.5067
38O	4.7825	0.4471	3.5028
39O	-3.9771	-2.8979	-2.5099
40O	4.1387	2.8319	2.4916
41O	-1.3526	-4.6877	1.7078
42O	1.6312	4.7210	-1.8526
43O	-0.5194	-2.0584	1.0991
44O	0.5974	2.1355	-1.1273
45O	-3.9659	-3.5150	1.5802
46O	4.1256	3.4174	-1.5834
47O	-6.7283	-3.1710	2.0828
48O	6.8600	2.9490	-2.1137
49O	-6.1675	-0.5281	1.2431
50O	6.1844	0.3214	-1.2629
51O	-5.8761	2.0873	1.6846
52O	5.7764	-2.2740	-1.6876
53O	-8.1393	1.2694	0.2385
54O	8.0739	-1.5381	-0.2301
55O	-5.9048	2.4697	-0.9754
56O	5.7808	-2.6585	0.9676
57O	-4.4880	4.6535	-2.1327
58O	4.1486	-4.7208	2.1372
59O	-2.2659	3.3670	-1.0515
60O	2.0972	-3.1642	0.9788
61O	1.6288	4.0143	3.1002
62O	-1.3688	-3.9999	-2.9678
63O	-2.9803	-0.5856	5.2606
64O	2.9679	0.5439	-5.2640
65O	-4.6963	-1.5614	3.2200
66O	4.7631	1.4210	-3.2335
67O	-1.3719	0.0682	3.0437
68O	1.3513	-0.0225	-3.0293
69O	-2.2146	2.7718	1.9000
70O	2.0940	-2.7573	-1.8305
71O	-0.3058	4.4929	0.5958
72O	0.2574	-4.6062	-0.6685
73O	-4.3181	3.8528	3.3851
74O	4.1451	-3.9367	-3.3774
75O	-3.8751	1.9232	-2.6913
76O	3.8062	-1.9626	2.6858
77P	-2.8625	0.0452	0.0136
78P	2.9201	-0.0438	-0.0022
79W	-3.0294	0.4461	-3.5468
80W	3.0363	-0.4464	3.5716
81W	-3.9945	2.7282	2.1199
82W	3.9221	-2.7818	-2.1235
83W	-2.0645	-3.1288	1.4522
84W	2.1821	3.1504	-1.4412
85W	-5.3904	-2.2297	1.5623
86W	5.4782	2.0777	-1.5845
87W	-3.0343	-0.5856	3.5413
88W	3.0264	0.5689	-3.5453
89W	-2.0789	-2.5838	-2.2661
90W	2.1954	2.6184	2.2753
91W	-6.4297	1.1007	0.2043
92W	6.3787	-1.2685	-0.1865
93W	-5.4017	-1.6655	-2.1065
94W	5.4884	1.5441	2.1073
95W	-4.0803	3.2252	-1.2660
96W	3.9235	-3.2604	1.2581
97O	-1.2696	5.5421	-0.3591
98H	-1.7740	4.7410	-0.7914
99H	-1.8493	5.8808	0.3452

Fe4-SK-O-H2O_addTS1T-7_20

Energy (POTENTIAL) = -7076.19609931 Eh

Atom	X	Y	Z
1 Fe	0.0037	-0.2127	1.8156
2 Fe	0.0171	0.2523	-1.7687
3 Fe	-0.7904	2.6178	0.3894
4 Fe	0.8697	-2.5815	-0.3147
5 H	-0.3230	-4.9306	0.1659
6 H	-0.3194	-4.7215	-1.3967
7 O	-1.3393	0.8900	-2.8982
8 O	1.3592	-0.8732	2.9366
9 O	0.5879	1.7208	1.6481
10O	-0.5367	-1.6956	-1.5942
11O	-5.4671	-2.3577	-0.2882
12O	5.5555	2.2601	0.3081
13O	-2.2368	-1.4193	-3.6716
14O	2.3107	1.4193	3.6961
15O	-2.9628	0.9074	-5.1956
16O	2.9747	-0.8974	5.2391
17O	-3.1657	-0.6367	-1.3595
18O	3.2337	0.6243	1.3997
19O	-1.3162	0.5556	0.1056
20O	1.3595	-0.5174	-0.0493
21O	-3.1682	-0.9838	1.2033
22O	3.2358	0.9498	-1.1643
23O	-3.8562	1.2799	0.2094
24O	3.8620	-1.3318	-0.1515
25O	-2.3193	-3.2074	-0.4042
26O	2.4108	3.2273	0.4261
27O	-2.2352	-2.3504	3.2217
28O	2.3245	2.2934	-3.1922
29O	-3.8333	1.1088	3.1909
30O	3.8061	-1.2047	-3.1061
31O	-4.1319	3.8705	0.5642
32O	4.0963	-3.9336	-0.4813

33O	-6.1296	-0.0568	-1.2775
34O	6.1693	-0.0408	1.3203
35O	-6.7729	-2.3536	-2.8109
36O	6.8515	2.2652	2.8349
37O	-4.6974	-0.5560	-3.4837
38O	4.7524	0.5000	3.5169
39O	-4.0131	-2.8963	-2.4410
40O	4.1121	2.8578	2.4643
41O	-1.4161	-4.6751	1.7792
42O	1.5981	4.6645	-1.8955
43O	-0.5399	-2.0578	1.1442
44O	0.6022	2.0765	-1.1325
45O	-4.0121	-3.4481	1.6439
46O	4.1152	3.3737	-1.6326
47O	-6.7739	-3.0277	2.1440
48O	6.8562	2.8977	-2.1363
49O	-6.1371	-0.4070	1.2750
50O	6.1751	0.2879	-1.2415
51O	-5.7941	2.2064	1.6893
52O	5.7751	-2.3192	-1.6275
53O	-8.0572	1.4277	0.2203
54O	8.0633	-1.5548	-0.1742
55O	-5.7851	2.5708	-0.9747
56O	5.7720	-2.6594	1.0347
57O	-4.1557	4.6641	-2.1396
58O	4.1354	-4.7105	2.2269
59O	-2.1115	3.1074	-0.9943
60O	2.0884	-3.1673	1.0422
61O	1.6036	4.0433	3.0281
62O	-1.4176	-4.0454	-2.8998
63O	-2.9567	-0.5301	5.3138
64O	2.9853	0.4390	-5.2644
65O	-4.6997	-1.4736	3.2720
66O	4.7633	1.3536	-3.2419
67O	-1.3490	0.0909	3.0843
68O	1.3651	-0.1123	-3.0303
69O	-2.1283	2.7201	1.8837
70O	2.0920	-2.8062	-1.7703
71O	-0.2887	4.1340	0.6080
72O	0.2232	-4.6244	-0.5874
73O	-4.1753	3.9201	3.3863
74O	4.1443	-4.0137	-3.2936
75O	-3.8174	1.9074	-2.6971
76O	3.8025	-1.9426	2.7379
77P	-2.8603	0.0553	0.0394
78P	2.9131	-0.0678	0.0094
79W	-3.0125	0.4270	-3.5459
80W	3.0305	-0.4188	3.5894
81W	-3.9173	2.7631	2.1376
82W	3.9186	-2.8368	-2.0624
83W	-2.1074	-3.1112	1.5053
84W	2.1829	3.0994	-1.4788
85W	-5.4125	-2.1259	1.6180
86W	5.4747	2.0332	-1.5998
87W	-3.0140	-0.5430	3.5960
88W	3.0383	0.4853	-3.5474
89W	-2.1072	-2.6097	-2.2214
90W	2.1841	2.6344	2.2421
91W	-6.3541	1.2107	0.1959
92W	6.3680	-1.2925	-0.1425
93W	-5.4105	-1.6267	-2.0631
94W	5.4714	1.5641	2.0951
95W	-3.9079	3.2195	-1.2379
96W	3.9137	-3.2657	1.3240
97O	-0.7627	6.2559	-1.2512
98H	-0.9153	5.5831	-0.5674
99H	0.0061	5.8815	-1.7114

Fe4-SK-O-H2O_addTS1B-7_20

Energy (POTENTIAL) = -7076.19819518 Eh

Atom	X	Y	Z
1 Fe	0.0026	-0.9000	1.5811
2 Fe	-0.0129	0.9581	-1.5156
3 Fe	-0.8209	2.2865	1.3632
4 Fe	0.8680	-2.2191	-1.3181
5 H	-0.3065	-4.5773	-1.8121
6 H	-0.3079	-3.7650	-3.1629
7 O	-1.3819	1.9702	-2.3098
8 O	1.3566	-1.9598	2.3450
9 O	0.5754	0.9312	2.2060
10O	-0.5496	-0.9093	-2.1352
11O	-5.4647	-2.0765	-1.1959
12O	5.5338	1.9797	1.1983
13O	-2.2564	0.1466	-3.9403
14O	2.2996	-0.1705	3.9692
15O	-2.9999	2.8735	-4.4323
16O	2.9739	-2.9096	4.4439
17O	-3.1862	-0.0507	-1.5095
18O	3.2203	0.0301	1.5435
19O	-1.3363	0.4871	0.3044
20O	1.3484	-0.4349	-0.2444
21O	-3.1713	-1.3755	0.7106
22O	3.2185	1.3614	-0.6716
23O	-3.8805	1.0937	0.6829
24O	3.8540	-1.1332	-0.6630
25O	-2.3159	-2.7855	-1.6401
26O	2.3923	2.7991	1.6984
27O	-2.2237	-3.4184	2.0309
28O	2.2951	3.4006	-1.9821
29O	-3.8387	-0.2301	3.3466
30O	3.7928	0.1754	-3.3123
31O	-4.1758	3.3368	2.0178
32O	4.0944	-3.3808	-2.0124
33O	-6.1525	0.4173	-1.1995
34O	6.1559	-0.5284	1.2002
35O	-6.7811	-1.0934	-3.5152
36O	6.8290	0.9774	3.5179
37O	-4.7244	0.8415	-3.4331
38O	4.7438	-0.9289	3.4296
39O	-4.0163	-1.7125	-3.3892
40O	4.0888	1.6518	3.4156
41O	-1.3925	-4.9859	-0.2097
42O	1.5909	5.0537	0.1713
43O	-0.5387	-2.3241	0.2329
44O	0.5716	2.3789	-0.1937
45O	-3.9973	-3.8281	0.1531
46O	4.0937	3.7734	-0.1305
47O	-6.7576	-3.6605	0.7760
48O	6.8350	3.5441	-0.7871
49O	-6.1429	-0.9017	1.0127
50O	6.1600	0.7951	-1.0155
51O	-5.8144	1.3503	2.4118
52O	5.7681	-1.4363	-2.4103
53O	-8.0877	1.1716	0.7679
54O	8.0558	-1.3162	-0.7676
55O	-5.8394	2.7194	0.1006
56O	5.7702	-2.8215	-0.1107
57O	-4.2641	5.1255	-0.1557
58O	4.1390	-5.1862	0.1474
59O	-2.1719	3.2841	0.2533
60O	2.0868	-3.2985	-0.3052
61O	1.5633	2.4964	4.4043
62O	-1.4126	-2.5614	-4.2651
63O	-2.9521	-2.5650	4.6697
64O	2.9525	2.5437	-4.6287
65O	-4.6927	-2.6502	2.4233
66O	4.7379	2.5729	-2.4146
67O	-1.3509	-1.1156	2.8661
68O	1.3426	1.1306	-2.8074
69O	-2.1465	1.7888	2.7681

70O	2.0884	-1.8383	-2.7393
71O	-0.3262	3.6044	2.1405
72O	0.2349	-3.9913	-2.3798
73O	-4.1890	2.2720	4.6331
74O	4.1421	-2.3166	-4.6198
75O	-3.8796	2.8114	-1.7525
76O	3.8023	-2.8591	1.7352
77P	-2.8764	0.0401	0.0479
78P	2.9009	-0.0441	-0.0081
79W	-3.0483	1.7886	-3.0999
80W	3.0279	-1.8089	3.1252
81W	-3.9355	1.6994	3.0295
82W	3.9154	-1.7371	-3.0184
83W	-2.0952	-3.4454	0.1512
84W	2.1711	3.4526	-0.0853
85W	-5.4053	-2.6129	0.6446
86W	5.4579	2.5311	-0.6420
87W	-3.0111	-1.9099	3.0819
88W	3.0118	1.8963	-3.0381
89W	-2.1120	-1.5155	-3.0755
90W	2.1534	1.5192	3.1240
91W	-6.3831	1.0015	0.6537
92W	6.3595	-1.0954	-0.6344
93W	-5.4216	-0.7043	-2.5435
94W	5.4497	0.6270	2.5594
95W	-3.9807	3.4491	0.1065
96W	3.9118	-3.5003	-0.0940
97O	-0.8940	5.4105	-1.2633
98H	-1.2758	4.6143	-0.8514
99H	-0.0554	5.5166	-0.7864

Fe_4-SK species. Grimme's correction tests B3LYP-D3bj, B3LYP-D3 and B3LYP-D2 with BS2.

GD3bjFe4H2O_5_20

Energy (POTENTIAL) = -7001.34118358 Eh

Atom	X	Y	Z
1 Fe	-0.0417	0.0376	1.7445
2 Fe	-0.0517	0.0550	-1.7678
3 Fe	2.5815	0.7969	0.0321
4 Fe	-2.6369	-0.8187	-0.0394
5 H	-4.9000	0.3413	0.7722
6 H	5.0120	-0.2608	-0.8027
7 H	5.0133	-0.3451	0.7568
8 H	-4.9069	0.3577	-0.8061
9 O	0.4607	1.3158	-3.0140
10 O	-0.5264	-1.3317	2.9752
11 O	1.9039	-0.5240	1.3270
12 O	-1.9509	0.5559	-1.3976
13 O	-2.3236	5.4781	0.0013
14 O	2.2914	-5.4499	-0.0325
15 O	-1.9109	2.2492	-3.4832
16 O	1.8862	-2.2259	3.4327
17 O	0.2009	2.9237	-5.3280
18 O	-0.2281	-2.8731	5.2972
19 O	-0.8845	3.1653	-1.2908
20 O	0.8584	-3.1500	1.2773
21 O	0.3836	1.2872	-0.0109
22 O	-0.5144	-1.3269	-0.0148
23 O	-0.8811	3.1559	1.2852
24 O	0.8672	-3.1529	-1.2836
25 O	1.2430	3.7609	-0.0035
26 O	-1.2595	-3.8334	0.0233
27 O	-3.2554	2.3593	-0.0102
28 O	3.2563	-2.3138	-0.0291
29 O	-1.9134	2.2253	3.4705
30 O	1.8789	-2.2062	-3.4510
31 O	1.5572	3.6890	2.9684
32 O	-1.5589	-3.7829	-2.9593

33	O	3.9037	3.9743	0.0147
34	O	-3.8812	-4.0960	0.0068
35	O	-0.1584	6.0870	-1.2851
36	O	0.1824	-6.0935	1.2950
37	O	-2.6191	6.8130	-2.4943
38	O	2.6743	-6.7448	2.5013
39	O	-0.9664	4.6879	-3.4034
40	O	0.9857	-4.6718	3.3942
41	O	-3.1924	4.0645	-2.0828
42	O	3.1971	-4.0244	2.0169
43	O	-4.4285	1.4580	2.3366
44	O	4.3784	-1.3232	-2.3950
45	O	-1.9423	0.5527	1.3659
46	O	1.9021	-0.4889	-1.3374
47	O	-3.1863	4.0463	2.0757
48	O	3.2762	-3.9629	-2.1100
49	O	-2.6111	6.7951	2.5135
50	O	2.7654	-6.6822	-2.5286
51	O	-0.1606	6.0712	1.2863
52	O	0.2305	-6.0634	-1.2211
53	O	2.4669	5.6386	1.3634
54	O	-2.3505	-5.7502	-1.3384
55	O	1.5708	7.9440	0.0080
56	O	-1.5133	-8.0067	0.1029
57	O	2.4769	5.6409	-1.3314
58	O	-2.5129	-5.7477	1.4051
59	O	4.3759	3.9890	-2.7867
60	O	-4.4071	-4.0342	2.8020
61	O	2.9954	1.9680	-1.3826
62	O	-3.0053	-2.0391	1.4215
63	O	4.3922	-1.4275	2.3536
64	O	-4.4329	1.4825	-2.3640
65	O	0.1822	2.8802	5.3271
66	O	-0.2176	-2.9039	-5.2964
67	O	-0.9647	4.6659	3.4067
68	O	0.9685	-4.6883	-3.3597
69	O	0.4652	1.2984	2.9979
70	O	-0.5270	-1.3294	-2.9889
71	O	2.9469	1.9602	1.3868
72	O	-2.9917	-2.0813	-1.4362
73	O	4.8135	0.2429	0.0068
74	O	-4.6923	-0.1909	-0.0235
75	O	4.3741	3.9860	2.7937
76	O	-4.3583	-4.1712	-2.7670
77	O	1.5586	3.7076	-2.9566
78	O	-1.5661	-3.7808	2.9562
79	P	-0.0303	2.8405	-0.0048
80	P	-0.0164	-2.8620	-0.0038
81	W	-0.0633	2.9901	-3.6373
82	W	0.0217	-2.9488	3.6061
83	W	3.0446	3.7998	1.7313
84	W	-3.0372	-3.8990	-1.7148
85	W	-2.9124	2.1400	1.8676
86	W	2.8902	-2.0185	-1.8839
87	W	-1.8447	5.4111	1.8622
88	W	2.0017	-5.2916	-1.8956
89	W	-0.0705	2.9599	3.6353
90	W	0.0179	-2.9558	-3.6019
91	W	-2.9186	2.1630	-1.8887
92	W	2.8882	-2.0916	1.8465
93	W	1.2827	6.2572	-0.0005
94	W	-1.3047	-6.3102	0.1299
95	W	-1.8479	5.4278	-1.8525
96	W	1.8727	-5.3689	1.8837
97	W	3.0525	3.7766	-1.7181
98	W	-3.0734	-3.8304	1.7507

GD3bjFe4H2O_6_21

Energy (POTENTIAL) = -7001.61513224 Eh

Atom		X	Y	Z
1	Fe	0.0000	0.0000	1.7693
2	Fe	0.0000	0.0000	-1.7693
3	Fe	2.6044	0.8705	0.0000
4	Fe	-2.6044	-0.8705	0.0000
5	H	-4.8577	0.3272	0.7891
6	H	4.8577	-0.3272	-0.7891
7	H	4.8577	-0.3272	0.7891
8	H	-4.8577	0.3272	-0.7891
9	O	0.5132	1.3301	-2.9983
10	O	-0.5132	-1.3301	2.9983
11	O	1.8889	-0.5503	1.3695
12	O	-1.8889	0.5503	-1.3695
13	O	-2.3430	5.4429	0.0000
14	O	2.3430	-5.4429	0.0000
15	O	-1.8837	2.2203	-3.4765
16	O	1.8837	-2.2203	3.4765
17	O	0.2153	2.9019	-5.3231
18	O	-0.2153	-2.9019	5.3231
19	O	-0.8575	3.1519	-1.2841
20	O	0.8575	-3.1519	1.2841
21	O	0.4935	1.3111	0.0000
22	O	-0.4935	-1.3111	0.0000
23	O	-0.8575	3.1519	1.2841
24	O	0.8575	-3.1519	-1.2841
25	O	1.2556	3.8120	0.0000
26	O	-1.2556	-3.8120	0.0000
27	O	-3.2400	2.3327	0.0000
28	O	3.2400	-2.3327	0.0000
29	O	-1.8837	2.2203	3.4765
30	O	1.8837	-2.2203	-3.4765
31	O	1.5586	3.7716	2.9724
32	O	-1.5586	-3.7716	-2.9724
33	O	3.8931	4.0568	0.0000
34	O	-3.8931	-4.0568	0.0000
35	O	-0.1979	6.0941	-1.2884
36	O	0.1979	-6.0941	1.2884
37	O	-2.6717	6.7613	-2.5027
38	O	2.6717	-6.7613	2.5027
39	O	-0.9797	4.6694	-3.4011
40	O	0.9797	-4.6694	3.4011
41	O	-3.1905	4.0117	-2.0776
42	O	3.1905	-4.0117	2.0776
43	O	-4.3873	1.4049	2.3495
44	O	4.3873	-1.4049	-2.3495
45	O	-1.8889	0.5503	1.3695
46	O	1.8889	-0.5503	-1.3695
47	O	-3.1905	4.0117	2.0776
48	O	3.1905	-4.0117	-2.0776
49	O	-2.6717	6.7613	2.5027
50	O	2.6717	-6.7613	-2.5027
51	O	-0.1979	6.0941	1.2884
52	O	0.1979	-6.0941	-1.2884
53	O	2.4377	5.7240	1.3431
54	O	-2.4377	-5.7240	-1.3431
55	O	1.4698	8.0078	0.0000
56	O	-1.4698	-8.0078	0.0000
57	O	2.4377	5.7240	-1.3431
58	O	-2.4377	-5.7240	1.3431
59	O	4.3760	4.1173	-2.7859
60	O	-4.3760	-4.1173	2.7859
61	O	2.9711	2.0616	-1.4370
62	O	-2.9711	-2.0616	1.4370
63	O	4.3873	-1.4049	2.3495
64	O	-4.3873	1.4049	-2.3495
65	O	0.2153	2.9019	5.3231
66	O	-0.2153	-2.9019	-5.3231
67	O	-0.9797	4.6694	3.4011
68	O	0.9797	-4.6694	-3.4011
69	O	0.5132	1.3301	2.9983
70	O	-0.5132	-1.3301	-2.9983
71	O	2.9711	2.0616	1.4370
72	O	-2.9711	-2.0616	-1.4370
73	O	4.6611	0.2188	0.0000
74	O	-4.6611	-0.2188	0.0000
75	O	4.3760	4.1173	2.7859
76	O	-4.3760	-4.1173	-2.7859
77	O	1.5586	3.7716	-2.9724
78	O	-1.5586	-3.7716	2.9724
79	P	0.0088	2.8529	0.0000
80	P	-0.0088	-2.8529	0.0000
81	W	-0.0421	2.9709	-3.6287
82	W	0.0421	-2.9709	3.6287
83	W	3.0429	3.8866	1.7320
84	W	-3.0429	-3.8866	-1.7320
85	W	-2.8787	2.1041	1.8725
86	W	2.8787	-2.1041	-1.8725
87	W	-1.8732	5.3885	1.8609
88	W	1.8732	-5.3885	-1.8609
89	W	-0.0421	2.9709	3.6287
90	W	0.0421	-2.9709	-3.6287
91	W	-2.8787	2.1041	-1.8725
92	W	2.8787	-2.1041	1.8725
93	W	1.2263	6.3115	0.0000
94	W	-1.2263	-6.3115	0.0000
95	W	-1.8732	5.3885	-1.8609
96	W	1.8732	-5.3885	1.8609
97	W	3.0429	3.8866	-1.7320
98	W	-3.0429	-3.8866	1.7320

GD3bjFe4O_7_20

Energy (POTENTIAL) = -7000.47775661 Eh

Atom		X	Y	Z
1	Fe	0.0126	-0.0591	1.7636
2	Fe	0.0091	-0.0486	-1.7659
3	Fe	0.8234	-2.6998	-0.0006
4	Fe	-0.8518	2.5684	0.0057
5	H	0.3441	4.8255	0.7953
6	H	0.3430	4.8260	-0.7837
7	O	1.3492	-0.5402	-3.0008
8	O	-1.3184	0.4775	2.9918
9	O	-0.5720	-1.9335	1.3863
10	O	0.5559	1.8453	-1.3631
11	O	5.4275	2.3617	0.0028
12	O	-5.4916	-2.2991	-0.0063
13	O	2.2143	1.8668	-3.4737
14	O	-2.2648	-1.8963	3.4684
15	O	2.9180	-0.2226	-5.3262
16	O	-2.8938	0.1982	5.3184
17	O	3.1538	0.8357	-1.2801
18	O	-3.1736	-0.8630	1.2780
19	O	1.3193	-0.5553	0.0002
20	O	-1.3115	0.4617	0.0004
21	O	3.1529	0.8329	1.2846
22	O	-3.1738	-0.8540	-1.2856
23	O	3.8438	-1.2679	0.0013
24	O	-3.8014	1.2682	0.0041
25	O	2.3157	3.2187	0.0053
26	O	-2.3825	-3.2867	-0.0112
27	O	2.2138	1.8572	3.4808
28	O	-2.2675	-1.8749	-3.4838
29	O	3.8285	-1.5546	2.9904
30	O	-3.7528	1.5768	-2.9624
31	O	4.1103	-3.8972	-0.0029
32	O	-4.0117	3.9082	0.0111
33	O	6.1056	0.2215	-1.2853
34	O	-6.1092	-0.1506	1.2898
35	O	6.7497	2.6953	-2.4941
36	O	-6.8068	-2.6207	2.4987
37	O	4.6724	0.9982	-3.4051
38	O	-4.6954	-0.9544	3.3966

39	O	3.9935	3.1897	-2.0695
40	O	-4.0725	-3.1763	2.0682
41	O	1.3777	4.3506	2.3571
42	O	-1.5441	-4.3905	-2.4859
43	O	0.5561	1.8386	1.3697
44	O	-0.5757	-1.9219	-1.4005
45	O	3.9927	3.1838	2.0781
46	O	-4.0723	-3.1626	-2.0875
47	O	6.7494	2.6897	2.5001
48	O	-6.8076	-2.6046	-2.5128
49	O	6.1065	0.2182	1.2867
50	O	-6.1089	-0.1426	-1.2892
51	O	5.7750	-2.4209	1.3426
52	O	-5.7016	2.4840	-1.3350
53	O	8.0405	-1.4361	-0.0034
54	O	-7.9982	1.5413	0.0067
55	O	5.7715	-2.4169	-1.3478
56	O	-5.6993	2.4753	1.3511
57	O	4.1655	-4.3687	-2.7999
58	O	-4.0708	4.3816	2.8017
59	O	2.1161	-2.9624	-1.4843
60	O	-2.0291	2.9636	1.4481
61	O	-1.5489	-4.4087	2.4553
62	O	1.3789	4.3588	-2.3424
63	O	2.9171	-0.2343	5.3283
64	O	-2.8976	0.2305	-5.3203
65	O	4.6722	0.9904	3.4078
66	O	-4.6975	-0.9336	-3.4029
67	O	1.3509	-0.5513	3.0017
68	O	-1.3192	0.4974	-2.9959
69	O	2.1197	-2.9695	1.4868
70	O	-2.0319	2.9670	-1.4328
71	O	0.3186	-4.2244	-0.0049
72	O	-0.2093	4.6488	0.0062
73	O	4.1743	-4.3740	2.7951
74	O	-4.0728	4.3963	-2.7779
75	O	3.8235	-1.5482	-2.9896
76	O	-3.7486	1.5609	2.9719
77	P	2.8547	-0.0424	0.0012
78	P	-2.8612	0.0041	-0.0009
79	W	2.9886	0.0254	-3.6277
80	W	-2.9641	-0.0613	3.6218
81	W	3.9113	-3.0490	1.7294
82	W	-3.8557	3.0573	-1.7249
83	W	2.0953	2.8476	1.8783
84	W	-2.1433	-2.9021	-1.8773
85	W	5.3842	1.8723	1.8591
86	W	-5.4190	-1.8297	-1.8694
87	W	2.9893	0.0161	3.6302
88	W	-2.9658	-0.0390	-3.6252
89	W	2.0961	2.8538	-1.8690
90	W	-2.1450	-2.9154	1.8565
91	W	6.3361	-1.2266	-0.0013
92	W	-6.3037	1.2715	0.0047
93	W	5.3844	1.8767	-1.8547
94	W	-5.4193	-1.8412	1.8582
95	W	3.9079	-3.0449	-1.7317
96	W	-3.8529	3.0480	1.7421

GD3bjFe4OH_5_21

Energy (POTENTIAL) = -7000.66540052 Eh

	Atom	X	Y	Z
1	Fe	0.0883	0.5858	-1.6885
2	Fe	-0.0806	-0.6481	1.6053
3	Fe	-0.9293	-2.5374	-0.9313
4	Fe	0.8530	2.4134	0.9071
5	H	-0.2767	4.8436	0.8558
6	H	-0.6144	-4.2285	-2.4604
7	H	-0.3199	4.3406	2.3531
8	O	-1.4170	-1.4930	2.6166
9	O	1.4362	1.5072	-2.6503
10	O	0.6655	-1.2940	-2.0280
11	O	-0.5703	1.2809	1.8799
12	O	-5.4197	2.2056	0.6911
13	O	5.5377	-2.1624	-0.6655
14	O	-2.2545	0.6420	3.8660
15	O	2.4400	-0.5790	-3.8897
16	O	-2.9668	-1.9122	4.9511
17	O	3.0680	2.0380	-4.8799
18	O	-3.1742	0.3811	1.4436
19	O	3.2909	-0.3165	-1.4522
20	O	-1.3093	-0.5179	-0.1965
21	O	1.3566	0.4378	0.1556
22	O	-3.1072	1.2161	-0.9772
23	O	3.1978	-1.2395	0.9364
24	O	-3.8354	-1.1926	-0.4589
25	O	3.8470	1.2137	0.4894
26	O	-2.3013	3.0492	1.0200
27	O	2.3596	-3.1222	-1.1343
28	O	-2.1578	2.9042	-2.7064
29	O	2.1575	-2.9880	2.5340
30	O	-3.6534	-0.5321	-3.2822
31	O	3.6838	0.4222	3.3720
32	O	-4.0477	-3.6670	-1.2827
33	O	4.0569	3.6416	1.4157
34	O	-6.1471	-0.2117	1.2545
35	O	6.1864	0.2803	-1.1257
36	O	-6.7658	1.8021	3.1638
37	O	6.8879	-1.6264	-3.1334
38	O	-4.7153	-0.1275	3.5005
39	O	4.8549	0.2888	-3.4335
40	O	-4.0104	2.3700	2.9537
41	O	4.1607	-2.2790	-2.9405
42	O	-1.3450	4.8957	-0.8167
43	O	1.3844	-5.0477	0.7608
44	O	-0.5070	2.2075	-0.6903
45	O	0.4539	-2.3395	0.5354
46	O	-3.9613	3.6826	-0.9754
47	O	3.9763	-3.8116	0.8658
48	O	-6.6937	3.3460	-1.5941
49	O	6.6714	-3.4796	1.5452
50	O	-6.0621	0.6035	-1.2119
51	O	6.0690	-0.6423	1.2013
52	O	-5.7687	-1.8446	-2.1393
53	O	5.6999	1.7429	2.2077
54	O	-8.0543	-1.3133	-0.5159
55	O	8.0160	1.4713	0.6556
56	O	-5.7821	-2.7239	0.3807
57	O	5.7811	2.8501	-0.3103
58	O	-4.1961	-5.0191	1.2294
59	O	4.0843	5.1071	-1.0323
60	O	-2.1498	-3.2556	0.4651
61	O	2.0699	3.2921	-0.3004
62	O	1.5612	-3.2841	-3.8655
63	O	-1.3905	3.3523	3.6248
64	O	-2.8165	1.4805	-5.1378
65	O	2.7696	-1.6797	5.0333
66	O	-4.5967	2.0044	-2.9536
67	O	4.6297	-2.0963	2.8878
68	O	-1.2206	0.5111	-3.0326
69	O	1.2514	-0.5940	2.9307
70	O	-2.0014	-2.2954	-2.2398
71	O	2.0231	2.2883	2.3992
72	O	-0.3295	-4.0860	-1.5406
73	O	0.2370	4.3816	1.5487
74	O	-4.1403	-3.1948	-4.0184
75	O	4.0545	3.1303	4.1891
76	O	-3.9094	-2.4082	2.3154
77	O	3.8653	2.5066	-2.1805
78	P	-2.8520	-0.0270	-0.0458
79	P	2.9207	0.0207	0.0340
80	W	-3.0366	-1.1268	3.4319
81	W	3.0915	1.2113	-3.3812
82	W	-3.9987	-2.2924	-2.5719
83	W	3.8397	2.2600	2.7312
84	W	-2.0522	3.3225	-0.8657
85	W	2.0076	-3.4595	0.7238
86	W	-5.3329	2.3775	-1.2297
87	W	5.2945	-2.5412	1.1642
88	W	-2.8750	1.2035	-3.4491
89	W	2.8897	-1.2897	3.3702
90	W	-2.1138	2.1047	2.6759
91	W	2.1714	-2.1166	-2.7719
92	W	-6.3613	-1.1073	-0.4003
93	W	6.3265	1.2703	0.4824
94	W	-5.3992	1.2170	2.3211
95	W	5.4839	-1.0926	-2.3168
96	W	-3.9398	-3.4157	0.6801
97	W	3.8720	3.4849	-0.5310

GD3bjFe4OH_6_20

Energy (POTENTIAL) = -7000.90322949 Eh

	Atom	X	Y	Z
1	Fe	0.0712	0.7063	-1.5469
2	Fe	-0.0749	-0.6904	1.6902
3	Fe	0.8258	2.4579	1.0330
4	Fe	-0.8507	-2.3802	-0.9948
5	H	0.3599	-4.2335	-2.5152
6	H	-0.0929	4.5612	0.9045
7	H	0.3251	-4.8106	-1.0463
8	O	1.2509	-0.6749	3.0298
9	O	-1.2400	0.7344	-2.8631
10	O	-0.4431	2.3627	-0.3708
11	O	0.5381	-2.2598	0.5962
12	O	5.4464	-2.1558	-0.8004
13	O	-5.4695	2.1536	0.8519
14	O	2.2094	-3.0294	2.5780
15	O	-2.0749	3.1362	-2.3220
16	O	2.8829	-1.6987	5.0713
17	O	-2.7153	1.9712	-4.9145
18	O	3.1113	-1.2736	0.9299
19	O	-3.1674	1.2559	-0.8553
20	O	1.3031	0.4793	0.2242
21	O	-1.3042	-0.4440	-0.1520
22	O	3.1764	-0.3343	-1.4527
23	O	-3.2044	0.2530	1.5064
24	O	3.8182	1.1671	0.5088
25	O	-3.7916	-1.1862	-0.5341
26	O	2.3373	-3.0124	-1.1474
27	O	-2.3228	3.0199	1.3447
28	O	2.2426	-0.4862	-3.8943
29	O	-2.3802	0.3027	3.9630
30	O	3.8797	2.5002	-2.2407
31	O	-3.8416	-2.6279	2.0533
32	O	3.9957	3.6281	1.4026
33	O	-4.0124	-3.5685	-1.6168
34	O	6.0647	-0.6236	1.1732
35	O	-6.0648	0.7216	-1.2384
36	O	6.7404	-3.3723	1.4286
37	O	-6.7139	3.4664	-1.3275
38	O	4.6385	-2.1194	2.8551
39	O	-4.5417	2.3310	-2.7600
40	O	4.0073	-3.7116	0.8073
41	O	-3.9689	3.8001	-0.6130
42	O	1.4039	-3.2086	-3.7503
43	O	-1.5767	2.9876	4.0726
44	O	0.5865	-1.2146	-1.9183
45	O	-0.6271	1.1473	2.1215
46	O	4.0216	-2.2267	-3.0539
47	O	-4.1146	2.0758	3.1346

48	O	6.7743	-1.6192	-3.2544
49	O	-6.8621	1.4334	3.2337
50	O	6.1288	0.2941	-1.2520
51	O	-6.1284	-0.3207	1.1201
52	O	5.7460	2.7597	-0.2966
53	O	-5.7410	-2.7789	0.1339
54	O	8.0230	1.3557	0.5740
55	O	-7.9863	-1.3413	-0.7682
56	O	5.7139	1.7877	2.1902
57	O	-5.6503	-1.6699	-2.3164
58	O	4.0546	3.0548	4.1183
59	O	-3.9878	-2.8842	-4.3582
60	O	1.9709	2.1904	2.3129
61	O	-1.9879	-2.1336	-2.4957
62	O	-1.3832	5.1136	-0.3215
63	O	1.4025	-4.9436	0.6121
64	O	2.9085	2.1165	-4.8766
65	O	-3.0503	-2.3476	4.7792
66	O	4.6982	0.2903	-3.5118
67	O	-4.8016	-0.4926	3.4265
68	O	1.4020	1.5952	-2.5413
69	O	-1.4067	-1.6876	2.5810
70	O	2.0953	3.2636	-0.3708
71	O	-2.0717	-3.3088	0.1360
72	O	0.3663	4.0626	1.6162
73	O	-0.2005	-4.3304	-1.7174
74	O	4.1280	5.0626	-1.0678
75	O	-4.1474	-5.1356	0.7514
76	O	3.6668	0.3974	3.3017
77	O	-3.6663	-0.2175	-3.3866
78	P	2.8452	0.0088	0.0523
79	P	-2.8641	-0.0293	-0.0059
80	W	2.9190	-1.3448	3.3934
81	W	-2.8699	1.4871	-3.2761
82	W	3.8770	3.4390	-0.5636
83	W	-3.8983	-3.4897	0.3387
84	W	2.1186	-1.9913	-2.7514
85	W	-2.1729	1.8869	2.9009
86	W	5.4015	-1.0842	-2.3833
87	W	-5.4540	0.9615	2.3804
88	W	3.0028	1.2698	-3.3887
89	W	-3.0668	-1.4178	3.3380
90	W	2.0889	-3.3618	0.7269
91	W	-2.0920	3.5296	-0.4931
92	W	6.3295	1.1377	0.4466
93	W	-6.2946	-1.1247	-0.6106
94	W	5.3643	-2.4046	1.1086
95	W	-5.3650	2.4580	-1.0189
96	W	3.9147	2.2041	2.6377
97	W	-3.8063	-2.1046	-2.8422

GD3bjFe4OH_7_21

Energy (POTENTIAL) = -7001.15039421 Eh

	Atom	X	Y	Z
1	Fe	-0.0307	-0.0397	-1.7506
2	Fe	-0.0178	-0.0901	1.7545
3	Fe	-0.7900	-2.7667	-0.0243
4	Fe	0.8542	2.5661	0.0329
5	H	-0.3381	4.8377	-0.7204
6	H	0.1884	-4.7901	-0.9121
7	H	-0.3321	4.8148	0.8585
8	O	-1.3415	-0.5863	2.9978
9	O	1.3110	0.5101	-2.9772
10	O	0.5682	-1.9225	-1.3936
11	O	-0.5477	1.8275	1.3978
12	O	-5.4257	2.3762	0.0428
13	O	5.4877	-2.3058	-0.0350
14	O	-2.2051	1.8116	3.5116
15	O	2.2477	-1.8610	-3.4918
16	O	-2.9140	-0.3101	5.3249
17	O	2.8691	0.2632	-5.3164
18	O	-3.1479	0.8236	1.2997
19	O	3.1679	-0.8512	-1.2927
20	O	-1.3107	-0.5289	-0.0071
21	O	1.3121	0.4581	0.0079
22	O	-3.1542	0.8681	-1.2661
23	O	3.1742	-0.8779	1.2703
24	O	-3.8336	-1.2560	-0.0192
25	O	3.8025	1.2617	0.0084
26	O	-2.3108	3.2256	0.0561
27	O	2.3848	-3.2811	-0.0312
28	O	-2.2153	1.9300	-3.4461
29	O	2.2731	-1.9278	3.4579
30	O	-3.8292	-1.4858	-3.0217
31	O	3.7577	1.5366	2.9792
32	O	-4.1026	-3.8858	-0.0668
33	O	4.0186	3.9038	0.0337
34	O	-6.0967	0.2095	1.2930
35	O	6.1050	-0.1419	-1.3072
36	O	-6.7418	2.6599	2.5473
37	O	6.7959	-2.5970	-2.5475
38	O	-4.6648	0.9438	3.4260
39	O	4.6791	-0.9201	-3.4166
40	O	-3.9848	3.1596	2.1311
41	O	4.0597	-3.1571	-2.1151
42	O	-1.3777	4.4025	-2.2724
43	O	1.5580	-4.4314	2.4435
44	O	-0.5543	1.8699	-1.3415
45	O	0.5654	-1.9674	1.3727
46	O	-3.9917	3.2312	-2.0188
47	O	4.0749	-3.1981	2.0394
48	O	-6.7506	2.7469	-2.4457
49	O	6.8075	-2.6481	2.4671
50	O	-6.1049	0.2546	-1.2773
51	O	6.1095	-0.1694	1.2734
52	O	-5.7651	-2.3831	-1.3812
53	O	5.7072	2.4569	1.3580
54	O	-8.0295	-1.4303	-0.0164
55	O	7.9996	1.5270	0.0006
56	O	-5.7599	-2.4301	1.3109
57	O	5.6996	2.4841	-1.3275
58	O	-4.1580	-4.4143	2.7164
59	O	4.0693	4.4101	-2.7517
60	O	-2.1020	-2.9919	1.4281
61	O	2.0331	2.9736	-1.4079
62	O	1.4967	-4.3824	-2.4543
63	O	-1.3685	4.3219	2.4230
64	O	-2.9226	-0.1228	-5.3334
65	O	2.8996	0.1617	5.3146
66	O	-4.6763	1.0648	-3.3900
67	O	4.7012	-0.9837	3.3812
68	O	-1.3553	-0.4887	-3.0096
69	O	1.3242	0.4433	2.9881
70	O	-2.1105	-2.9110	-1.5328
71	O	2.0398	2.9507	1.4714
72	O	-0.2840	-4.5303	-0.1033
73	O	0.2180	4.6496	0.0647
74	O	-4.1443	-4.3109	-2.8698
75	O	4.0883	4.3574	2.8264
76	O	-3.8109	-1.5971	2.9631
77	O	3.7455	1.5924	-2.9575
78	P	-2.8431	-0.0299	0.0011
79	P	2.8601	-0.0005	-0.0005
80	W	-2.9852	-0.0323	3.6310
81	W	2.9500	-0.0155	-3.6233
82	W	-3.8919	-2.9998	-1.7834
83	W	3.8644	3.0318	1.7579
84	W	-2.0950	2.8897	-1.8221
85	W	2.1396	-2.9333	1.8447
86	W	-5.3850	1.9167	-1.8215
87	W	5.4173	-1.8646	1.8372
88	W	-2.9937	0.0976	-3.6310
89	W	2.9694	-0.0870	3.6161
90	W	-2.0857	2.8248	1.9245
91	W	2.1389	-2.8839	-1.8901
92	W	-6.3250	-1.2193	-0.0170
93	W	6.3046	1.2601	0.0017
94	W	-5.3772	1.8542	1.8897
95	W	5.4120	-1.8243	-1.8920
96	W	-3.8965	-3.0706	1.6750
97	W	3.8544	3.0641	-1.7071

GD3bjFe4Or_6_21

Energy (POTENTIAL) = -7000.24055678 Eh

	Atom	X	Y	Z
1	Fe	-0.0073	-0.0690	1.7615
2	Fe	-0.0072	-0.0614	-1.7619
3	Fe	0.7982	-2.7064	-0.0057
4	Fe	-0.8643	2.5760	0.0053
5	H	0.3058	4.8556	0.7997
6	H	0.3061	4.8588	-0.7793
7	O	1.3512	-0.5380	-3.0161
8	O	-1.3092	0.4804	2.9835
9	O	-0.5519	-1.9429	1.3957
10	O	0.5727	1.8547	-1.3603
11	O	5.4305	2.2708	0.0051
12	O	-5.4771	-2.3027	-0.0052
13	O	2.2120	1.9001	-3.4925
14	O	-2.2507	-1.8929	3.4680
15	O	2.8599	-0.1508	-5.3698
16	O	-2.8841	0.1999	5.3185
17	O	3.1472	0.8211	-1.2824
18	O	-3.1606	-0.8643	1.2794
19	O	1.3136	-0.5619	-0.0011
20	O	-1.2988	0.4608	0.0008
21	O	3.1469	0.8156	1.2866
22	O	-3.1603	-0.8592	-1.2835
23	O	3.8255	-1.3024	-0.0023
24	O	-3.7905	1.2649	0.0024
25	O	2.3371	3.2383	0.0070
26	O	-2.3663	-3.2796	-0.0072
27	O	2.2116	1.8856	3.5009
28	O	-2.2503	-1.8780	-3.4764
29	O	3.8299	-1.5170	3.0455
30	O	-3.7390	1.5713	-2.9646
31	O	4.0503	-3.9184	-0.0078
32	O	-3.9983	3.9033	0.0080
33	O	6.0841	0.1489	-1.3044
34	O	-6.0970	-0.1513	1.2880
35	O	6.7499	2.6580	-2.4838
36	O	-6.8001	-2.6163	2.4970
37	O	4.6661	0.9945	-3.4162
38	O	-4.6830	-0.9566	3.3984
39	O	4.0027	3.1729	-2.0636
40	O	-4.0635	-3.1779	2.0722
41	O	1.3856	4.3642	2.3453
42	O	-1.5470	-4.4039	-2.4816
43	O	0.5725	1.8489	1.3683
44	O	-0.5517	-1.9369	-1.4039
45	O	4.0025	3.1644	2.0774
46	O	-4.0632	-3.1690	-2.0862
47	O	6.7495	2.6476	2.4959
48	O	-6.7996	-2.6056	-2.5090
49	O	6.0838	0.1434	1.3059
50	O	-6.0968	-0.1459	-1.2894
51	O	5.7440	-2.4992	1.3120
52	O	-5.6903	2.4806	-1.3387
53	O	8.0284	-1.4546	-0.0024
54	O	-7.9884	1.5403	0.0027
55	O	5.7442	-2.4937	-1.3216

56	O	-5.6904	2.4749	1.3482
57	O	4.1939	-4.2855	-2.8724
58	O	-4.0618	4.3817	2.7976
59	O	2.1614	-3.0003	-1.4587
60	O	-2.0211	2.9523	1.4486
61	O	-1.5476	-4.4146	2.4624
62	O	1.3862	4.3741	-2.3266
63	O	2.8593	-0.1731	5.3698
64	O	-2.8835	0.2225	-5.3180
65	O	4.6656	0.9803	3.4211
66	O	-4.6825	-0.9421	-3.4032
67	O	1.3506	-0.5503	3.0146
68	O	-1.3086	0.4930	-2.9821
69	O	2.1611	-3.0062	1.4467
70	O	-2.0210	2.9581	-1.4366
71	O	0.2936	-4.2292	-0.0088
72	O	-0.2302	4.6407	0.0097
73	O	4.1933	-4.2973	2.8552
74	O	-4.0614	4.3937	-2.7795
75	O	3.8304	-1.5044	-3.0512
76	O	-3.7393	1.5586	2.9706
77	P	2.8482	-0.0559	0.0002
78	P	-2.8537	0.0006	-0.0003
79	W	2.9360	0.0976	-3.6764
80	W	-2.9625	-0.0608	3.6251
81	W	3.9280	-2.9461	1.8301
82	W	-3.8493	3.0554	-1.7284
83	W	2.0886	2.8617	1.8650
84	W	-2.1467	-2.9159	-1.8796
85	W	5.3699	1.8474	1.8764
86	W	-5.4139	-1.8311	-1.8655
87	W	2.9355	0.0823	3.6774
88	W	-2.9622	-0.0451	-3.6258
89	W	2.0890	2.8695	-1.8525
90	W	-2.1471	-2.9241	1.8666
91	W	6.3331	-1.2191	-0.0020
92	W	-6.2961	1.2719	0.0022
93	W	5.3703	1.8551	-1.8679
94	W	-5.4143	-1.8390	1.8570
95	W	3.9285	-2.9385	-1.8418
96	W	-3.8494	3.0478	1.7410

GD3bjFeOHFe2FeOH_8_21

Energy (POTENTIAL) = -7000.67879620 Eh

Atom	X	Y	Z
1 Fe	0.0130	0.1356	1.7302
2 Fe	-0.0130	-0.1356	-1.7302
3 Fe	0.7666	-2.7291	0.1972
4 Fe	-0.7666	2.7291	-0.1974
5 H	-0.2058	-4.6860	1.2138
6 H	0.2056	4.6858	-1.2144
7 O	1.3234	-0.7358	-2.9396
8 O	-1.3234	0.7358	2.9396
9 O	-0.5658	-1.7885	1.5154
10 O	0.5659	1.7885	-1.5154
11 O	5.4738	2.3183	-0.1945
12 O	-5.4738	-2.3182	0.1946
13 O	2.2380	1.5985	-3.6132
14 O	-2.2380	-1.5985	3.6133
15 O	2.8887	-0.6468	-5.2871
16 O	-2.8887	0.6469	5.2872
17 O	3.1652	0.7418	-1.3461
18 O	-3.1652	-0.7418	1.3462
19 O	1.3099	-0.4989	0.0408
20 O	-1.3099	0.4989	-0.0408
21 O	3.1762	0.9420	1.2078
22 O	-3.1763	-0.9420	-1.2077
23 O	3.8223	-1.2674	0.0939
24 O	-3.8223	1.2674	-0.0938
25 O	2.3707	3.2487	-0.2573
26 O	-2.3708	-3.2487	0.2574
27 O	2.2691	2.1430	3.3218
28 O	-2.2691	-2.1430	-3.3217
29 O	3.8101	-1.3102	3.1050
30 O	-3.8101	1.3101	-3.1051
31 O	4.0576	-3.8941	0.3059
32 O	-4.0575	3.8941	-0.3059
33 O	6.1078	0.0724	-1.3139
34 O	-6.1078	-0.0723	1.3140
35 O	6.7823	2.4361	-2.7154
36 O	-6.7823	-2.4360	2.7155
37 O	4.6779	0.6960	-3.4786
38 O	-4.6779	-0.6960	3.4786
39 O	4.0402	3.0036	-2.3251
40 O	-4.0402	-3.0035	2.3252
41 O	1.5410	4.5604	2.1265
42 O	-1.5410	-4.5604	-2.1264
43 O	0.5716	2.0092	1.2407
44 O	-0.5716	-2.0092	-1.2406
45 O	4.0600	3.3252	1.8121
46 O	-4.0601	-3.3252	-1.8120
47 O	6.8007	2.8280	2.2713
48 O	-6.8007	-2.8280	-2.2712
49 O	6.1227	0.2784	1.2524
50 O	-6.1227	-0.2784	-1.2523
51 O	5.7437	-2.3377	1.5219
52 O	-5.7438	2.3378	-1.5219
53 O	8.0192	-1.5026	0.0966
54 O	-8.0192	1.5026	-0.0965
55 O	5.7314	-2.5525	-1.1610
56 O	-5.7313	2.5526	1.1610
57 O	4.1053	-4.5923	-2.4434
58 O	-4.1052	4.5924	2.4433
59 O	2.0668	-3.0751	-1.2416
60 O	-2.0667	3.0751	1.2415
61 O	-1.4670	-4.1758	2.7478
62 O	1.4670	4.1758	-2.7478
63 O	2.9144	0.2039	5.3262
64 O	-2.9145	-0.2040	-5.3261
65 O	4.7083	1.2312	3.3144
66 O	-4.7083	-1.2312	-3.3143
67 O	1.3424	-0.2692	3.0249
68 O	-1.3424	0.2692	-3.0249
69 O	2.0851	-2.8038	1.7104
70 O	-2.0852	2.8037	-1.7104
71 O	0.2746	-4.4951	0.3905
72 O	-0.2748	4.4951	-0.3910
73 O	4.1054	-4.1376	3.1345
74 O	-4.1054	4.1376	-3.1346
75 O	3.7837	-1.7911	-2.8540
76 O	-3.7836	1.7912	2.8540
77 P	2.8487	-0.0283	0.0014
78 P	-2.8487	0.0283	-0.0013
79 W	2.9689	-0.2569	-3.6130
80 W	-2.9689	0.2569	3.6130
81 W	3.8643	-2.8925	1.9673
82 W	-3.8644	2.8925	-1.9673
83 W	2.1353	3.0263	1.6343
84 W	-2.1353	-3.0263	-1.6343
85 W	5.4159	1.9842	1.7026
86 W	-5.4159	-1.9842	-1.7025
87 W	2.9851	0.3266	3.6111
88 W	-2.9852	-0.3266	-3.6110
89 W	2.1254	2.7198	-2.0886
90 W	-2.1254	-2.7198	2.0887
91 W	6.3163	-1.2626	0.0860
92 W	-6.3163	1.2626	-0.0860
93 W	5.4042	1.6942	-2.0062
94 W	-5.4042	-1.6942	2.0062
95 W	3.8597	-3.1849	-1.4814
96 W	-3.8596	3.1849	1.4814

GD3Fe4H2O_5_20

Energy (POTENTIAL) = -7001.07542931 Eh

Atom	X	Y	Z
1 Fe	-0.0400	0.0403	1.7531
2 Fe	-0.0542	0.0555	-1.7810
3 Fe	2.5823	0.7881	0.0327
4 Fe	-2.6296	-0.8061	-0.0379
5 H	-4.9357	0.2967	0.7711
6 H	5.0320	-0.2019	-0.8109
7 H	5.0333	-0.3160	0.7437
8 H	-4.9429	0.3193	-0.8012
9 O	0.4511	1.3243	-3.0185
10 O	-0.5142	-1.3372	2.9784
11 O	1.9123	-0.5305	1.3339
12 O	-1.9602	0.5613	-1.4054
13 O	-2.3214	5.4912	0.0014
14 O	2.2980	-5.4657	-0.0349
15 O	-1.9194	2.2656	-3.4880
16 O	1.8965	-2.2404	3.4358
17 O	0.1974	2.9405	-5.3279
18 O	-0.2218	-2.8891	5.2960
19 O	-0.8809	3.1840	-1.2928
20 O	0.8551	-3.1677	1.2788
21 O	0.3877	1.2928	-0.0105
22 O	-0.5167	-1.3268	-0.0115
23 O	-0.8780	3.1748	1.2874
24 O	0.8620	-3.1641	-1.2857
25 O	1.2501	3.7744	-0.0027
26 O	-1.2699	-3.8388	0.0238
27 O	-3.2689	2.3652	-0.0111
28 O	3.2680	-2.3203	-0.0296
29 O	-1.9219	2.2402	3.4749
30 O	1.8894	-2.2205	-3.4559
31 O	1.5520	3.7014	2.9659
32 O	-1.5549	-3.7954	-2.9527
33 O	3.9138	3.9803	0.0155
34 O	-3.8949	-4.1022	0.0098
35 O	-0.1520	6.0969	-1.2858
36 O	0.1790	-6.1066	1.2884
37 O	-2.6140	6.8304	-2.4920
38 O	2.6707	-6.7615	2.5004
39 O	-0.9685	4.7065	-3.4105
40 O	0.9869	-4.6902	3.3978
41 O	-3.1975	4.0821	-2.0830
42 O	3.2018	-4.0419	2.0171
43 O	-4.4385	1.4811	2.3526
44 O	4.3888	-1.3384	-2.4072
45 O	-1.9510	0.5593	1.3713
46 O	1.9098	-0.4956	-1.3452
47 O	-3.1914	4.0626	2.0746
48 O	3.2842	-3.9792	-2.1109
49 O	-2.6092	6.8108	2.5121
50 O	2.7787	-6.7040	-2.5306
51 O	-0.1550	6.0816	1.2891
52 O	0.2300	-6.0847	-1.2252
53 O	2.4766	5.6507	1.3655
54 O	-2.3632	-5.7642	-1.3336
55 O	1.5801	7.9545	0.0091
56 O	-1.5282	-8.0267	0.1064
57 O	2.4860	5.6532	-1.3334
58 O	-2.5190	-5.7613	1.4099
59 O	4.3762	3.9906	-2.7877
60 O	-4.4065	-4.0366	2.8062
61 O	2.9914	1.9729	-1.3811
62 O	-3.0046	-2.0441	1.4206
63 O	4.4042	-1.4483	2.3623
64 O	-4.4432	1.5071	-2.3813
65 O	0.1784	2.8953	5.3273

66	O	-0.2118	-2.9284	-5.2938
67	O	-0.9693	4.6837	3.4151
68	O	0.9767	-4.7082	-3.3614
69	O	0.4568	1.3090	3.0000
70	O	-0.5167	-1.3404	-2.9934
71	O	2.9426	1.9665	1.3885
72	O	-2.9907	-2.0874	-1.4323
73	O	4.8035	0.2749	0.0059
74	O	-4.6962	-0.2202	-0.0238
75	O	4.3735	3.9867	2.7975
76	O	-4.3599	-4.1728	-2.7675
77	O	1.5549	3.7161	-2.9521
78	O	-1.5627	-3.7866	2.9533
79	P	-0.0263	2.8505	-0.0045
80	P	-0.0212	-2.8686	-0.0035
81	W	-0.0688	3.0057	-3.6374
82	W	0.0272	-2.9614	3.6045
83	W	3.0469	3.8043	1.7308
84	W	-3.0417	-3.9041	-1.7103
85	W	-2.9246	2.1563	1.8730
86	W	2.9020	-2.0301	-1.8904
87	W	-1.8420	5.4255	1.8644
88	W	2.0138	-5.3136	-1.8989
89	W	-0.0762	2.9754	3.6358
90	W	0.0235	-2.9748	-3.5989
91	W	-2.9314	2.1806	-1.8945
92	W	2.9010	-2.1078	1.8500
93	W	1.2940	6.2673	0.0006
94	W	-1.3188	-6.3302	0.1311
95	W	-1.8444	5.4427	-1.8536
96	W	1.8713	-5.3835	1.8847
97	W	3.0555	3.7823	-1.7150
98	W	-3.0769	-3.8349	1.7488

GD3Fe4H2O_6_21freq

Energy (POTENTIAL) = -7001.34847730 Eh

	Atom	X	Y	Z
1	Fe	0.0000	0.0000	1.7956
2	Fe	0.0000	0.0000	-1.7956
3	Fe	2.5969	0.8592	0.0000
4	Fe	-2.5969	-0.8592	0.0000
5	H	-4.8882	0.2987	0.7861
6	H	4.8882	-0.2987	-0.7861
7	H	4.8882	-0.2987	0.7861
8	H	-4.8882	0.2987	-0.7861
9	O	0.5060	1.3408	-3.0096
10	O	-0.5060	-1.3408	3.0096
11	O	1.8976	-0.5568	1.3788
12	O	-1.8976	0.5568	-1.3788
13	O	-2.3363	5.4617	0.0000
14	O	2.3363	-5.4617	0.0000
15	O	-1.8890	2.2406	-3.4815
16	O	1.8890	-2.2406	3.4815
17	O	0.2136	2.9278	-5.3249
18	O	-0.2136	-2.9278	5.3249
19	O	-0.8488	3.1738	-1.2872
20	O	0.8488	-3.1738	1.2872
21	O	0.4995	1.3204	0.0000
22	O	-0.4995	-1.3204	0.0000
23	O	-0.8488	3.1738	1.2872
24	O	0.8488	-3.1738	-1.2872
25	O	1.2675	3.8286	0.0000
26	O	-1.2675	-3.8286	0.0000
27	O	-3.2462	2.3423	0.0000
28	O	3.2462	-2.3423	0.0000
29	O	-1.8890	2.2406	3.4815
30	O	1.8890	-2.2406	-3.4815
31	O	1.5597	3.7823	2.9697
32	O	-1.5597	-3.7823	-2.9697
33	O	3.9104	4.0642	0.0000
34	O	-3.9104	-4.0642	0.0000
35	O	-0.1863	6.1067	-1.2902
36	O	0.1863	-6.1067	1.2902
37	O	-2.6626	6.7831	-2.5005
38	O	2.6626	-6.7831	2.5005
39	O	-0.9781	4.6922	-3.4090
40	O	0.9781	-4.6922	3.4090
41	O	-3.1905	4.0334	-2.0771
42	O	3.1905	-4.0334	2.0771
43	O	-4.3944	1.4329	2.3644
44	O	4.3944	-1.4329	-2.3644
45	O	-1.8976	0.5568	1.3788
46	O	1.8976	-0.5568	-1.3788
47	O	-3.1905	4.0334	2.0771
48	O	3.1905	-4.0334	-2.0771
49	O	-2.6626	6.7831	2.5005
50	O	2.6626	-6.7831	-2.5005
51	O	-0.1863	6.1067	1.2902
52	O	0.1863	-6.1067	-1.2902
53	O	2.4527	5.7366	1.3453
54	O	-2.4527	-5.7366	-1.3453
55	O	1.4860	8.0201	0.0000
56	O	-1.4860	-8.0201	0.0000
57	O	2.4527	5.7366	-1.3453
58	O	-2.4527	-5.7366	1.3453
59	O	4.3814	4.1170	-2.7882
60	O	-4.3814	-4.1170	2.7882
61	O	2.9717	2.0679	-1.4328
62	O	-2.9717	-2.0679	1.4328
63	O	4.3944	-1.4329	2.3644
64	O	-4.3944	1.4329	-2.3644
65	O	0.2136	2.9278	5.3249
66	O	-0.2136	-2.9278	-5.3249
67	O	-0.9781	4.6922	3.4090
68	O	0.9781	-4.6922	-3.4090
69	O	0.5060	1.3408	3.0096
70	O	-0.5060	-1.3408	-3.0096
71	O	2.9717	2.0679	1.4328
72	O	-2.9717	-2.0679	-1.4328
73	O	4.6636	0.2382	0.0000
74	O	-4.6636	-0.2382	0.0000
75	O	4.3814	4.1170	2.7882
76	O	-4.3814	-4.1170	-2.7882
77	O	1.5597	3.7823	-2.9697
78	O	-1.5597	-3.7823	2.9697
79	P	0.0173	2.8665	0.0000
80	P	-0.0173	-2.8665	0.0000
81	W	-0.0437	2.9924	-3.6304
82	W	0.0437	-2.9924	3.6304
83	W	3.0512	3.8921	1.7293
84	W	-3.0512	-3.8921	-1.7293
85	W	-2.8863	2.1233	1.8785
86	W	2.8863	-2.1233	-1.8785
87	W	-1.8663	5.4072	1.8624
88	W	1.8663	-5.4072	-1.8624
89	W	-0.0437	2.9924	3.6304
90	W	0.0437	-2.9924	-3.6304
91	W	-2.8863	2.1233	-1.8785
92	W	2.8863	-2.1233	1.8785
93	W	1.2429	6.3237	0.0000
94	W	-1.2429	-6.3237	0.0000
95	W	-1.8663	5.4072	-1.8624
96	W	1.8663	-5.4072	1.8624
97	W	3.0512	3.8921	-1.7293
98	W	-3.0512	-3.8921	1.7293

GD3Fe4H2O_6_21

Energy (POTENTIAL) = -7001.34847730 Eh

	Atom	X	Y	Z
1	Fe	0.0000	0.0000	1.7956
2	Fe	0.0000	0.0000	-1.7956
3	Fe	2.5958	0.8624	0.0000
4	Fe	-2.5958	-0.8624	0.0000
5	H	-4.8885	0.2927	0.7861
6	H	4.8885	-0.2927	-0.7861
7	H	4.8885	-0.2927	0.7861
8	H	-4.8885	0.2927	-0.7861
9	O	0.5043	1.3414	-3.0096
10	O	-0.5043	-1.3414	3.0096
11	O	1.8983	-0.5544	1.3788
12	O	-1.8983	0.5544	-1.3788
13	O	-2.3430	5.4588	0.0000
14	O	2.3430	-5.4588	0.0000
15	O	-1.8917	2.2383	-3.4815
16	O	1.8917	-2.2383	3.4815
17	O	0.2099	2.9281	-5.3249
18	O	-0.2099	-2.9281	5.3249
19	O	-0.8528	3.1727	-1.2872
20	O	0.8528	-3.1727	1.2872
21	O	0.4978	1.3210	0.0000
22	O	-0.4978	-1.3210	0.0000
23	O	-0.8528	3.1727	1.2872
24	O	0.8528	-3.1727	-1.2872
25	O	1.2628	3.8302	0.0000
26	O	-1.2628	-3.8302	0.0000
27	O	-3.2492	2.3383	0.0000
28	O	3.2492	-2.3383	0.0000
29	O	-1.8917	2.2383	3.4815
30	O	1.8917	-2.2383	-3.4815
31	O	1.5550	3.7842	2.9697
32	O	-1.5550	-3.7842	-2.9697
33	O	3.9053	4.0690	0.0000
34	O	-3.9053	-4.0690	0.0000
35	O	-0.1938	6.1065	-1.2902
36	O	0.1938	-6.1065	1.2902
37	O	-2.6710	6.7798	-2.5005
38	O	2.6710	-6.7798	2.5005
39	O	-0.9839	4.6910	-3.4090
40	O	0.9839	-4.6910	3.4090
41	O	-3.1955	4.0294	-2.0771
42	O	3.1955	-4.0294	2.0771
43	O	-4.3962	1.4274	2.3644
44	O	4.3962	-1.4274	-2.3644
45	O	-1.8983	0.5544	1.3788
46	O	1.8983	-0.5544	-1.3788
47	O	-3.1955	4.0294	2.0771
48	O	3.1955	-4.0294	-2.0771
49	O	-2.6710	6.7798	2.5005
50	O	2.6710	-6.7798	-2.5005
51	O	-0.1938	6.1065	1.2902
52	O	0.1938	-6.1065	-1.2902
53	O	2.4455	5.7396	1.3453
54	O	-2.4455	-5.7396	-1.3453
55	O	1.4761	8.0219	0.0000
56	O	-1.4761	-8.0219	0.0000
57	O	2.4455	5.7396	-1.3453
58	O	-2.4455	-5.7396	1.3453
59	O	4.3763	4.1225	-2.7882
60	O	-4.3763	-4.1225	2.7882
61	O	2.9691	2.0716	-1.4328
62	O	-2.9691	-2.0716	1.4328
63	O	4.3962	-1.4274	2.3644
64	O	-4.3962	1.4274	-2.3644
65	O	0.2099	2.9281	5.3249
66	O	-0.2099	-2.9281	-5.3249
67	O	-0.9839	4.6910	3.4090
68	O	0.9839	-4.6910	-3.4090
69	O	0.5043	1.3414	3.0096
70	O	-0.5043	-1.3414	-3.0096
71	O	2.9691	2.0716	1.4328

72	O	-2.9691	-2.0716	-1.4328
73	O	4.6633	0.2440	0.0000
74	O	-4.6633	-0.2440	0.0000
75	O	4.3763	4.1225	2.7882
76	O	-4.3763	-4.1225	-2.7882
77	O	1.5550	3.7842	-2.9697
78	O	-1.5550	-3.7842	2.9697
79	P	0.0138	2.8666	0.0000
80	P	-0.0138	-2.8666	0.0000
81	W	-0.0475	2.9924	-3.6304
82	W	0.0475	-2.9924	3.6304
83	W	3.0464	3.8959	1.7293
84	W	-3.0464	-3.8959	-1.7293
85	W	-2.8889	2.1197	1.8785
86	W	2.8889	-2.1197	-1.8785
87	W	-1.8730	5.4049	1.8624
88	W	1.8730	-5.4049	-1.8624
89	W	-0.0475	2.9924	3.6304
90	W	0.0475	-2.9924	-3.6304
91	W	-2.8889	2.1197	-1.8785
92	W	2.8889	-2.1197	1.8785
93	W	1.2350	6.3252	0.0000
94	W	-1.2350	-6.3252	0.0000
95	W	-1.8730	5.4049	-1.8624
96	W	1.8730	-5.4049	1.8624
97	W	3.0464	3.8959	-1.7293
98	W	-3.0464	-3.8959	1.7293

GD3Fe4O_7_20freq

Energy (POTENTIAL) = -7000.21030068 Eh

Atom		X	Y	Z
1	Fe	-0.0125	-0.0955	-1.7916
2	Fe	-0.0085	-0.0224	1.7962
3	Fe	-0.8135	-2.6930	0.0499
4	Fe	0.8471	2.5534	-0.0509
5	H	-0.3055	4.8352	-0.8786
6	H	-0.3036	4.8643	0.6939
7	O	-1.3601	-0.4823	3.0236
8	O	1.3317	0.4115	-3.0124
9	O	0.5753	-1.9702	-1.3595
10	O	-0.5548	1.8750	1.3398
11	O	-5.4374	2.3665	-0.0437
12	O	5.5051	-2.3091	0.0457
13	O	-2.2265	1.9348	3.4458
14	O	2.2800	-1.9706	-3.4400
15	O	-2.9441	-0.1208	5.3327
16	O	2.9219	0.0943	-5.3240
17	O	-3.1706	0.8540	1.2694
18	O	3.1958	-0.8851	-1.2673
19	O	-1.3285	-0.5652	0.0098
20	O	1.3255	0.4635	-0.0092
21	O	-3.1710	0.8055	-1.3011
22	O	3.1963	-0.8316	1.3030
23	O	-3.8644	-1.2725	0.0232
24	O	3.8242	1.2689	-0.0271
25	O	-2.3150	3.2254	-0.0617
26	O	2.3943	-3.2902	0.0678
27	O	-2.2280	1.8017	-3.5178
28	O	2.2836	-1.8271	3.5197
29	O	-3.8429	-1.6016	-2.9579
30	O	3.7695	1.6187	2.9316
31	O	-4.1301	-3.9057	0.0741
32	O	4.0320	3.9125	-0.0808
33	O	-6.1169	0.2472	1.2843
34	O	6.1217	-0.1797	-1.2892
35	O	-6.7616	2.7463	2.4447
36	O	6.8234	-2.6737	-2.4516
37	O	-4.6905	1.0669	3.3955
38	O	4.7160	-1.0264	-3.3886
39	O	-4.0035	3.2331	2.0134
40	O	4.0876	-3.2240	-2.0143
41	O	-1.3941	4.3159	-2.4471
42	O	1.5611	-4.3621	2.5611
43	O	-0.5561	1.8210	-1.4119
44	O	0.5786	-1.9107	1.4403
45	O	-4.0045	3.1536	-2.1336
46	O	4.0887	-3.1375	2.1431
47	O	-6.7634	2.6513	-2.5438
48	O	6.8256	-2.5698	2.5544
49	O	-6.1187	0.1980	-1.2908
50	O	6.1231	-0.1264	1.2917
51	O	-5.7954	-2.4462	-1.2999
52	O	5.7229	2.5051	1.2924
53	O	-8.0575	-1.4320	0.0304
54	O	8.0164	1.5348	-0.0355
55	O	-5.7928	-2.3943	1.3948
56	O	5.7203	2.4494	-1.3982
57	O	-4.1770	-4.3154	2.8812
58	O	4.0818	4.3254	-2.8811
59	O	-2.1320	-2.9336	1.5315
60	O	2.0456	2.9298	-1.4950
61	O	1.5631	-4.4665	-2.3777
62	O	-1.3926	4.4065	2.2793
63	O	-2.9452	-0.3221	-5.3247
64	O	2.9275	0.3124	5.3169
65	O	-4.6923	0.9374	-3.4318
66	O	4.7193	-0.8862	3.4261
67	O	-1.3629	-0.5998	-3.0035
68	O	1.3336	0.5368	2.9984
69	O	-2.1349	-2.9928	-1.4243
70	O	2.0485	2.9852	1.3752
71	O	-0.3278	-4.2245	0.0815
72	O	0.2402	4.6438	-0.0892
73	O	-4.1847	-4.4205	-2.7174
74	O	4.0856	4.4382	2.7014
75	O	-3.8381	-1.4888	3.0156
76	O	3.7648	1.4985	-2.9975
77	P	-2.8662	-0.0484	0.0007
78	P	2.8774	0.0043	-0.0000
79	W	-3.0088	0.0965	3.6299
80	W	2.9875	-0.1348	-3.6231
81	W	-3.9251	-3.0800	-1.6703
82	W	3.8706	3.0840	1.6674
83	W	-2.1066	2.8234	-1.9339
84	W	2.1589	-2.8820	1.9326
85	W	-5.3976	1.8431	-1.8924
86	W	5.4358	-1.8054	1.9012
87	W	-3.0110	-0.0416	-3.6312
88	W	2.9906	0.0142	3.6266
89	W	-2.1055	2.8955	1.8245
90	W	2.1585	-2.9605	-1.8119
91	W	-6.3523	-1.2292	0.0249
92	W	6.3210	1.2704	-0.0285
93	W	-5.3963	1.9140	1.8232
94	W	5.4347	-1.8826	-1.8282
95	W	-3.9221	-3.0144	1.7845
96	W	3.8676	3.0139	-1.7933

GD3Fe4O_7_20

Energy (POTENTIAL) = -7000.21030068 Eh

Atom		X	Y	Z
1	Fe	0.0142	-0.0620	1.7930
2	Fe	0.0112	-0.0523	-1.7955
3	Fe	0.8128	-2.6925	-0.0020
4	Fe	-0.8421	2.5567	0.0056
5	H	0.3129	4.8515	0.7932
6	H	0.3114	4.8528	-0.7796
7	O	1.3625	-0.5353	-3.0141
8	O	-1.3297	0.4680	3.0044
9	O	-0.5756	-1.9434	1.3940
10	O	0.5594	1.8523	-1.3725
11	O	5.4422	2.3628	0.0035
12	O	-5.5054	-2.3017	-0.0063
13	O	2.2317	1.8730	-3.4788
14	O	-2.2808	-1.9052	3.4737
15	O	2.9475	-0.2164	-5.3289
16	O	-2.9209	0.1934	5.3208
17	O	3.1741	0.8298	-1.2833
18	O	-3.1948	-0.8572	1.2820
19	O	1.3301	-0.5649	0.0006
20	O	-1.3228	0.4669	0.0007
21	O	3.1738	0.8268	1.2876
22	O	-3.1946	-0.8491	-1.2889
23	O	3.8653	-1.2751	0.0004
24	O	-3.8206	1.2752	0.0037
25	O	2.3208	3.2253	0.0054
26	O	-2.3956	-3.2864	-0.0102
27	O	2.2313	1.8630	3.4861
28	O	-2.2825	-1.8847	-3.4874
29	O	3.8426	-1.5514	2.9869
30	O	-3.7647	1.5726	-2.9608
31	O	4.1281	-3.9090	-0.0038
32	O	-4.0255	3.9196	0.0106
33	O	6.1198	0.2196	-1.2867
34	O	-6.1200	-0.1483	1.2906
35	O	6.7675	2.6971	-2.4909
36	O	-6.8248	-2.6206	2.4966
37	O	4.6948	1.0035	-3.4124
38	O	-4.7158	-0.9593	3.4050
39	O	4.0098	3.1945	-2.0691
40	O	-4.0894	-3.1816	2.0699
41	O	1.4005	4.3587	2.3709
42	O	-1.5630	-4.4031	-2.4840
43	O	0.5600	1.8469	1.3797
44	O	-0.5781	-1.9334	-1.4064
45	O	4.0097	3.1882	2.0787
46	O	-4.0893	-3.1686	-2.0883
47	O	6.7678	2.6903	2.4984
48	O	-6.8256	-2.6053	-2.5104
49	O	6.1208	0.2160	1.2889
50	O	-6.1207	-0.1407	-1.2909
51	O	5.7946	-2.4273	1.3446
52	O	-5.7176	2.4900	-1.3380
53	O	8.0582	-1.4393	-0.0028
54	O	-8.0125	1.5458	0.0063
55	O	5.7927	-2.4231	-1.3506
56	O	-5.7158	2.4818	1.3532
57	O	4.1753	-4.3684	-2.8033
58	O	-4.0755	4.3819	2.8031
59	O	2.1314	-2.9607	-1.4787
60	O	-2.0406	2.9598	1.4425
61	O	-1.5664	-4.4202	2.4559
62	O	1.4002	4.3659	-2.3564
63	O	2.9457	-0.2294	5.3304
64	O	-2.9236	0.2234	-5.3223
65	O	4.6947	0.9946	3.4160
66	O	-4.7172	-0.9396	-3.4112
67	O	1.3637	-0.5462	3.0141
68	O	-1.3300	0.4870	-3.0077
69	O	2.1334	-2.9677	1.4776
70	O	-2.0426	2.9645	-1.4283
71	O	0.3254	-4.2238	-0.0067
72	O	-0.2329	4.6468	0.0072
73	O	4.1814	-4.3745	2.7963
74	O	-4.0778	4.3961	-2.7805
75	O	3.8395	-1.5442	-2.9877
76	O	-3.7617	1.5572	2.9695
77	P	2.8684	-0.0497	0.0011
78	P	-2.8751	0.0093	-0.0008
79	W	3.0120	0.0309	-3.6301

80	W	-2.9863	-0.0656	3.6242
81	W	3.9235	-3.0524	1.7256
82	W	-3.8646	3.0601	-1.7226
83	W	2.1114	2.8567	1.8843
84	W	-2.1593	-2.9115	-1.8819
85	W	5.4014	1.8722	1.8610
86	W	-5.4351	-1.8309	-1.8704
87	W	3.0122	0.0212	3.6322
88	W	-2.9874	-0.0448	-3.6271
89	W	2.1113	2.8624	-1.8747
90	W	-2.1599	-2.9238	1.8634
91	W	6.3532	-1.2346	-0.0014
92	W	-6.3174	1.2795	0.0044
93	W	5.4011	1.8775	-1.8552
94	W	-5.4350	-1.8422	1.8598
95	W	3.9215	-3.0479	-1.7298
96	W	-3.8625	3.0512	1.7387

GD3Fe4OH_5_21

Energy (POTENTIAL) = -7000.39672139 Eh

	Atom	X	Y	Z
1	Fe	0.0958	0.6171	-1.7171
2	Fe	-0.0927	-0.6516	1.6445
3	Fe	-0.9217	-2.5197	-0.9248
4	Fe	0.8404	2.4088	0.9056
5	H	-0.2341	4.8767	0.8657
6	H	-0.4994	-4.1661	-2.4874
7	H	-0.2944	4.3759	2.3570
8	O	-1.4337	-1.4856	2.6453
9	O	1.4484	1.5211	-2.6738
10	O	0.6727	-1.2675	-2.0108
11	O	-0.5812	1.2911	1.9024
12	O	-5.4450	2.2070	0.6898
13	O	5.5386	-2.1887	-0.6753
14	O	-2.2850	0.6525	3.8803
15	O	2.4536	-0.5669	-3.9079
16	O	-3.0053	-1.9028	4.9609
17	O	3.1007	2.0333	-4.8940
18	O	-3.2014	0.3815	1.4508
19	O	3.2659	-0.3619	-1.4676
20	O	-1.3258	-0.5277	-0.1804
21	O	1.3556	0.4492	0.1540
22	O	-3.1304	1.2097	-0.9795
23	O	3.1981	-1.2444	0.9412
24	O	-3.8575	-1.1997	-0.4505
25	O	3.8559	1.2026	0.4663
26	O	-2.3169	3.0600	1.0277
27	O	2.3898	-3.0988	-1.1116
28	O	-2.1780	2.9130	-2.7037
29	O	2.1749	-3.0065	2.5475
30	O	-3.6677	-0.5305	-3.2826
31	O	3.7010	0.4142	3.3576
32	O	-4.0571	-3.6767	-1.2869
33	O	4.0686	3.6445	1.4073
34	O	-6.1638	-0.2174	1.2499
35	O	6.1888	0.2636	-1.1179
36	O	-6.7989	1.8027	3.1532
37	O	6.9059	-1.6383	-3.1287
38	O	-4.7502	-0.1269	3.5080
39	O	4.8751	0.2833	-3.4305
40	O	-4.0402	2.3745	2.9576
41	O	4.1774	-2.2844	-2.9593
42	O	-1.3811	4.9137	-0.8262
43	O	1.3996	-5.0539	0.7506
44	O	-0.5153	2.2257	-0.6876
45	O	0.4565	-2.3437	0.5495
46	O	-3.9855	3.6847	-0.9712
47	O	3.9910	-3.8310	0.8761
48	O	-6.7163	3.3402	-1.6011
49	O	6.6977	-3.5093	1.5304
50	O	-6.0778	0.5976	-1.2170
51	O	6.0915	-0.6572	1.1972
52	O	-5.7773	-1.8543	-2.1453
53	O	5.7140	1.7414	2.1992
54	O	-8.0677	-1.3257	-0.5242
55	O	8.0379	1.4681	0.6424
56	O	-5.8010	-2.7361	0.3817
57	O	5.8001	2.8486	-0.3165
58	O	-4.2063	-5.0192	1.2355
59	O	4.0930	5.0935	-1.0518
60	O	-2.1569	-3.2655	0.4569
61	O	2.0763	3.2874	-0.3009
62	O	1.5860	-3.2481	-3.8121
63	O	-1.4265	3.3630	3.6432
64	O	-2.8395	1.4837	-5.1351
65	O	2.8153	-1.6800	5.0347
66	O	-4.6188	2.0093	-2.9599
67	O	4.6573	-2.1087	2.8805
68	O	-1.2324	0.5235	-3.0377
69	O	1.2652	-0.6137	2.9434
70	O	-2.0066	-2.2873	-2.2318
71	O	2.0341	2.2759	2.3840
72	O	-0.3065	-4.0620	-1.5383
73	O	0.2580	4.3829	1.5502
74	O	-4.1382	-3.2026	-4.0218
75	O	4.0631	3.1159	4.1758
76	O	-3.9190	-2.4007	2.3103
77	O	3.8763	2.4864	-2.1786
78	P	-2.8695	-0.0319	-0.0398
79	P	2.9142	0.0098	0.0282
80	W	-3.0684	-1.1151	3.4428
81	W	3.1084	1.1996	-3.3995
82	W	-4.0035	-2.3004	-2.5751
83	W	3.8516	2.2566	2.7113
84	W	-2.0763	3.3368	-0.8649
85	W	2.0171	-3.4630	0.7363
86	W	-5.3545	2.3733	-1.2350
87	W	5.3188	-2.5700	1.1584
88	W	-2.8954	1.2074	-3.4463
89	W	2.9173	-1.2972	3.3689
90	W	-2.1397	2.1171	2.6879
91	W	2.2053	-2.0719	-2.7301
92	W	-6.3750	-1.1209	-0.4045
93	W	6.3470	1.2728	0.4781
94	W	-5.4263	1.2183	2.3197
95	W	5.4951	-1.1084	-2.3226
96	W	-3.9474	-3.4185	0.6793
97	W	3.8774	3.4750	-0.5393

GD3Fe4OH_6_20

Energy (POTENTIAL) = -7000.64683927 Eh

	Atom	X	Y	Z
1	Fe	-0.0949	-0.5356	-1.6638
2	Fe	0.0937	0.5100	1.7932
3	Fe	-0.8348	-2.5595	0.7310
4	Fe	0.8504	2.4684	-0.7045
5	H	-0.3111	4.4992	-2.0278
6	H	0.1145	-4.6433	0.3987
7	H	-0.2591	4.9075	-0.5091
8	O	-1.2543	0.3280	3.0932
9	O	1.2492	-0.4004	-2.9439
10	O	0.4630	-2.2734	-0.6489
11	O	-0.5318	2.1870	0.8606
12	O	-5.4596	2.2534	-0.5394
13	O	5.4850	-2.2446	0.5852
14	O	-2.2131	2.7173	2.9131
15	O	2.1141	-2.8248	-2.7030
16	O	-2.8987	1.1000	5.2312
17	O	2.7391	-1.3851	-5.1279
18	O	-3.1488	1.1302	1.0642
19	O	3.1422	-1.2131	-0.9775
20	O	-1.3287	-0.5268	0.1463
21	O	1.3206	0.4601	-0.0954
22	O	-3.2074	0.4858	-1.4235
23	O	3.2322	-0.4366	1.4724
24	O	-3.8534	-1.2417	0.3409
25	O	3.8234	1.1950	-0.4103
26	O	-2.3399	3.1311	-0.7947
27	O	2.3696	-3.1220	0.9832
28	O	-2.2836	0.9426	-3.8246
29	O	2.4092	-0.7708	3.9183
30	O	-3.9302	-2.2228	-2.5169
31	O	3.8720	2.3512	2.3392
32	O	-4.0510	-3.7778	0.9767
33	O	4.0346	3.7242	-1.1926
34	O	-6.0823	0.5004	1.2455
35	O	6.0795	-0.5682	-1.3148
36	O	-6.7465	3.2046	1.8171
37	O	6.7502	-3.2773	-1.7397
38	O	-4.6497	1.7916	3.0917
39	O	4.5747	-1.9777	-3.0241
40	O	-4.0116	3.6048	1.2328
41	O	4.0122	-3.6951	-1.0810
42	O	-1.4296	3.6275	-3.3706
43	O	1.5953	-3.4527	3.6987
44	O	-0.5987	1.4315	-1.7895
45	O	0.6426	-1.3873	1.9785
46	O	-4.0476	2.5805	-2.7767
47	O	4.1396	-2.4407	2.8766
48	O	-6.8079	2.0117	-3.0258
49	O	6.8899	-1.8257	3.0325
50	O	-6.1623	-0.1305	-1.2689
51	O	6.1533	0.1791	1.1536
52	O	-5.8022	-2.7046	-0.6083
53	O	5.7676	2.7350	0.4644
54	O	-8.0577	-1.3869	0.4334
55	O	8.0130	1.4147	-0.6048
56	O	-5.7459	-2.0189	1.9792
57	O	5.6767	1.9328	-2.1036
58	O	-4.0833	-3.5092	3.7420
59	O	4.0009	3.3495	-3.9992
60	O	-2.0033	-2.4534	2.0232
61	O	2.0070	2.4067	-2.2213
62	O	1.4511	-4.9343	-0.9373
63	O	-1.4116	4.8503	1.1872
64	O	-2.9923	-1.5220	-5.1031
65	O	3.1218	1.7748	5.0245
66	O	-4.7495	0.1335	-3.5246
67	O	4.8386	0.0725	3.4742
68	O	-1.4373	-1.2876	-2.7487
69	O	1.4344	1.3668	2.7947
70	O	-2.1560	-3.2188	-0.7584
71	O	2.0935	3.2399	0.5228
72	O	-0.3857	-4.2239	1.1335
73	O	0.2465	4.4738	-1.2237
74	O	-4.1964	-4.9167	-1.6422
75	O	4.1632	4.9957	1.3303
76	O	-3.6806	-0.7728	3.2257
77	O	3.6834	0.5963	-3.3236
78	P	-2.8725	-0.0363	0.0336
79	P	2.8723	0.0036	-0.0009
80	W	-2.9326	0.9477	3.5235
81	W	2.8800	-1.1194	-3.4399
82	W	-3.9303	-3.3628	-0.9587
83	W	3.9214	3.4116	0.7205
84	W	-2.1425	2.3062	-2.5147
85	W	2.1937	-2.2071	2.6835
86	W	-5.4320	1.3719	-2.2340
87	W	5.4794	-1.2489	2.2505
88	W	-3.0616	-0.8572	-3.5246

89	W	3.1176	1.0197	3.4849
90	W	-2.0941	3.2663	1.1128
91	W	2.1556	-3.3589	-0.8964
92	W	-6.3629	-1.1718	0.3204
93	W	6.3204	1.1860	-0.4739
94	W	-5.3747	2.2736	1.3883
95	W	5.3940	-2.3229	-1.3142
96	W	-3.9475	-2.5005	2.3641
97	W	3.8214	2.3973	-2.5848

GD3Fe4OH_7_21freq

Energy (POTENTIAL) = -7000.88386026 Eh

	Atom	X	Y	Z
1	Fe	0.0319	0.0016	-1.7728
2	Fe	0.0188	0.1437	1.7746
3	Fe	0.7822	2.7909	-0.0961
4	Fe	-0.8391	-2.5544	0.0997
5	H	0.3123	-4.8824	-0.5897
6	H	-0.2074	4.8235	-0.9982
7	H	0.3078	-4.8185	0.9818
8	O	1.3543	0.6621	2.9903
9	O	-1.3207	-0.5781	-2.9702
10	O	-0.5784	1.9019	-1.4567
11	O	0.5555	-1.7966	1.4548
12	O	5.4452	-2.3696	0.1041
13	O	-5.5109	2.2922	-0.0946
14	O	2.2258	-1.7219	3.5626
15	O	-2.2734	1.7728	-3.5465
16	O	2.9408	0.4498	5.3152
17	O	-2.8941	-0.4082	-5.3067
18	O	3.1721	-0.7804	1.3228
19	O	-3.1921	0.8060	-1.3170
20	O	1.3200	0.5322	-0.0217
21	O	-1.3210	-0.4618	0.0210
22	O	3.1779	-0.8931	-1.2463
23	O	-3.1978	0.9026	1.2504
24	O	3.8505	1.2684	-0.0542
25	O	-3.8176	-1.2750	0.0451
26	O	2.3208	-3.2290	0.1402
27	O	-2.4028	3.2824	-0.1193
28	O	2.2345	-2.0228	-3.3997
29	O	-2.2958	2.0286	3.4103
30	O	3.8394	1.4099	-3.0533
31	O	-3.7642	-1.4575	3.0186
32	O	4.1217	3.8997	-0.1687
33	O	-4.0206	-3.9205	0.1425
34	O	6.1113	-0.1669	1.2985
35	O	-6.1180	0.0881	-1.3079
36	O	6.7637	-2.5856	2.6142
37	O	-6.8242	2.5078	-2.6120
38	O	4.6889	-0.8517	3.4568
39	O	-4.7037	0.8206	-3.4461
40	O	4.0062	-3.1028	2.2128
41	O	-4.0898	3.0953	-2.1971
42	O	1.4031	-4.4665	-2.1707
43	O	-1.5906	4.5093	2.3240
44	O	0.5609	-1.9116	-1.3004
45	O	-0.5764	2.0172	1.3310
46	O	4.0117	-3.2830	-1.9351
47	O	-4.1018	3.2496	1.9540
48	O	6.7713	-2.8041	-2.3728
49	O	-6.8331	2.6972	2.3958
50	O	6.1186	-0.2792	-1.2740
51	O	-6.1221	0.1860	1.2738
52	O	5.7846	2.3585	-1.4466
53	O	-5.7156	-2.4400	1.4300
54	O	8.0464	1.4380	-0.0562
55	O	-8.0099	-1.5521	0.0477
56	O	5.7800	2.4751	1.2477
57	O	-5.7095	-2.5390	-1.2588
58	O	4.1739	4.4877	2.6025
59	O	-4.0651	-4.4920	-2.6303
60	O	2.1156	3.0402	1.3430
61	O	-2.0368	-3.0103	-1.3222
62	O	-1.5392	4.3280	-2.5801
63	O	1.3962	-4.2622	2.5495
64	O	2.9482	-0.0160	-5.3350
65	O	-2.9209	-0.0153	5.3197
66	O	4.6990	-1.1511	-3.3689
67	O	-4.7238	1.0698	3.3632
68	O	1.3678	0.4046	-3.0284
69	O	-1.3331	-0.3511	3.0078
70	O	2.1228	2.8909	-1.6028
71	O	-2.0410	-2.9089	1.5466
72	O	0.2883	4.5551	-0.2070
73	O	-0.2354	-4.6462	0.1865
74	O	4.1623	4.2395	-2.9845
75	O	-4.0777	-4.2861	2.9492
76	O	3.8239	1.6752	2.9141
77	O	-3.7540	-1.6756	-2.9085
78	P	2.8567	0.0389	-0.0007
79	P	-2.8741	-0.0086	0.0009
80	W	3.0070	0.1258	3.6293
81	W	-2.9719	-0.0837	-3.6216
82	W	3.9062	2.9622	-1.8595
83	W	-3.8628	-2.9924	1.8402
84	W	2.1124	-2.9428	-1.7516
85	W	-2.1640	2.9913	1.7696
86	W	5.4037	-1.9597	-1.7725
87	W	-5.4386	1.9022	1.7898
88	W	3.0158	-0.1942	-3.6277
89	W	-2.9885	0.1879	3.6152
90	W	2.1049	-2.7796	2.0029
91	W	-2.1658	2.8398	-1.9755
92	W	6.3414	1.2309	-0.0511
93	W	-6.3152	-1.2833	0.0413
94	W	5.3967	-1.7986	1.9390
95	W	-5.4352	1.7586	-1.9398
96	W	3.9122	3.1216	1.5907
97	W	-3.8574	-3.1207	-1.6175

GD3Fe4OH_7_21

Energy (POTENTIAL) = -7000.88386026 Eh

	Atom	X	Y	Z
1	Fe	-0.0326	-0.0478	-1.7732
2	Fe	-0.0184	-0.0965	1.7767
3	Fe	-0.7872	-2.7907	-0.0235
4	Fe	0.8436	2.5550	0.0312
5	H	-0.3039	4.8661	-0.7189
6	H	0.1985	-4.8481	-0.8721
7	H	-0.2990	4.8435	0.8537
8	O	-1.3544	-0.5804	3.0061
9	O	1.3206	0.4978	-2.9859
10	O	0.5745	-1.9402	-1.4074
11	O	-0.5519	1.8357	1.4062
12	O	-5.4410	2.3815	0.0424
13	O	5.5068	-2.3033	-0.0370
14	O	-2.2215	1.8193	3.5157
15	O	2.2689	-1.8691	-3.5004
16	O	-2.9397	-0.3042	5.3250
17	O	2.8929	0.2637	-5.3176
18	O	-3.1702	0.8210	1.3017
19	O	3.1902	-0.8456	-1.2974
20	O	-1.3209	-0.5299	-0.0084
21	O	1.3218	0.4602	0.0073
22	O	-3.1768	0.8660	-1.2694
23	O	3.1967	-0.8747	1.2716
24	O	-3.8528	-1.2622	-0.0206
25	O	3.8198	1.2693	0.0092
26	O	-2.3151	3.2360	0.0548
27	O	2.3970	-3.2883	-0.0348
28	O	-2.2322	1.9370	-3.4521
29	O	2.2935	-1.9418	3.4607
30	O	-3.8430	-1.4825	-3.0150
31	O	3.7679	1.5301	2.9769
32	O	-4.1286	-3.8951	-0.0658
33	O	4.0275	3.9162	0.0370
34	O	-6.1105	0.2122	1.2945
35	O	6.1173	-0.1330	-1.3082
36	O	-6.7582	2.6659	2.5464
37	O	6.8188	-2.5873	-2.5484
38	O	-4.6862	0.9510	3.4337
39	O	4.7010	-0.9190	-3.4259
40	O	-3.9999	3.1674	2.1306
41	O	4.0835	-3.1589	-2.1172
42	O	-1.3960	4.4107	-2.2881
43	O	1.5835	-4.4491	2.4403
44	O	-0.5580	1.8781	-1.3511
45	O	0.5733	-1.9821	1.3824
46	O	-4.0067	3.2384	-2.0206
47	O	4.0968	-3.2039	2.0364
48	O	-6.7672	2.7531	-2.4447
49	O	6.8292	-2.6449	2.4627
50	O	-6.1186	0.2568	-1.2800
51	O	6.1222	-0.1629	1.2752
52	O	-5.7892	-2.3851	-1.3833
53	O	5.7204	2.4671	1.3624
54	O	-8.0490	-1.4243	-0.0169
55	O	8.0127	1.5390	0.0032
56	O	-5.7839	-2.4308	1.3132
57	O	5.7135	2.4953	-1.3281
58	O	-4.1809	-4.4099	2.7200
59	O	4.0720	4.4144	-2.7499
60	O	-2.1205	-2.9997	1.4221
61	O	2.0416	2.9712	-1.4026
62	O	1.5306	-4.3967	-2.4669
63	O	-1.3877	4.3306	2.4358
64	O	-2.9501	-0.1188	-5.3337
65	O	2.9229	0.1505	5.3155
66	O	-4.6982	1.0707	-3.3976
67	O	4.7231	-0.9889	3.3876
68	O	-1.3696	-0.4813	-3.0173
69	O	1.3348	0.4281	2.9961
70	O	-2.1285	-2.9280	-1.5265
71	O	2.0467	2.9453	1.4678
72	O	-0.2964	-4.5581	-0.0881
73	O	0.2436	4.6494	0.0631
74	O	-4.1709	-4.3087	-2.8716
75	O	4.0863	4.3553	2.8330
76	O	-3.8258	-1.5908	2.9573
77	O	3.7559	1.5922	-2.9539
78	P	-2.8568	-0.0335	0.0001
79	P	2.8741	0.0039	-0.0013
80	W	-3.0059	-0.0246	3.6313
81	W	2.9707	-0.0165	-3.6246
82	W	-3.9121	-3.0028	-1.7807
83	W	3.8687	3.0333	1.7586
84	W	-2.1078	2.8998	-1.8288
85	W	2.1593	-2.9472	1.8460
86	W	-5.4009	1.9223	-1.8228
87	W	5.4359	-1.8637	1.8364
88	W	-3.0168	0.1044	-3.6316
89	W	2.9895	-0.0976	3.6168
90	W	-2.0992	2.8354	1.9287
91	W	2.1601	-2.8943	-1.9018
92	W	-6.3436	-1.2202	-0.0177
93	W	6.3174	1.2731	0.0044
94	W	-5.3928	1.8589	1.8917
95	W	5.4314	-1.8183	-1.8957
96	W	-3.9171	-3.0714	1.6725

97	W	3.8623	3.0706	-1.7013

GD3Fe4Or_6_21

Energy (POTENTIAL) = -6999.97655280 Eh

	Atom	X	Y	Z
1	Fe	0.0012	-0.0622	1.7813
2	Fe	0.0017	-0.0546	-1.7814
3	Fe	0.7921	-2.6979	-0.0058
4	Fe	-0.8752	2.5785	0.0054
5	H	0.2067	4.9354	0.7953
6	H	0.2067	4.9386	-0.7746
7	O	1.3620	-0.5275	-3.0203
8	O	-1.3179	0.4784	2.9857
9	O	-0.5499	-1.9453	1.3988
10	O	0.5759	1.9012	-1.3728
11	O	5.4623	2.2627	0.0053
12	O	-5.4832	-2.3065	-0.0053
13	O	2.2324	1.9127	-3.4760
14	O	-2.2583	-1.8964	3.4710
15	O	2.8835	-0.1376	-5.3624
16	O	-2.9000	0.1999	5.3173
17	O	3.2096	0.7581	-1.2864
18	O	-3.1760	-0.8557	1.2818
19	O	1.3361	-0.5804	-0.0011
20	O	-1.3062	0.4791	0.0010
21	O	3.2093	0.7526	1.2901
22	O	-3.1756	-0.8503	-1.2859
23	O	3.8561	-1.3610	-0.0027
24	O	-3.8109	1.2737	0.0024
25	O	2.3141	3.2991	0.0073
26	O	-2.3724	-3.2772	-0.0071
27	O	2.2318	1.8978	3.4847
28	O	-2.2574	-1.8818	-3.4791
29	O	3.8401	-1.5368	3.0524
30	O	-3.7544	1.5695	-2.9619
31	O	4.0722	-3.9601	-0.0084
32	O	-4.0257	3.9157	0.0080
33	O	6.1096	0.1320	-1.3039
34	O	-6.1064	-0.1534	1.2897
35	O	6.7659	2.6456	-2.4822
36	O	-6.8085	-2.6216	2.4964
37	O	4.6916	0.9904	-3.4257
38	O	-4.6964	-0.9616	3.4058
39	O	4.0149	3.1664	-2.0461
40	O	-4.0708	-3.1831	2.0740
41	O	1.3974	4.4258	2.3949
42	O	-1.5526	-4.4100	-2.4818
43	O	0.5756	1.8953	1.3810
44	O	-0.5494	-1.9395	-1.4066
45	O	4.0145	3.1576	2.0603
46	O	-4.0702	-3.1745	-2.0879
47	O	6.7654	2.6349	2.4946
48	O	-6.8078	-2.6113	-2.5084
49	O	6.1093	0.1263	1.3055
50	O	-6.1061	-0.1480	-1.2916
51	O	5.7687	-2.5227	1.3204
52	O	-5.7148	2.4825	-1.3413
53	O	8.0494	-1.4849	-0.0024
54	O	-8.0073	1.5312	0.0024
55	O	5.7691	-2.5169	-1.3303
56	O	-5.7150	2.4768	1.3507
57	O	4.2068	-4.3115	-2.8786
58	O	-4.0849	4.3828	2.8006
59	O	2.1800	-3.0181	-1.4564
60	O	-2.0439	2.9583	1.4460
61	O	-1.5532	-4.4204	2.4628
62	O	1.3979	4.4361	-2.3755
63	O	2.8828	-0.1607	5.3621
64	O	-2.8992	0.2225	-5.3166
65	O	4.6909	0.9756	3.4306
66	O	-4.6955	-0.9475	-3.4104
67	O	1.3614	-0.5403	3.0184
68	O	-1.3174	0.4909	-2.9837
69	O	2.1795	-3.0242	1.4434
70	O	-2.0435	2.9643	-1.4338
71	O	0.2963	-4.2250	-0.0091
72	O	-0.3076	4.6694	0.0098
73	O	4.2058	-4.3240	2.8604
74	O	-4.0842	4.3949	-2.7824
75	O	3.8408	-1.5235	-3.0586
76	O	-3.7549	1.5568	2.9680
77	P	2.8881	-0.1013	0.0000
78	P	-2.8644	0.0111	-0.0002
79	W	2.9631	0.0961	-3.6669
80	W	-2.9782	-0.0611	3.6242
81	W	3.9446	-2.9717	1.8349
82	W	-3.8710	3.0608	-1.7263
83	W	2.0851	2.9308	1.8845
84	W	-2.1533	-2.9210	-1.8846
85	W	5.3899	1.8293	1.8723
86	W	-5.4221	-1.8348	-1.8674
87	W	2.9626	0.0802	3.6677
88	W	-2.9777	-0.0454	-3.6246
89	W	2.0856	2.9389	-1.8712
90	W	-2.1538	-2.9290	1.8716
91	W	6.3540	-1.2493	-0.0021
92	W	-6.3135	1.2723	0.0020
93	W	5.3903	1.8372	-1.8636
94	W	-5.4226	-1.8423	1.8591
95	W	3.9451	-2.9637	-1.8473
96	W	-3.8713	3.0531	1.7390

GD3FeOHFe2FeOH_8_21freq

Energy (POTENTIAL) = -7000.41245890 Eh

	Atom	X	Y	Z
1	Fe	0.0146	0.1374	1.7477
2	Fe	-0.0146	-0.1373	-1.7475
3	Fe	0.7617	-2.7531	0.2009
4	Fe	-0.7617	2.7531	-0.2009
5	H	-0.2358	-4.7457	1.1703
6	H	0.2356	4.7457	-1.1705
7	O	1.3331	-0.7279	-2.9462
8	O	-1.3332	0.7280	2.9462
9	O	-0.5724	-1.8028	1.5282
10	O	0.5724	1.8028	-1.5281
11	O	5.4936	2.3215	-0.1974
12	O	-5.4936	-2.3215	0.1974
13	O	2.2570	1.6057	-3.6206
14	O	-2.2571	-1.6055	3.6207
15	O	2.9092	-0.6443	-5.2871
16	O	-2.9093	0.6444	5.2871
17	O	3.1884	0.7384	-1.3493
18	O	-3.1883	-0.7383	1.3494
19	O	1.3189	-0.4947	0.0422
20	O	-1.3189	0.4948	-0.0421
21	O	3.1999	0.9428	1.2094
22	O	-3.1998	-0.9428	-1.2093
23	O	3.8405	-1.2729	0.0975
24	O	-3.8406	1.2728	-0.0974
25	O	2.3811	3.2603	-0.2588
26	O	-2.3811	-3.2603	0.2590
27	O	2.2892	2.1557	3.3254
28	O	-2.2891	-2.1557	-3.3253
29	O	3.8218	-1.3058	3.0981
30	O	-3.8218	1.3057	-3.0982
31	O	4.0825	-3.9038	0.3095
32	O	-4.0824	3.9038	-0.3096
33	O	6.1223	0.0701	-1.3153
34	O	-6.1223	-0.0700	1.3152
35	O	6.8026	2.4322	-2.7195
36	O	-6.8029	-2.4321	2.7196
37	O	4.6993	0.6961	-3.4873
38	O	-4.6994	-0.6960	3.4873
39	O	4.0611	3.0071	-2.3282
40	O	-4.0612	-3.0070	2.3283
41	O	1.5625	4.5759	2.1347
42	O	-1.5623	-4.5760	-2.1345
43	O	0.5784	2.0272	1.2498
44	O	-0.5784	-2.0272	-1.2497
45	O	4.0799	3.3343	1.8110
46	O	-4.0797	-3.3343	-1.8109
47	O	6.8208	2.8327	2.2673
48	O	-6.8207	-2.8328	-2.2673
49	O	6.1376	0.2791	1.2540
50	O	-6.1375	-0.2791	-1.2541
51	O	5.7666	-2.3407	1.5268
52	O	-5.7666	2.3406	-1.5269
53	O	8.0387	-1.5003	0.0994
54	O	-8.0387	1.5003	-0.0997
55	O	5.7544	-2.5560	-1.1613
56	O	-5.7544	2.5560	1.1612
57	O	4.1255	-4.5905	-2.4428
58	O	-4.1256	4.5905	2.4427
59	O	2.0859	-3.0800	-1.2285
60	O	-2.0860	3.0801	1.2285
61	O	-1.4986	-4.1886	2.7593
62	O	1.4984	4.1888	-2.7591
63	O	2.9411	0.2121	5.3239
64	O	-2.9410	-0.2123	-5.3239
65	O	4.7315	1.2376	3.3185
66	O	-4.7314	-1.2378	-3.3185
67	O	1.3564	-0.2551	3.0280
68	O	-1.3563	0.2552	-3.0280
69	O	2.1007	-2.8189	1.7071
70	O	-2.1006	2.8188	-1.7072
71	O	0.2806	-4.5229	0.3782
72	O	-0.2806	4.5229	-0.3783
73	O	4.1280	-4.1343	3.1396
74	O	-4.1279	4.1341	-3.1398
75	O	3.7949	-1.7876	-2.8476
76	O	-3.7950	1.7876	2.8475
77	P	2.8623	-0.0304	0.0022
78	P	-2.8623	0.0304	-0.0021
79	W	2.9868	-0.2518	-3.6136
80	W	-2.9869	0.2519	3.6136
81	W	3.8823	-2.8957	1.9666
82	W	-3.8822	2.8955	-1.9667
83	W	2.1515	3.0409	1.6390
84	W	-2.1514	-3.0410	-1.6389
85	W	5.4342	1.9904	1.7005
86	W	-5.4342	-1.9905	-1.7005
87	W	3.0087	0.3362	3.6090
88	W	-3.0085	-0.3362	-3.6089
89	W	2.1445	2.7301	-2.0964
90	W	-2.1445	-2.7300	2.0965
91	W	6.3351	-1.2659	0.0896
92	W	-6.3351	1.2659	-0.0898
93	W	5.4228	1.6927	-2.0111
94	W	-5.4230	-1.6926	2.0112
95	W	3.8801	-3.1861	-1.4764
96	W	-3.8802	3.1861	1.4763

GD3FeOHFe2FeOH_8_21

Energy (POTENTIAL) = -7000.41245890 Eh

	Atom	X	Y	Z
1	Fe	0.0157	-0.0392	-1.7526
2	Fe	-0.0156	0.0391	1.7524
3	Fe	0.7673	2.7584	-0.0459
4	Fe	-0.7672	-2.7585	0.0458
5	H	-0.2255	4.8043	-0.9027

6	H	0.2254	-4.8043	0.9028
7	O	1.3323	0.5589	2.9832
8	O	-1.3323	-0.5590	-2.9833
9	O	-0.5677	1.8868	-1.4252
10	O	0.5678	-1.8868	1.4250
11	O	5.4889	-2.3400	0.0705
12	O	-5.4889	2.3400	-0.0705
13	O	2.2512	-1.8107	3.5263
14	O	-2.2512	1.8105	-3.5265
15	O	2.9065	0.3411	5.3168
16	O	-2.9066	-0.3413	-5.3168
17	O	3.1860	-0.8192	1.3078
18	O	-3.1858	0.8192	-1.3079
19	O	1.3200	0.4936	-0.0136
20	O	-1.3199	-0.4938	0.0134
21	O	3.1989	-0.8800	-1.2583
22	O	-3.1988	0.8800	1.2582
23	O	3.8431	1.2686	-0.0236
24	O	-3.8431	-1.2686	0.0234
25	O	2.3745	-3.2745	0.0772
26	O	-2.3744	3.2744	-0.0774
27	O	2.2875	-1.9705	-3.4396
28	O	-2.2873	1.9705	3.4394
29	O	3.8267	1.4697	-3.0177
30	O	-3.8267	-1.4696	3.0176
31	O	4.0904	3.9068	-0.0876
32	O	-4.0903	-3.9068	0.0877
33	O	6.1212	-0.1560	1.3132
34	O	-6.1212	0.1559	-1.3132
35	O	6.7958	-2.5945	2.5832
36	O	-6.7960	2.5943	-2.5834
37	O	4.6953	-0.8999	3.4458
38	O	-4.6953	0.8998	-3.4458
39	O	4.0534	-3.1410	2.1586
40	O	-4.0535	3.1409	-2.1588
41	O	1.5551	-4.4522	-2.3868
42	O	-1.5549	4.4522	2.3865
43	O	0.5754	-1.9552	-1.3612
44	O	-0.5753	1.9551	1.3610
45	O	4.0747	-3.2357	-1.9924
46	O	-4.0745	3.2357	1.9923
47	O	6.8169	-2.7148	-2.4181
48	O	-6.8168	2.7150	2.4181
49	O	6.1380	-0.2207	-1.2638
50	O	-6.1379	0.2207	1.2638
51	O	5.7724	2.4110	-1.3895
52	O	-5.7723	-2.4110	1.3896
53	O	8.0418	1.4873	-0.0101
54	O	-8.0417	-1.4874	0.0103
55	O	5.7586	2.4753	1.3064
56	O	-5.7585	-2.4754	-1.3063
57	O	4.1327	4.4381	2.6989
58	O	-4.1328	-4.4381	-2.6988
59	O	2.0911	3.0021	1.4005
60	O	-2.0910	-3.0022	-1.4005
61	O	-1.4882	4.3397	-2.5212
62	O	1.4881	-4.3398	2.5209
63	O	2.9447	0.0807	-5.3256
64	O	-2.9445	-0.0806	5.3255
65	O	4.7316	-1.0592	-3.3797
66	O	-4.7314	1.0593	3.3796
67	O	1.3592	0.4217	-3.0081
68	O	-1.3591	-0.4218	3.0080
69	O	2.1076	2.9059	-1.5451
70	O	-2.1074	-2.9059	1.5451
71	O	0.2898	4.5364	-0.1240
72	O	-0.2897	-4.5365	0.1240
73	O	4.1385	4.2954	-2.9004
74	O	-4.1383	-4.2953	2.9004
75	O	3.7963	1.6175	2.9457
76	O	-3.7963	-1.6176	-2.9457
77	P	2.8624	0.0247	0.0013
78	P	-2.8623	-0.0247	-0.0015
79	W	2.9846	0.0429	3.6239
80	W	-2.9846	-0.0430	-3.6239
81	W	3.8895	2.9935	-1.7988
82	W	-3.8893	-2.9934	1.7988
83	W	2.1468	-2.9486	-1.8055
84	W	-2.1466	2.9486	1.8053
85	W	5.4316	-1.9029	-1.8059
86	W	-5.4315	1.9029	1.8059
87	W	3.0107	-0.1394	-3.6203
88	W	-3.0106	0.1395	3.6201
89	W	2.1376	-2.8476	1.9414
90	W	-2.1375	2.8475	-1.9416
91	W	6.3376	1.2562	-0.0145
92	W	-6.3376	-1.2563	0.0146
93	W	5.4180	-1.8136	1.9165
94	W	-5.4181	1.8136	-1.9167
95	W	3.8853	3.0905	1.6551
96	W	-3.8853	-3.0906	-1.6550

GD3largeFe4H2O_7_20from5

Energy (POTENTIAL) = -7001.53686371 Eh

Atom	X	Y	Z
1 Fe	-0.0275	-0.0145	1.7982
2 Fe	-0.0311	-0.0299	-1.7737
3 Fe	2.5757	0.8471	0.0081
4 Fe	-2.6603	-0.8026	0.0205
5 H	-4.9834	0.3853	0.7586
6 H	4.8589	-0.3222	-0.7794
7 H	4.8595	-0.3240	0.7926
8 H	-4.9911	0.3070	-0.7965
9 O	0.4776	1.3300	-2.9980
10 O	-0.5243	-1.3588	3.0093
11 O	1.8824	-0.5469	1.3897
12 O	-1.9088	0.5911	-1.3864
13 O	-2.2968	5.5071	0.0010
14 O	2.3943	-5.4567	-0.0027
15 O	-1.9023	2.2739	-3.4798
16 O	1.8697	-2.2387	3.4784
17 O	0.2104	2.9121	-5.3178
18 O	-0.2389	-2.9632	5.3143
19 O	-0.8453	3.1937	-1.2790
20 O	0.8285	-3.1939	1.2826
21 O	0.4890	1.3330	0.0116
22 O	-0.4902	-1.3178	0.0051
23 O	-0.8365	3.2096	1.2940
24 O	0.8409	-3.1909	-1.2845
25 O	1.2831	3.8336	-0.0029
26 O	-1.3045	-3.8221	-0.0221
27 O	-3.2558	2.3795	0.0160
28 O	3.2303	-2.3254	0.0051
29 O	-1.8874	2.3225	3.5178
30 O	1.8790	-2.2271	-3.4740
31 O	1.5793	3.7836	2.9634
32 O	-1.5450	-3.8344	-2.9851
33 O	3.9282	4.0457	-0.0077
34 O	-3.9280	-4.1659	-0.0151
35 O	-0.1475	6.1222	-1.3027
36 O	0.2316	-6.1106	1.2733
37 O	-2.6285	6.8086	-2.5060
38 O	2.6891	-6.7804	2.4975
39 O	-0.9547	4.7058	-3.4055
40 O	0.9958	-4.7000	3.4116
41 O	-3.1752	4.0700	-2.0648
42 O	3.1967	-4.0187	2.0764
43 O	-4.3936	1.5081	2.4072
44 O	4.3826	-1.4104	-2.3566
45 O	-1.8846	0.6268	1.4519
46 O	1.8789	-0.5502	-1.3750
47 O	-3.1603	4.0961	2.0835
48 O	3.2065	-4.0126	-2.0751
49 O	-2.6097	6.8347	2.5038
50 O	2.7053	-6.7743	-2.5021
51 O	-0.1418	6.1401	1.2786
52 O	0.2379	-6.1164	-1.2906
53 O	2.4886	5.7362	1.3320
54 O	-2.4054	-5.8062	-1.3602
55 O	1.5424	8.0246	-0.0241
56 O	-1.4313	-8.0545	-0.0056
57 O	2.4847	5.7244	-1.3592
58 O	-2.4054	-5.7920	1.3428
59 O	4.3924	4.0857	-2.7999
60 O	-4.3845	-4.2278	2.7806
61 O	2.9760	2.0521	-1.4322
62 O	-3.0672	-2.1303	1.4882
63 O	4.3786	-1.4214	2.3741
64 O	-4.4046	1.4819	-2.3657
65 O	0.2384	2.9544	5.3323
66 O	-0.2161	-2.9432	-5.3212
67 O	-0.9273	4.7445	3.4072
68 O	1.0126	-4.6928	-3.4181
69 O	0.4892	1.3469	3.0284
70 O	-0.5248	-1.3655	-2.9950
71 O	2.9812	2.0634	1.4344
72 O	-3.0976	-2.1390	-1.5457
73 O	4.6622	0.2261	0.0075
74 O	-4.8050	-0.2103	0.0086
75 O	4.3992	4.1099	2.7833
76 O	-4.3684	-4.2517	-2.8287
77 O	1.5688	3.7640	-2.9697
78 O	-1.5600	-3.8236	2.9605
79 P	0.0231	2.8810	0.0068
80 P	-0.0414	-2.8636	-0.0048
81 W	-0.0489	2.9811	-3.6208
82 W	0.0150	-3.0266	3.6152
83 W	3.0642	3.8864	1.7254
84 W	-3.0741	-3.9078	-1.7428
85 W	-2.8768	2.1603	1.8912
86 W	2.8745	-2.1166	-1.8774
87 W	-1.8273	5.4443	1.8715
88 W	1.8895	-5.4092	-1.8550
89 W	-0.0365	3.0026	3.6371
90 W	0.0302	-3.0220	-3.6216
91 W	-2.8878	2.1419	-1.8609
92 W	2.8700	-2.1200	1.8870
93 W	1.2772	6.3287	-0.0145
94 W	-1.2442	-6.3452	-0.0146
95 W	-1.8422	5.4260	-1.8618
96 W	1.8784	-5.4116	1.8514
97 W	3.0621	3.8719	-1.7343
98 W	-3.0796	-3.9158	1.7017

GD3largeFe4OH_8_20

Energy (POTENTIAL) = -7001.06323877 Eh

Atom	X	Y	Z
1 Fe	-0.0071	0.0186	-1.7484
2 Fe	-0.0127	-0.1184	1.7743
3 Fe	-0.7874	-2.7734	-0.0908
4 Fe	0.7996	2.6116	0.1111
5 H	-0.2991	4.9841	-0.5940
6 H	0.2104	-4.8033	-0.9754
7 H	-0.3534	4.9114	0.9610
8 O	-1.3684	-0.6425	3.0062
9 O	1.3485	0.5752	-2.9369
10 O	0.5614	-1.8993	-1.4525
11 O	-0.6133	1.7808	1.5199
12 O	-5.4764	2.3657	0.0955
13 O	5.4911	-2.3740	-0.0842

14	O	-2.2970	1.7319	3.5913
15	O	2.2558	-1.7937	-3.5332
16	O	-2.9753	-0.4536	5.3174
17	O	2.9249	0.3719	-5.2605
18	O	-3.2026	0.7870	1.3220
19	O	3.1995	-0.7991	-1.3327
20	O	-1.3367	-0.5192	-0.0155
21	O	1.3131	0.4433	0.0201
22	O	-3.1913	0.9075	-1.2455
23	O	3.2077	-0.8945	1.2382
24	O	-3.8661	-1.2592	-0.0646
25	O	3.8090	1.2970	0.0245
26	O	-2.3359	3.2509	0.1491
27	O	2.3693	-3.2791	-0.1047
28	O	-2.2543	2.0477	-3.4057
29	O	2.2708	-2.0065	3.4092
30	O	-3.8328	-1.3969	-3.0616
31	O	3.8026	1.4492	3.0079
32	O	-4.1306	-3.8895	-0.1826
33	O	4.1323	3.9197	0.1222
34	O	-6.1437	0.1639	1.2784
35	O	6.1301	-0.1712	-1.2999
36	O	-6.7974	2.5805	2.6069
37	O	6.8132	-2.5938	-2.5913
38	O	-4.7381	0.8333	3.4463
39	O	4.7152	-0.8962	-3.4464
40	O	-4.0467	3.0985	2.2104
41	O	4.0581	-3.1350	-2.1788
42	O	-1.4187	4.4819	-2.1786
43	O	1.5501	-4.4940	2.3502
44	O	-0.5827	1.9226	-1.3154
45	O	0.5498	-2.0057	1.3398
46	O	-4.0253	3.2912	-1.9307
47	O	4.0633	-3.2669	1.9667
48	O	-6.7763	2.8156	-2.3896
49	O	6.8084	-2.7474	2.4105
50	O	-6.1350	0.2818	-1.2955
51	O	6.1192	-0.2546	1.2666
52	O	-5.7905	-2.3517	-1.4680
53	O	5.7746	2.3704	1.4298
54	O	-8.0639	-1.4375	-0.0895
55	O	8.0518	1.4620	0.0541
56	O	-5.7995	-2.4725	1.2255
57	O	5.7943	2.4653	-1.2666
58	O	-4.2002	-4.4765	2.5912
59	O	4.2296	4.4461	-2.6861
60	O	-2.1343	-3.0343	1.3377
61	O	2.1159	3.1385	-1.4438
62	O	1.5047	-4.3398	-2.5606
63	O	-1.4341	4.2649	2.5828
64	O	-2.9313	0.0346	-5.3353
65	O	2.9379	0.0414	5.3064
66	O	-4.7052	1.1555	-3.3733
67	O	4.7131	-1.0991	3.3716
68	O	-1.3609	-0.3738	-3.0215
69	O	1.3423	0.3750	3.0009
70	O	-2.1273	-2.8803	-1.6068
71	O	2.1073	2.9916	1.5980
72	O	-0.3142	-4.5501	-0.1980
73	O	0.2378	4.7862	0.1963
74	O	-4.1612	-4.2250	-3.0008
75	O	4.1951	4.2789	2.9357
76	O	-3.8409	-1.6682	2.9010
77	O	3.8216	1.6225	-2.8972
78	P	-2.8713	-0.0283	-0.0009
79	P	2.8640	0.0228	-0.0098
80	W	-3.0206	-0.1125	3.6312
81	W	3.0072	0.0531	-3.5696
82	W	-3.9088	-2.9482	-1.8701
83	W	3.8922	3.0078	1.8111
84	W	-2.1089	2.9528	-1.7419
85	W	2.1384	-2.9812	1.7871
86	W	-5.4085	1.9708	-1.7814
87	W	5.4266	-1.9321	1.7906
88	W	-3.0030	0.2143	-3.6253
89	W	3.0081	-0.1622	3.5981
90	W	-2.1201	2.7811	2.0057
91	W	2.1478	-2.8507	-1.9656
92	W	-6.3574	-1.2201	-0.0740
93	W	6.3424	1.2571	0.0348
94	W	-5.4212	1.7966	1.9386
95	W	5.4359	-1.8131	-1.9211
96	W	-3.9314	-3.1061	1.5822
97	W	3.8852	3.1197	-1.6357

GD3largeFe4Or_8_19

Energy (POTENTIAL) = -7000.39198949 Eh

Atom		X	Y	Z
1	Fe	-0.0003	-0.0458	1.7948
2	Fe	-0.0181	-0.0316	-1.7709
3	Fe	0.8068	-2.6860	0.0019
4	Fe	-0.7931	2.6116	0.0209
5	H	0.3714	4.9366	0.7758
6	H	0.3131	4.9474	-0.7809
7	O	1.3532	-0.5127	-3.0034
8	O	-1.3443	0.4812	3.0062
9	O	-0.5647	-1.9371	1.4061
10	O	0.5872	1.8560	-1.3818
11	O	5.4781	2.3356	0.0059
12	O	-5.5057	-2.3582	-0.0084
13	O	2.2588	1.8859	-3.4780
14	O	-2.2809	-1.8872	3.4702
15	O	2.9326	-0.2114	-5.3222
16	O	-2.9542	0.2178	5.3113
17	O	3.1898	0.8283	-1.2753
18	O	-3.2141	-0.8377	1.2777
19	O	1.3426	-0.5611	0.0108
20	O	-1.3163	0.4495	0.0051
21	O	3.2044	0.8164	1.2939
22	O	-3.2113	-0.8441	-1.2854
23	O	3.8745	-1.2855	-0.0024
24	O	-3.8062	1.3121	-0.0198
25	O	2.3441	3.2356	0.0214
26	O	-2.3820	-3.2754	-0.0036
27	O	2.3026	1.8586	3.5218
28	O	-2.2712	-1.8798	-3.4772
29	O	3.8496	-1.5671	2.9815
30	O	-3.8122	1.5562	-2.9781
31	O	4.1237	-3.9202	-0.0120
32	O	-4.1149	3.9363	-0.0065
33	O	6.1357	0.1959	-1.2981
34	O	-6.1216	-0.1902	1.2737
35	O	6.7826	2.6805	-2.4955
36	O	-6.8249	-2.6420	2.4950
37	O	4.7048	0.9889	-3.4075
38	O	-4.7236	-0.9752	3.4081
39	O	4.0343	3.1852	-2.0552
40	O	-4.0785	-3.1871	2.0695
41	O	1.4472	4.3494	2.4128
42	O	-1.5485	-4.3990	-2.4806
43	O	0.6209	1.8233	1.4503
44	O	-0.5690	-1.9264	-1.4032
45	O	4.0554	3.1642	2.0863
46	O	-4.0732	-3.1870	-2.0841
47	O	6.8046	2.6575	2.5037
48	O	-6.8197	-2.6467	-2.5119
49	O	6.1509	0.1869	1.2788
50	O	-6.1280	-0.1904	-1.2916
51	O	5.8031	-2.4509	1.3318
52	O	-5.7809	2.4443	-1.3538
53	O	8.0691	-1.4710	-0.0229
54	O	-8.0434	1.4956	-0.0012
55	O	5.7911	-2.4412	-1.3628
56	O	-5.7649	2.4375	1.3477
57	O	4.1662	-4.3718	-2.8152
58	O	-4.1803	4.3852	2.7941
59	O	2.1281	-2.9654	-1.4799
60	O	-2.0941	3.0529	1.5001
61	O	-1.5592	-4.4068	2.4732
62	O	1.4319	4.3722	-2.3579
63	O	2.9721	-0.2537	5.3385
64	O	-2.9375	0.2208	-5.3188
65	O	4.7411	0.9529	3.4149
66	O	-4.7184	-0.9763	-3.4203
67	O	1.3713	-0.5375	3.0314
68	O	-1.3523	0.4975	-2.9924
69	O	2.1391	-2.9767	1.4766
70	O	-2.1041	3.0897	-1.5484
71	O	0.3183	-4.2178	-0.0019
72	O	-0.2216	4.7819	0.0178
73	O	4.1885	-4.3867	2.7896
74	O	-4.2084	4.3827	-2.8222
75	O	3.8293	-1.5474	-2.9881
76	O	-3.7981	1.5576	2.9598
77	P	2.8807	-0.0549	0.0073
78	P	-2.8694	0.0299	-0.0057
79	W	2.9999	0.0371	-3.6208
80	W	-3.0180	-0.0379	3.6101
81	W	3.9290	-3.0584	1.7224
82	W	-3.8737	3.0812	-1.7385
83	W	2.1310	2.8431	1.8954
84	W	-2.1542	-2.9066	-1.8799
85	W	5.4273	1.8473	1.8709
86	W	-5.4384	-1.8550	-1.8626
87	W	3.0203	0.0152	3.6395
88	W	-3.0154	-0.0353	-3.6182
89	W	2.1181	2.8618	-1.8573
90	W	-2.1574	-2.9112	1.8734
91	W	6.3633	-1.2505	-0.0130
92	W	-6.3351	1.2818	-0.0117
93	W	5.4122	1.8652	-1.8544
94	W	-5.4403	-1.8525	1.8495
95	W	3.9171	-3.0524	-1.7347
96	W	-3.8795	3.0781	1.7111

GD2Fe4H2O_5_20

Energy (POTENTIAL) = -7001.44567952 Eh

Atom		X	Y	Z
1	Fe	-0.0323	0.0341	1.7232
2	Fe	-0.0400	0.0505	-1.7512
3	Fe	2.5604	0.8092	0.0292
4	Fe	-2.6140	-0.8154	-0.0312
5	H	-4.8809	0.3076	0.7708
6	H	4.9376	-0.2070	-0.8240
7	H	4.9434	-0.3252	0.7366
8	H	-4.8837	0.3245	-0.8094
9	O	0.4979	1.3183	-2.9725
10	O	-0.5491	-1.3260	2.9374
11	O	1.8975	-0.5170	1.3051
12	O	-1.9345	0.5504	-1.3788
13	O	-2.3089	5.4406	0.0017
14	O	2.2745	-5.4504	-0.0239
15	O	-1.8879	2.2222	-3.4657
16	O	1.8770	-2.1969	3.4148
17	O	0.2351	2.9044	-5.2932
18	O	-0.2420	-2.8510	5.2649
19	O	-0.8394	3.1906	-1.2960
20	O	0.8211	-3.1583	1.2834
21	O	0.4162	1.3074	-0.0098
22	O	-0.5264	-1.3201	-0.0126

23	O	-0.8413	3.1808	1.2901
24	O	0.8270	-3.1516	-1.2910
25	O	1.2956	3.7785	0.0029
26	O	-1.3038	-3.8170	0.0179
27	O	-3.2578	2.3480	-0.0155
28	O	3.2596	-2.3099	-0.0297
29	O	-1.9001	2.1932	3.4455
30	O	1.8746	-2.1928	-3.4373
31	O	1.5410	3.7216	2.9537
32	O	-1.5538	-3.7904	-2.9490
33	O	3.9195	3.9713	0.0207
34	O	-3.8925	-4.0847	0.0051
35	O	-0.1439	6.0664	-1.2827
36	O	0.1729	-6.0922	1.3158
37	O	-2.6097	6.7926	-2.4763
38	O	2.6744	-6.7372	2.5030
39	O	-0.9663	4.6773	-3.4086
40	O	0.9907	-4.6557	3.3984
41	O	-3.1778	4.0353	-2.0814
42	O	3.1814	-4.0047	2.0104
43	O	-4.4318	1.4218	2.3309
44	O	4.3853	-1.3084	-2.3943
45	O	-1.9310	0.5474	1.3386
46	O	1.8995	-0.4875	-1.3282
47	O	-3.1782	4.0166	2.0672
48	O	3.2461	-3.9624	-2.0929
49	O	-2.6111	6.7730	2.4930
50	O	2.7455	-6.6967	-2.5183
51	O	-0.1490	6.0526	1.2915
52	O	0.2161	-6.0577	-1.2146
53	O	2.4811	5.6548	1.3617
54	O	-2.3455	-5.7505	-1.3363
55	O	1.5503	7.9528	0.0130
56	O	-1.5012	-8.0216	0.1011
57	O	2.4943	5.6580	-1.3226
58	O	-2.5129	-5.7469	1.3898
59	O	4.3608	3.9784	-2.7754
60	O	-4.3928	-4.0232	2.8024
61	O	2.9650	1.9694	-1.3764
62	O	-2.9874	-2.0290	1.4250
63	O	4.3950	-1.3971	2.3481
64	O	-4.4266	1.4447	-2.3742
65	O	0.1982	2.8518	5.2961
66	O	-0.2237	-2.8899	-5.2705
67	O	-0.9778	4.6510	3.4166
68	O	0.9632	-4.6863	-3.3555
69	O	0.4981	1.3003	2.9558
70	O	-0.5426	-1.3208	-2.9644
71	O	2.9190	1.9674	1.3948
72	O	-2.9737	-2.0650	-1.4395
73	O	4.7057	0.2620	-0.0025
74	O	-4.6389	-0.2083	-0.0255
75	O	4.3492	3.9763	2.8007
76	O	-4.3446	-4.1514	-2.7634
77	O	1.5536	3.7378	-2.9291
78	O	-1.5579	-3.7961	2.9375
79	P	0.0082	2.8651	-0.0033
80	P	-0.0442	-2.8642	-0.0037
81	W	-0.0409	2.9825	-3.6038
82	W	0.0111	-2.9374	3.5740
83	W	3.0280	3.7987	1.7245
84	W	-3.0270	-3.8773	-1.7055
85	W	-2.9218	2.1118	1.8565
86	W	2.8978	-2.0009	-1.8786
87	W	-1.8292	5.3903	1.8561
88	W	1.9781	-5.3078	-1.8860
89	W	-0.0598	2.9471	3.6049
90	W	0.0099	-2.9449	-3.5751
91	W	-2.9198	2.1314	-1.8877
92	W	2.8950	-2.0678	1.8402
93	W	1.2873	6.2614	0.0038
94	W	-1.2937	-6.3249	0.1276
95	W	-1.8300	5.4064	-1.8450
96	W	1.8619	-5.3686	1.8830
97	W	3.0440	3.7800	-1.6942
98	W	-3.0658	-3.8194	1.7414

GD2Fe4H2O_6_21

Energy (POTENTIAL) = -7001.72154724 Eh

Atom		X	Y	Z
1	Fe	0.0000	0.0000	1.7538
2	Fe	0.0000	0.0000	-1.7538
3	Fe	2.5943	0.8671	0.0000
4	Fe	-2.5943	-0.8671	0.0000
5	H	-4.8548	0.2970	0.7898
6	H	4.8548	-0.2970	-0.7898
7	H	4.8548	-0.2970	0.7898
8	H	-4.8548	0.2970	-0.7898
9	O	0.5367	1.3295	-2.9596
10	O	-0.5367	-1.3295	2.9596
11	O	1.8885	-0.5451	1.3487
12	O	-1.8885	0.5451	-1.3487
13	O	-2.3319	5.4199	0.0000
14	O	2.3319	-5.4199	0.0000
15	O	-1.8735	2.1951	-3.4562
16	O	1.8735	-2.1951	3.4562
17	O	0.2290	2.8811	-5.2899
18	O	-0.2290	-2.8811	5.2899
19	O	-0.8246	3.1738	-1.2904
20	O	0.8246	-3.1738	1.2904
21	O	0.5053	1.3265	0.0000
22	O	-0.5053	-1.3265	0.0000
23	O	-0.8246	3.1738	1.2904
24	O	0.8246	-3.1738	-1.2904
25	O	1.2974	3.8217	0.0000
26	O	-1.2974	-3.8217	0.0000
27	O	-3.2508	2.3246	0.0000
28	O	3.2508	-2.3246	0.0000
29	O	-1.8735	2.1951	3.4562
30	O	1.8735	-2.1951	-3.4562
31	O	1.5483	3.7916	2.9525
32	O	-1.5483	-3.7916	-2.9525
33	O	3.9073	4.0412	0.0000
34	O	-3.9073	-4.0412	0.0000
35	O	-0.1848	6.0744	-1.2895
36	O	0.1848	-6.0744	1.2895
37	O	-2.6635	6.7517	-2.4884
38	O	2.6635	-6.7517	2.4884
39	O	-0.9859	4.6596	-3.4059
40	O	0.9859	-4.6596	3.4059
41	O	-3.1814	3.9915	-2.0725
42	O	3.1814	-3.9915	2.0725
43	O	-4.3938	1.3765	2.3534
44	O	4.3938	-1.3765	-2.3534
45	O	-1.8885	0.5451	1.3487
46	O	1.8885	-0.5451	-1.3487
47	O	-3.1814	3.9915	2.0725
48	O	3.1814	-3.9915	-2.0725
49	O	-2.6635	6.7517	2.4884
50	O	2.6635	-6.7517	-2.4884
51	O	-0.1848	6.0744	1.2895
52	O	0.1848	-6.0744	-1.2895
53	O	2.4531	5.7276	1.3388
54	O	-2.4531	-5.7276	-1.3388
55	O	1.4612	8.0068	0.0000
56	O	-1.4612	-8.0068	0.0000
57	O	2.4531	5.7276	-1.3388
58	O	-2.4531	-5.7276	1.3388
59	O	4.3624	4.0976	-2.7857
60	O	-4.3624	-4.0976	2.7857
61	O	2.9483	2.0520	-1.4405
62	O	-2.9483	-2.0520	1.4405
63	O	4.3938	-1.3765	2.3534
64	O	-4.3938	1.3765	-2.3534
65	O	0.2290	2.8811	5.2899
66	O	-0.2290	-2.8811	-5.2899
67	O	-0.9859	4.6596	3.4059
68	O	0.9859	-4.6596	-3.4059
69	O	0.5367	1.3295	2.9596
70	O	-0.5367	-1.3295	-2.9596
71	O	2.9483	2.0520	1.4405
72	O	-2.9483	-2.0520	-1.4405
73	O	4.6276	0.2348	0.0000
74	O	-4.6276	-0.2348	0.0000
75	O	4.3624	4.0976	2.7857
76	O	-4.3624	-4.0976	-2.7857
77	O	1.5483	3.7916	-2.9525
78	O	-1.5483	-3.7916	2.9525
79	P	0.0350	2.8741	0.0000
80	P	-0.0350	-2.8741	0.0000
81	W	-0.0320	2.9631	-3.5958
82	W	0.0320	-2.9631	3.5958
83	W	3.0351	3.8748	1.7215
84	W	-3.0351	-3.8748	-1.7215
85	W	-2.8912	2.0799	1.8671
86	W	2.8912	-2.0799	-1.8671
87	W	-1.8603	5.3772	1.8545
88	W	1.8603	-5.3772	-1.8545
89	W	-0.0320	2.9631	3.5958
90	W	0.0320	-2.9631	-3.5958
91	W	-2.8912	2.0799	-1.8671
92	W	2.8912	-2.0799	1.8671
93	W	1.2334	6.3079	0.0000
94	W	-1.2334	-6.3079	0.0000
95	W	-1.8603	5.3772	-1.8545
96	W	1.8603	-5.3772	1.8545
97	W	3.0351	3.8748	-1.7215
98	W	-3.0351	-3.8748	1.7215

GD2Fe4O_7_20

Energy (POTENTIAL) = -7000.58276659 Eh

Atom		X	Y	Z
1	Fe	0.0105	-0.0520	1.7542
2	Fe	0.0107	-0.0447	-1.7544
3	Fe	0.8217	-2.6599	-0.0057
4	Fe	-0.8483	2.5563	0.0054
5	H	0.3067	4.8183	0.8002
6	H	0.3065	4.8214	-0.7803
7	O	1.3452	-0.5583	-2.9731
8	O	-1.3179	0.5129	2.9567
9	O	-0.5610	-1.9217	1.3609
10	O	0.5534	1.8484	-1.3405
11	O	5.4081	2.3460	0.0053
12	O	-5.4566	-2.2955	-0.0053
13	O	2.1923	1.8620	-3.4546
14	O	-2.2298	-1.8796	3.4494
15	O	2.9019	-0.2276	-5.2958
16	O	-2.8754	0.2182	5.2854
17	O	3.1677	0.8024	-1.2874
18	O	-3.1908	-0.8243	1.2871
19	O	1.3309	-0.5744	-0.0011
20	O	-1.3258	0.4812	0.0007
21	O	3.1674	0.7961	1.2919
22	O	-3.1911	-0.8183	-1.2917
23	O	3.8510	-1.3087	-0.0027
24	O	-3.8105	1.3110	0.0027
25	O	2.3127	3.2317	0.0069
26	O	-2.3727	-3.2889	-0.0072
27	O	2.1917	1.8476	3.4627
28	O	-2.2296	-1.8647	-3.4577

29	O	3.8401	-1.5459	2.9654
30	O	-3.7724	1.5636	-2.9443
31	O	4.0778	-3.9116	-0.0077
32	O	-3.9998	3.9207	0.0081
33	O	6.0887	0.2037	-1.2858
34	O	-6.0846	-0.1445	1.2895
35	O	6.7481	2.6836	-2.4769
36	O	-6.7872	-2.6192	2.4842
37	O	4.6649	1.0056	-3.4061
38	O	-4.6809	-0.9620	3.4033
39	O	3.9785	3.1789	-2.0613
40	O	-4.0402	-3.1659	2.0686
41	O	1.3555	4.3588	2.3609
42	O	-1.5026	-4.3976	-2.4762
43	O	0.5532	1.8429	1.3483
44	O	-0.5610	-1.9160	-1.3691
45	O	3.9782	3.1704	2.0752
46	O	-4.0401	-3.1571	-2.0827
47	O	6.7477	2.6732	2.4893
48	O	-6.7870	-2.6086	-2.4963
49	O	6.0887	0.1985	1.2874
50	O	-6.0849	-0.1391	-1.2906
51	O	5.7679	-2.4431	1.3363
52	O	-5.7055	2.4920	-1.3336
53	O	8.0351	-1.4426	-0.0025
54	O	-7.9973	1.5223	0.0030
55	O	5.7681	-2.4376	-1.3455
56	O	-5.7057	2.4864	1.3436
57	O	4.1249	-4.3514	-2.8054
58	O	-4.0550	4.3670	2.7981
59	O	2.0966	-2.9203	-1.4875
60	O	-2.0232	2.9375	1.4500
61	O	-1.5028	-4.4082	2.4571
62	O	1.3557	4.3686	-2.3424
63	O	2.9009	-0.2495	5.2955
64	O	-2.8749	0.2405	-5.2850
65	O	4.6644	0.9913	3.4111
66	O	-4.6808	-0.9473	-3.4078
67	O	1.3448	-0.5708	2.9710
68	O	-1.3174	0.5254	-2.9548
69	O	2.0964	-2.9265	1.4754
70	O	-2.0229	2.9445	-1.4378
71	O	0.3257	-4.1903	-0.0086
72	O	-0.2315	4.6079	0.0096
73	O	4.1243	-4.3632	2.7880
74	O	-4.0550	4.3790	-2.7800
75	O	3.8408	-1.5335	-2.9709
76	O	-3.7733	1.5506	2.9500
77	P	2.8712	-0.0695	0.0001
78	P	-2.8790	0.0336	-0.0003
79	W	2.9797	0.0214	-3.5969
80	W	-2.9561	-0.0465	3.5893
81	W	3.8837	-3.0401	1.7132
82	W	-3.8437	3.0466	-1.7159
83	W	2.0758	2.8610	1.8736
84	W	-2.1088	-2.9135	-1.8671
85	W	5.3798	1.8536	1.8554
86	W	-5.3989	-1.8245	-1.8611
87	W	2.9791	0.0065	3.5977
88	W	-2.9556	-0.0312	-3.5899
89	W	2.0760	2.8687	-1.8613
90	W	-2.1087	-2.9215	1.8545
91	W	6.3293	-1.2421	-0.0021
92	W	-6.2993	1.2721	0.0023
93	W	5.3801	1.8614	-1.8468
94	W	-5.3990	-1.8325	1.8524
95	W	3.8840	-3.0330	-1.7250
96	W	-3.8441	3.0391	1.7284

GD2Fe4OH_5_21

Energy (POTENTIAL) = -7000.76651337 Eh

	Atom	X	Y	Z
1	Fe	0.0617	0.6068	-1.6621
2	Fe	-0.0746	-0.6156	1.6290
3	Fe	-0.9007	-2.4511	-0.9274
4	Fe	0.8455	2.4169	0.8969
5	H	-0.2622	4.8370	0.8631
6	H	-0.3809	-4.0730	-2.4831
7	H	-0.2970	4.3272	2.3596
8	O	-1.4085	-1.4851	2.6018
9	O	1.4181	1.5184	-2.5981
10	O	0.6291	-1.2808	-1.9390
11	O	-0.5700	1.3106	1.8866
12	O	-5.4182	2.1872	0.6852
13	O	5.4811	-2.1888	-0.6762
14	O	-2.2538	0.6451	3.8580
15	O	2.3633	-0.5843	-3.8645
16	O	-2.9701	-1.9207	4.9134
17	O	3.0247	2.0160	-4.8490
18	O	-3.1871	0.3612	1.4515
19	O	3.2331	-0.3428	-1.4563
20	O	-1.3255	-0.5152	-0.1907
21	O	1.3376	0.4633	0.1772
22	O	-3.1284	1.1995	-0.9910
23	O	3.1452	-1.2469	0.9535
24	O	-3.8467	-1.2091	-0.4537
25	O	3.8256	1.2079	0.4874
26	O	-2.3171	3.0652	1.0401
27	O	2.3676	-3.0885	-1.0880
28	O	-2.1416	2.9092	-2.6723
29	O	2.1388	-2.9580	2.5779
30	O	-3.6666	-0.5132	-3.3081
31	O	3.7133	0.4183	3.3428
32	O	-3.9787	-3.6642	-1.3165
33	O	4.0656	3.6284	1.3903
34	O	-6.1217	-0.2391	1.2349
35	O	6.1521	0.2442	-1.1545
36	O	-6.7866	1.7709	3.1400
37	O	6.8432	-1.6780	-3.1434
38	O	-4.7210	-0.1393	3.4968
39	O	4.8047	0.2431	-3.4443
40	O	-4.0212	2.3568	2.9512
41	O	4.1023	-2.2992	-2.9438
42	O	-1.3466	4.9206	-0.7925
43	O	1.3443	-4.9823	0.7860
44	O	-0.5153	2.2214	-0.6497
45	O	0.4552	-2.2746	0.5573
46	O	-3.9647	3.6765	-0.9636
47	O	3.9524	-3.8016	0.9048
48	O	-6.7082	3.3217	-1.5830
49	O	6.6732	-3.4856	1.5316
50	O	-6.0380	0.5829	-1.2326
51	O	6.0503	-0.6580	1.1812
52	O	-5.7215	-1.8662	-2.1640
53	O	5.7141	1.7194	2.1731
54	O	-8.0184	-1.3479	-0.5481
55	O	8.0334	1.4106	0.6032
56	O	-5.7508	-2.7568	0.3507
57	O	5.7837	2.8042	-0.3323
58	O	-4.1106	-5.0212	1.1898
59	O	4.0918	5.0579	-1.0665
60	O	-2.0981	-3.2050	0.4533
61	O	2.0627	3.2674	-0.3188
62	O	1.4858	-3.2732	-3.7679
63	O	-1.3975	3.3692	3.6503
64	O	-2.7926	1.5089	-5.1076
65	O	2.7883	-1.6382	5.0397
66	O	-4.5931	2.0244	-2.9565
67	O	4.6311	-2.0857	2.8835
68	O	-1.2268	0.5000	-3.0033
69	O	1.2543	-0.5441	2.9513
70	O	-1.9735	-2.2266	-2.2576
71	O	2.0210	2.2738	2.3846
72	O	-0.2955	-4.0076	-1.5142
73	O	0.2399	4.3420	1.5413
74	O	-4.0617	-3.1936	-4.0646
75	O	4.0649	3.1066	4.1491
76	O	-3.9030	-2.4052	2.2832
77	O	3.8752	2.4521	-2.1737
78	P	-2.8748	-0.0345	-0.0439
79	P	2.8899	0.0160	0.0408
80	W	-3.0390	-1.1290	3.3968
81	W	3.0557	1.1855	-3.3520
82	W	-3.9414	-2.2894	-2.6172
83	W	3.8341	2.2349	2.6933
84	W	-2.0526	3.3474	-0.8367
85	W	1.9865	-3.4005	0.7533
86	W	-5.3404	2.3589	-1.2270
87	W	5.2935	-2.5463	1.1637
88	W	-2.8739	1.2104	-3.4230
89	W	2.8837	-1.2725	3.3690
90	W	-2.1081	2.1223	2.6921
91	W	2.1344	-2.0903	-2.7083
92	W	-6.3264	-1.1345	-0.4202
93	W	6.3394	1.2256	0.4554
94	W	-5.4069	1.1977	2.3091
95	W	5.4476	-1.1303	-2.3222
96	W	-3.8833	-3.4108	0.6459
97	W	3.8656	3.4444	-0.5410

GD2Fe4OH_6_20

Energy (POTENTIAL) = -7001.02153919 Eh

	Atom	X	Y	Z
1	Fe	-0.0628	-0.5091	-1.6364
2	Fe	0.0667	0.4985	1.7334
3	Fe	-0.8409	-2.4949	0.7579
4	Fe	0.8617	2.4844	-0.6996
5	H	-0.3108	4.4696	-2.0291
6	H	0.0134	-4.6085	0.3889
7	H	-0.2862	4.8801	-0.5032
8	O	-1.2478	0.3080	3.0551
9	O	1.2462	-0.3155	-2.9400
10	O	0.4598	-2.2212	-0.6511
11	O	-0.5285	2.1850	0.8248
12	O	-5.4266	2.2257	-0.5472
13	O	5.4207	-2.2516	0.5681
14	O	-2.1791	2.7211	2.8790
15	O	2.0609	-2.7650	-2.7255
16	O	-2.8462	1.1370	5.2040
17	O	2.7120	-1.3115	-5.1294
18	O	-3.1412	1.1221	1.0725
19	O	3.1358	-1.1748	-1.0104
20	O	-1.3254	-0.5235	0.1674
21	O	1.3226	0.4786	-0.1157
22	O	-3.1836	0.4578	-1.4237
23	O	3.2163	-0.4199	1.4536
24	O	-3.8443	-1.2470	0.3559
25	O	3.8152	1.2303	-0.4182
26	O	-2.3332	3.1356	-0.8140
27	O	2.3357	-3.1316	0.9472
28	O	-2.2338	0.9134	-3.8022
29	O	2.3237	-0.7922	3.8612
30	O	-3.8951	-2.2399	-2.4707
31	O	3.8719	2.3183	2.3391
32	O	-3.9743	-3.7658	1.0277
33	O	4.0256	3.7326	-1.1635
34	O	-6.0419	0.4828	1.2494
35	O	6.0458	-0.5657	-1.3133
36	O	-6.7351	3.1851	1.7884
37	O	6.7004	-3.2781	-1.7469

38	O	-4.6256	1.8053	3.0817
39	O	4.5427	-1.9555	-3.0410
40	O	-3.9884	3.5938	1.2143
41	O	3.9457	-3.6692	-1.1215
42	O	-1.3830	3.6150	-3.3830
43	O	1.5079	-3.4798	3.6475
44	O	-0.5816	1.4379	-1.7620
45	O	0.5997	-1.3989	1.9037
46	O	-4.0120	2.5461	-2.7817
47	O	4.0669	-2.4597	2.8477
48	O	-6.7767	1.9675	-3.0304
49	O	6.8266	-1.8650	3.0156
50	O	-6.1161	-0.1634	-1.2644
51	O	6.1084	0.1616	1.1608
52	O	-5.7421	-2.7348	-0.5736
53	O	5.7586	2.7201	0.4831
54	O	-8.0073	-1.4066	0.4384
55	O	8.0004	1.3773	-0.5761
56	O	-5.7055	-2.0320	2.0021
57	O	5.6775	1.9472	-2.0796
58	O	-4.0378	-3.4913	3.8043
59	O	4.0081	3.3699	-3.9641
60	O	-1.9794	-2.3878	2.0779
61	O	2.0012	2.4174	-2.2133
62	O	1.3591	-4.9024	-0.9916
63	O	-1.3753	4.8611	1.1437
64	O	-2.9297	-1.5712	-5.0458
65	O	3.0377	1.7415	4.9823
66	O	-4.7032	0.0998	-3.5127
67	O	4.7767	0.0296	3.4721
68	O	-1.3957	-1.3096	-2.6925
69	O	1.4075	1.3671	2.7134
70	O	-2.0877	-3.1592	-0.7094
71	O	2.0798	3.2274	0.5494
72	O	-0.3794	-4.1566	1.1662
73	O	0.2317	4.4516	-1.2141
74	O	-4.0765	-4.9308	-1.5786
75	O	4.1506	4.9658	1.3757
76	O	-3.6851	-0.7513	3.2560
77	O	3.7007	0.6244	-3.3103
78	P	-2.8727	-0.0422	0.0421
79	P	2.8738	0.0271	-0.0192
80	W	-2.9064	0.9591	3.4990
81	W	2.8577	-1.0643	-3.4380
82	W	-3.8574	-3.3640	-0.9073
83	W	3.9073	3.3908	0.7411
84	W	-2.0978	2.2989	-2.5198
85	W	2.1253	-2.2400	2.6389
86	W	-5.3990	1.3378	-2.2325
87	W	5.4251	-1.2697	2.2300
88	W	-3.0105	-0.8900	-3.4738
89	W	3.0628	0.9923	3.4387
90	W	-2.0645	3.2780	1.0793
91	W	2.0798	-3.3360	-0.9280
92	W	-6.3123	-1.1859	0.3292
93	W	6.3037	1.1694	-0.4587
94	W	-5.3561	2.2586	1.3717
95	W	5.3488	-2.3136	-1.3277
96	W	-3.9066	-2.4845	2.4243
97	W	3.8165	2.4069	-2.5576

GD2Fe4OH_7_21

Energy (POTENTIAL) = -7001.25591227 Eh

	Atom	X	Y	Z
1	Fe	-0.0275	-0.0452	-1.7327
2	Fe	-0.0155	-0.0946	1.7385
3	Fe	-0.8163	-2.7732	-0.0241
4	Fe	0.8516	2.5493	0.0347
5	H	-0.2952	4.8308	-0.7185
6	H	0.1933	-4.8140	-0.8870
7	H	-0.2915	4.8065	0.8615
8	O	-1.3438	-0.6078	2.9599
9	O	1.3091	0.5351	-2.9346
10	O	0.5659	-1.9207	-1.3778
11	O	-0.5435	1.8275	1.3775
12	O	-5.4010	2.3668	0.0401
13	O	5.4648	-2.2931	-0.0400
14	O	-2.1831	1.8046	3.4917
15	O	2.2247	-1.8469	-3.4756
16	O	-2.8977	-0.3177	5.2896
17	O	2.8473	0.2856	-5.2804
18	O	-3.1709	0.7934	1.3063
19	O	3.1905	-0.8136	-1.3022
20	O	-1.3256	-0.5333	-0.0057
21	O	1.3270	0.4715	0.0082
22	O	-3.1752	0.8348	-1.2747
23	O	3.1974	-0.8424	1.2761
24	O	-3.8432	-1.2961	-0.0170
25	O	3.8107	1.3059	0.0077
26	O	-2.3039	3.2376	0.0541
27	O	2.3832	-3.2895	-0.0360
28	O	-2.1887	1.9154	-3.4282
29	O	2.2524	-1.9228	3.4350
30	O	-3.8498	-1.4780	-2.9911
31	O	3.7789	1.5216	2.9572
32	O	-4.0963	-3.8966	-0.0628
33	O	4.0001	3.9182	0.0378
34	O	-6.0859	0.2024	1.2924
35	O	6.0878	-0.1251	-1.3099
36	O	-6.7333	2.6607	2.5307
37	O	6.7876	-2.5826	-2.5384
38	O	-4.6591	0.9529	3.4275
39	O	4.6704	-0.9192	-3.4243
40	O	-3.9651	3.1531	2.1251
41	O	4.0422	-3.1427	-2.1164
42	O	-1.3435	4.4045	-2.2794
43	O	1.5360	-4.4443	2.4387
44	O	-0.5493	1.8676	-1.3191
45	O	0.5632	-1.9660	1.3560
46	O	-3.9695	3.2219	-2.0184
47	O	4.0579	-3.1895	2.0308
48	O	-6.7394	2.7428	-2.4364
49	O	6.8006	-2.6400	2.4457
50	O	-6.0906	0.2448	-1.2801
51	O	6.0917	-0.1560	1.2716
52	O	-5.7758	-2.3951	-1.3747
53	O	5.7104	2.4732	1.3551
54	O	-8.0383	-1.4137	-0.0175
55	O	7.9999	1.5239	0.0000
56	O	-5.7725	-2.4389	1.3066
57	O	5.7016	2.5032	-1.3215
58	O	-4.1572	-4.3942	2.7219
59	O	4.0457	4.4016	-2.7468
60	O	-2.1013	-2.9736	1.4348
61	O	2.0215	2.9514	-1.4096
62	O	1.4760	-4.3884	-2.4630
63	O	-1.3382	4.3285	2.4238
64	O	-2.9031	-0.1442	-5.2956
65	O	2.8815	0.1691	5.2773
66	O	-4.6658	1.0686	-3.3926
67	O	4.6948	-0.9917	3.3822
68	O	-1.3534	-0.5178	-2.9720
69	O	1.3228	0.4635	2.9485
70	O	-2.1060	-2.9015	-1.5312
71	O	2.0296	2.9221	1.4776
72	O	-0.2767	-4.5271	-0.0865
73	O	0.2446	4.6060	0.0672
74	O	-4.1434	-4.2975	-2.8656
75	O	4.0646	4.3399	2.8322
76	O	-3.8349	-1.5826	2.9414
77	O	3.7643	1.5871	-2.9368
78	P	-2.8648	-0.0538	0.0016
79	P	2.8809	0.0277	-0.0016
80	W	-2.9775	-0.0350	3.5960
81	W	2.9416	-0.0009	-3.5883
82	W	-3.8915	-2.9935	-1.7699
83	W	3.8508	3.0218	1.7508
84	W	-2.0675	2.8996	-1.8183
85	W	2.1179	-2.9495	1.8340
86	W	-5.3739	1.9067	-1.8186
87	W	5.4074	-1.8520	1.8260
88	W	-2.9831	0.0848	-3.5939
89	W	2.9623	-0.0832	3.5788
90	W	-2.0607	2.8383	1.9160
91	W	2.1172	-2.8940	-1.8899
92	W	-6.3318	-1.2179	-0.0176
93	W	6.3023	1.2709	0.0019
94	W	-5.3685	1.8468	1.8824
95	W	5.4018	-1.8057	-1.8897
96	W	-3.8983	-3.0569	1.6706
97	W	3.8402	3.0595	-1.6936

GD2Fe4Or_6_21

Energy (POTENTIAL) = -7000.34540176 Eh

	Atom	X	Y	Z
1	Fe	-0.0035	-0.0552	1.7489
2	Fe	-0.0034	-0.0473	-1.7493
3	Fe	0.8096	-2.6574	-0.0058
4	Fe	-0.8650	2.5773	0.0055
5	H	0.2832	4.8561	0.8008
6	H	0.2835	4.8597	-0.7796
7	O	1.3486	-0.5533	-2.9823
8	O	-1.3065	0.5144	2.9472
9	O	-0.5352	-1.9272	1.3663
10	O	0.5700	1.8642	-1.3397
11	O	5.4106	2.2511	0.0052
12	O	-5.4404	-2.3029	-0.0053
13	O	2.1924	1.8939	-3.4738
14	O	-2.2109	-1.8781	3.4459
15	O	2.8392	-0.1606	-5.3410
16	O	-2.8628	0.2148	5.2830
17	O	3.1613	0.8055	-1.2915
18	O	-3.1750	-0.8260	1.2874
19	O	1.3334	-0.5763	-0.0012
20	O	-1.3112	0.4822	0.0008
21	O	3.1608	0.7999	1.2955
22	O	-3.1750	-0.8204	-1.2914
23	O	3.8520	-1.3045	-0.0025
24	O	-3.7991	1.3078	0.0026
25	O	2.3353	3.2564	0.0072
26	O	-2.3513	-3.2791	-0.0074
27	O	2.1918	1.8788	3.4823
28	O	-2.2106	-1.8630	-3.4546
29	O	3.8369	-1.5216	3.0374
30	O	-3.7615	1.5599	-2.9430
31	O	4.0125	-3.9368	-0.0082
32	O	-3.9952	3.9147	0.0083
33	O	6.0609	0.1272	-1.3079
34	O	-6.0731	-0.1520	1.2891
35	O	6.7449	2.6394	-2.4680
36	O	-6.7750	-2.6253	2.4834
37	O	4.6574	0.9939	-3.4203
38	O	-4.6654	-0.9687	3.4030
39	O	3.9917	3.1652	-2.0611
40	O	-4.0247	-3.1704	2.0694
41	O	1.3650	4.3767	2.3509
42	O	-1.4928	-4.4025	-2.4756
43	O	0.5698	1.8583	1.3478
44	O	-0.5352	-1.9211	-1.3751
45	O	3.9913	3.1562	2.0753

46	O	-4.0245	-3.1614	-2.0836
47	O	6.7445	2.6287	2.4804
48	O	-6.7747	-2.6145	-2.4955
49	O	6.0608	0.1215	1.3092
50	O	-6.0729	-0.1464	-1.2903
51	O	5.7235	-2.5290	1.3113
52	O	-5.6998	2.4849	-1.3335
53	O	8.0034	-1.4677	-0.0027
54	O	-7.9912	1.5113	0.0028
55	O	5.7236	-2.5236	-1.3211
56	O	-5.7000	2.4791	1.3436
57	O	4.1353	-4.3047	-2.8793
58	O	-4.0576	4.3640	2.7977
59	O	2.1389	-2.9591	-1.4572
60	O	-2.0185	2.9378	1.4514
61	O	-1.4931	-4.4133	2.4559
62	O	1.3656	4.3870	-2.3316
63	O	2.8384	-0.1835	5.3408
64	O	-2.8625	0.2378	-5.2826
65	O	4.6569	0.9789	3.4252
66	O	-4.6651	-0.9539	-3.4077
67	O	1.3480	-0.5662	2.9803
68	O	-1.3060	0.5270	-2.9457
69	O	2.1389	-2.9655	1.4445
70	O	-2.0184	2.9440	-1.4388
71	O	0.3102	-4.1855	-0.0090
72	O	-0.2404	4.6173	0.0100
73	O	4.1352	-4.3172	2.8612
74	O	-4.0573	4.3764	-2.7790
75	O	3.8375	-1.5083	-3.0432
76	O	-3.7619	1.5471	2.9493
77	P	2.8695	-0.0641	0.0001
78	P	-2.8696	0.0315	-0.0002
79	W	2.9285	0.0872	-3.6478
80	W	-2.9514	-0.0500	3.5898
81	W	3.9022	-2.9620	1.8330
82	W	-3.8462	3.0451	-1.7173
83	W	2.0701	2.8788	1.8616
84	W	-2.1033	-2.9205	-1.8723
85	W	5.3594	1.8301	1.8699
86	W	-5.3906	-1.8295	-1.8593
87	W	2.9279	0.0713	3.6487
88	W	-2.9511	-0.0342	-3.5905
89	W	2.0705	2.8870	-1.8487
90	W	-2.1036	-2.9287	1.8590
91	W	6.3075	-1.2326	-0.0023
92	W	-6.2950	1.2650	0.0024
93	W	5.3597	1.8382	-1.8613
94	W	-5.3909	-1.8376	1.8508
95	W	3.9022	-2.9540	-1.8451
96	W	-3.8463	3.0375	1.7302

GD2FeOHFe2FeOH_8_21

Energy (POTENTIAL) = -7000.78329308 Eh

	Atom	X	Y	Z
1	Fe	0.0109	0.1380	1.7120
2	Fe	-0.0107	-0.1382	-1.7120
3	Fe	0.7982	-2.7301	0.1998
4	Fe	-0.7982	2.7298	-0.1996
5	H	-0.2116	-4.7067	1.1906
6	H	0.2117	4.7063	-1.1908
7	O	1.3270	-0.7607	-2.8969
8	O	-1.3271	0.7611	2.8964
9	O	-0.5665	-1.7842	1.4999
10	O	0.5666	1.7843	-1.4996
11	O	5.4548	2.3063	-0.1944
12	O	-5.4548	-2.3064	0.1946
13	O	2.2198	1.5869	-3.5961
14	O	-2.2197	-1.5865	3.5962
15	O	2.8721	-0.6583	-5.2484
16	O	-2.8718	0.6588	5.2483
17	O	3.1908	0.7052	-1.3529
18	O	-3.1908	-0.7048	1.3529
19	O	1.3256	-0.5032	0.0412
20	O	-1.3254	0.5034	-0.0412
21	O	3.1997	0.9076	1.2180
22	O	-3.1995	-0.9074	-1.2180
23	O	3.8328	-1.3095	0.0962
24	O	-3.8320	1.3102	-0.0966
25	O	2.3722	3.2579	-0.2598
26	O	-2.3721	-3.2576	0.2601
27	O	2.2515	2.1335	3.3021
28	O	-2.2512	-2.1337	-3.3018
29	O	3.8315	-1.3008	3.0716
30	O	-3.8315	1.3005	-3.0715
31	O	4.0533	-3.9057	0.3073
32	O	-4.0538	3.9056	-0.3078
33	O	6.1010	0.0610	-1.3131
34	O	-6.1011	-0.0610	1.3130
35	O	6.7775	2.4301	-2.7036
36	O	-6.7774	-2.4298	2.7039
37	O	4.6757	0.6968	-3.4813
38	O	-4.6757	-0.6964	3.4814
39	O	4.0249	2.9901	-2.3235
40	O	-4.0249	-2.9897	2.3237
41	O	1.5217	4.5707	2.1322
42	O	-1.5215	-4.5709	-2.1317
43	O	0.5699	2.0106	1.2251
44	O	-0.5697	-2.0105	-1.2248
45	O	4.0449	3.3156	1.8087
46	O	-4.0446	-3.3158	-1.8084
47	O	6.7959	2.8246	2.2576
48	O	-6.7957	-2.8253	-2.2575
49	O	6.1145	0.2683	1.2546
50	O	-6.1148	-0.2687	-1.2547
51	O	5.7569	-2.3504	1.5178
52	O	-5.7572	2.3502	-1.5181
53	O	8.0338	-1.4869	0.0993
54	O	-8.0341	1.4867	-0.0996
55	O	5.7482	-2.5639	-1.1537
56	O	-5.7486	2.5637	1.1535
57	O	4.1077	-4.5766	-2.4437
58	O	-4.1084	4.5768	2.4432
59	O	2.0716	-3.0526	-1.2458
60	O	-2.0721	3.0531	1.2455
61	O	-1.4459	-4.1787	2.7542
62	O	1.4460	4.1789	-2.7538
63	O	2.8993	0.1866	5.2840
64	O	-2.8992	-0.1871	-5.2838
65	O	4.7050	1.2350	3.3132
66	O	-4.7048	-1.2354	-3.3131
67	O	1.3402	-0.2937	2.9857
68	O	-1.3402	0.2936	-2.9855
69	O	2.0820	-2.7943	1.7120
70	O	-2.0821	2.7944	-1.7121
71	O	0.2662	-4.4857	0.3740
72	O	-0.2662	4.4854	-0.3743
73	O	4.1067	-4.1210	3.1343
74	O	-4.1068	4.1206	-3.1347
75	O	3.8114	-1.7805	-2.8321
76	O	-3.8114	1.7809	2.8320
77	P	2.8718	-0.0540	0.0025
78	P	-2.8716	0.0543	-0.0025
79	W	2.9629	-0.2625	-3.5753
80	W	-2.9629	0.2630	3.5752
81	W	3.8659	-2.8858	1.9557
82	W	-3.8658	2.8855	-1.9560
83	W	2.1134	3.0410	1.6260
84	W	-2.1131	-3.0411	-1.6257
85	W	5.4105	1.9751	1.6971
86	W	-5.4104	-1.9754	-1.6969
87	W	2.9773	0.3172	3.5688
88	W	-2.9773	-0.3176	-3.5686
89	W	2.1040	2.7289	-2.0844
90	W	-2.1040	-2.7287	2.0847
91	W	6.3285	-1.2629	0.0889
92	W	-6.3287	1.2628	-0.0893
93	W	5.3987	1.6815	-2.0013
94	W	-5.3987	-1.6812	2.0014
95	W	3.8667	-3.1724	-1.4745
96	W	-3.8673	3.1725	1.4741

GD2H2O

Energy (POTENTIAL) = -76.4251652220 Eh

	Atom	X	Y	Z
1	O	0.0176	0.0000	0.0123
2	H	0.0732	0.0000	0.9767
3	H	0.9429	0.0000	-0.2653

GD3H2O

Energy (POTENTIAL) = -76.4251353127 Eh

	Atom	X	Y	Z
1	O	0.0175	0.0000	0.0123
2	H	0.0733	0.0000	0.9766
3	H	0.9428	0.0000	-0.2651

GD3bjH2O

Energy (POTENTIAL) = -76.4257012912 Eh

	Atom	X	Y	Z
1	O	0.0175	0.0000	0.0123
2	H	0.0734	0.0000	0.9766
3	H	0.9428	0.0000	-0.2651

Fe_4-SK species. Small basis sets BS1

bs1Fe4-SK-OH2_-6_21

Energy (POTENTIAL) = -7000.22662587 Eh

	Atom	X	Y	Z
1	Fe	0.0000	0.0000	1.8351
2	Fe	0.0000	0.0000	-1.8351
3	Fe	2.6565	0.8640	0.0000
4	Fe	-2.6565	-0.8640	0.0000
5	H	-4.9267	0.3079	0.7925
6	H	4.9267	-0.3079	-0.7925
7	H	4.9267	-0.3079	0.7925
8	H	-4.9267	0.3079	-0.7925
9	O	0.4933	1.3528	-3.0289
10	O	-0.4933	-1.3528	3.0289
11	O	1.9029	-0.5594	1.3924
12	O	-1.9029	0.5594	-1.3924
13	O	-2.3178	5.5020	0.0000
14	O	2.3178	-5.5020	0.0000
15	O	-1.8906	2.2653	-3.4925
16	O	1.8906	-2.2653	3.4925
17	O	0.2284	2.9625	-5.3467
18	O	-0.2284	-2.9625	5.3467
19	O	-0.8351	3.2024	-1.3313
20	O	0.8351	-3.2024	1.3313
21	O	0.5306	1.3300	0.0000
22	O	-0.5306	-1.3300	0.0000
23	O	-0.8351	3.2024	1.3313
24	O	0.8351	-3.2024	-1.3313
25	O	1.3491	3.8764	0.0000
26	O	-1.3491	-3.8764	0.0000
27	O	-3.2067	2.3398	0.0000
28	O	3.2067	-2.3398	0.0000
29	O	-1.8906	2.2653	3.4925
30	O	1.8906	-2.2653	-3.4925
31	O	1.5656	3.7754	2.9435
32	O	-1.5656	-3.7754	-2.9435

33O	3.9436	4.1038	0.0000
34O	-3.9436	-4.1038	0.0000
35O	-0.1825	6.1368	-1.2797
36O	0.1825	-6.1368	1.2797
37O	-2.6780	6.8413	-2.5165
38O	2.6780	-6.8413	2.5165
39O	-0.9783	4.7201	-3.4116
40O	0.9783	-4.7201	3.4116
41O	-3.1736	4.0498	-2.0749
42O	3.1736	-4.0498	2.0749
43O	-4.4294	1.4265	2.3448
44O	4.4294	-1.4265	-2.3448
45O	-1.9029	0.5594	1.3924
46O	1.9029	-0.5594	-1.3924
47O	-3.1736	4.0498	2.0749
48O	3.1736	-4.0498	-2.0749
49O	-2.6780	6.8413	2.5165
50O	2.6780	-6.8413	-2.5165
51O	-0.1825	6.1368	1.2797
52O	0.1825	-6.1368	-1.2797
53O	2.4713	5.7690	1.3420
54O	-2.4713	-5.7690	-1.3420
55O	1.5030	8.0911	0.0000
56O	-1.5030	-8.0911	0.0000
57O	2.4713	5.7690	-1.3420
58O	-2.4713	-5.7690	1.3420
59O	4.4062	4.1418	-2.8068
60O	-4.4062	-4.1418	2.8068
61O	3.0035	2.0936	-1.4142
62O	-3.0035	-2.0936	1.4142
63O	4.4294	-1.4265	2.3448
64O	-4.4294	1.4265	-2.3448
65O	0.2284	2.9625	5.3467
66O	-0.2284	-2.9625	-5.3467
67O	-0.9783	4.7201	3.4116
68O	0.9783	-4.7201	-3.4116
69O	0.4933	1.3528	3.0289
70O	-0.4933	-1.3528	-3.0289
71O	3.0035	2.0936	1.4142
72O	-3.0035	-2.0936	-1.4142
73O	4.6816	0.2147	0.0000
74O	-4.6816	-0.2147	0.0000
75O	4.4062	4.1418	2.8068
76O	-4.4062	-4.1418	-2.8068
77O	1.5656	3.7754	-2.9435
78O	-1.5656	-3.7754	2.9435
79P	0.0601	2.8655	0.0000
80P	-0.0601	-2.8655	0.0000
81W	-0.0453	3.0169	-3.6286
82W	0.0453	-3.0169	3.6286
83W	3.0651	3.9190	1.7197
84W	-3.0651	-3.9190	-1.7197
85W	-2.8894	2.1263	1.8850
86W	2.8894	-2.1263	-1.8850
87W	-1.8675	5.4476	1.8689
88W	1.8675	-5.4476	-1.8689
89W	-0.0453	3.0169	3.6286
90W	0.0453	-3.0169	-3.6286
91W	-2.8894	2.1263	-1.8850
92W	2.8894	-2.1263	1.8850
93W	1.2565	6.3706	0.0000
94W	-1.2565	-6.3706	0.0000
95W	-1.8675	5.4476	-1.8689
96W	1.8675	-5.4476	1.8689
97W	3.0651	3.9190	-1.7197
98W	-3.0651	-3.9190	1.7197

bs1Fe4-SK-OH_-7_21

Energy (POTENTIAL) = -6999.77492492 Eh

Atom	X	Y	Z
1 Fe	-0.0312	-0.0599	-1.8135
2 Fe	-0.0175	-0.0704	1.8189
3 Fe	-0.8163	-2.8327	0.0004
4 Fe	0.8436	2.6165	0.0019
5 H	-0.3077	4.8988	-0.7834
6 H	0.1588	-4.8764	-0.8904
7 H	-0.3024	4.8954	0.8029
8 O	-1.3715	-0.5248	3.0269
9 O	1.3331	0.4496	-3.0078
10O	0.5752	-1.9554	-1.3989
11O	-0.5558	1.8669	1.3963
12O	-5.4882	2.3774	0.0114
13O	5.5393	-2.2871	0.0015
14O	-2.2521	1.8691	3.5019
15O	2.2930	-1.9161	-3.4796
16O	-2.9836	-0.2468	5.3410
17O	2.9329	0.2051	-5.3347
18O	-3.2013	0.8319	1.3343
19O	3.2167	-0.8468	-1.3245
20O	-1.3324	-0.5453	-0.0038
21O	1.3292	0.4976	0.0041
22O	-3.2066	0.8463	-1.3276
23O	3.2213	-0.8369	1.3338
24O	-3.9046	-1.3319	-0.0072
25O	3.8653	1.3548	-0.0059
26O	-2.3165	3.2049	0.0151
27O	2.3807	-3.2560	0.0156
28O	-2.2560	1.9059	-3.4857
29O	2.3091	-1.8913	3.5008
30O	-3.8465	-1.5162	-2.9748
31O	3.7603	1.5776	2.9315
32O	-4.1907	-3.9225	-0.0263
33O	4.0683	3.9536	-0.0129
34O	-6.1542	0.2392	1.2773
35O	6.1461	-0.1502	-1.2883
36O	-6.8206	2.7286	2.5301
37O	6.8705	-2.6426	-2.5189
38O	-4.7220	0.9991	3.4172
39O	4.7297	-0.9660	-3.4100
40O	-4.0216	3.1864	2.0896
41O	4.0926	-3.1710	-2.0661
42O	-1.3900	4.4245	-2.3224
43O	1.5810	-4.4439	2.5233
44O	-0.5600	1.8768	-1.3850
45O	0.5688	-1.9696	1.4275
46O	-4.0250	3.2091	-2.0577
47O	4.1024	-3.1565	2.0833
48O	-6.8264	2.7568	-2.4999
49O	6.8774	-2.6261	2.5217
50O	-6.1585	0.2530	-1.2762
51O	6.1461	-0.1425	1.2736
52O	-5.8323	-2.4035	-1.3564
53O	5.7521	2.5038	1.3305
54O	-8.1331	-1.4253	-0.0035
55O	8.0823	1.5531	-0.0124
56O	-5.8262	-2.4189	1.3335
57O	5.7463	2.4953	-1.3537
58O	-4.2314	-4.3952	2.7862
59O	4.0963	4.4007	-2.8248
60O	-2.1624	-3.0238	1.4325
61O	2.0662	2.9880	-1.4194
62O	1.5178	-4.4579	-2.4036
63O	-1.3851	4.4006	2.3640
64O	-2.9851	-0.1859	-5.3498
65O	2.9515	0.2437	5.3342
66O	-4.7281	1.0432	-3.4124
67O	4.7436	-0.9418	3.4114
68O	-1.3852	-0.4987	-3.0266
69O	1.3419	0.4624	3.0098
70O	-2.1743	-2.9750	-1.4790
71O	2.0726	2.9985	1.4116
72O	-0.2839	-4.5758	-0.0772
73O	0.2221	4.6622	0.0078
74O	-4.2224	-4.3581	-2.8473
75O	4.1105	4.4207	2.7958
76O	-3.8248	-1.5579	2.9443
77O	3.7501	1.5572	-2.9424
78P	-2.8604	-0.0664	-0.0021
79P	2.8704	0.0507	0.0028
80W	-3.0369	0.0272	3.6203
81W	2.9977	-0.0686	-3.6146
82W	-3.9594	-3.0329	-1.7403
83W	3.8953	3.0748	1.7096
84W	-2.1118	2.8881	-1.8712
85W	2.1540	-2.9235	1.9019
86W	-5.4449	1.9176	-1.8562
87W	5.4686	-1.8369	1.8738
88W	-3.0444	0.0697	-3.6263
89W	3.0107	-0.0444	3.6160
90W	-2.1052	2.8680	1.8988
91W	2.1563	-2.9223	-1.8629
92W	-6.4045	-1.2138	-0.0060
93W	6.3627	1.2874	-0.0091
94W	-5.4394	1.8984	1.8742
95W	5.4666	-1.8468	-1.8693
96W	-3.9597	-3.0605	1.6948
97W	3.8868	3.0618	-1.7288

bs1Fe4-SK-O_-7_20

Energy (POTENTIAL) = -6999.10250866 Eh

Atom	X	Y	Z
1 Fe	0.0091	-0.0528	1.8411
2 Fe	0.0092	-0.0448	-1.8413
3 Fe	0.8162	-2.6865	-0.0054
4 Fe	-0.8490	2.6128	0.0054
5 H	0.3120	4.8845	0.8028
6 H	0.3117	4.8876	-0.7831
7 O	1.3712	-0.5159	-3.0374
8 O	-1.3456	0.4659	3.0276
9 O	-0.5706	-1.9414	1.4057
10O	0.5577	1.8649	-1.3849
11O	5.4918	2.3501	0.0051
12O	-5.5331	-2.2997	-0.0053
13O	2.2558	1.8814	-3.4884
14O	-2.2947	-1.9041	3.4821
15O	2.9838	-0.2195	-5.3509
16O	-2.9612	0.2071	5.3416
17O	3.1942	0.8203	-1.3280
18O	-3.2207	-0.8452	1.3274
19O	1.3356	-0.5908	-0.0010
20O	-1.3345	0.5027	0.0010
21O	3.1943	0.8141	1.3323
22O	-3.2207	-0.8397	-1.3314
23O	3.9101	-1.3506	-0.0029
24O	-3.8727	1.3517	0.0026
25O	2.3183	3.1896	0.0069
26O	-2.3681	-3.2651	-0.0072
27O	2.2558	1.8670	3.4967
28O	-2.2942	-1.8890	-3.4906
29O	3.8305	-1.5587	2.9606
30O	-3.7650	1.5683	-2.9352
31O	4.1654	-3.9439	-0.0078
32O	-4.0781	3.9473	0.0082
33O	6.1516	0.2193	-1.2761
34O	-6.1471	-0.1616	1.2797
35O	6.8308	2.7176	-2.5087
36O	-6.8690	-2.6551	2.5116
37O	4.7224	1.0094	-3.4110
38O	-4.7391	-0.9716	3.4099
39O	4.0288	3.1804	-2.0622

40O	-4.0884	-3.1730	2.0679
41O	1.3960	4.3959	2.3535
42O	-1.5513	-4.4372	-2.4986
43O	0.5578	1.8586	1.3935
44O	-0.5705	-1.9352	-1.4140
45O	4.0287	3.1720	2.0759
46O	-4.0881	-3.1639	-2.0821
47O	6.8307	2.7074	2.5204
48O	-6.8686	-2.6440	-2.5238
49O	6.1517	0.2142	1.2777
50O	-6.1470	-0.1561	-1.2810
51O	5.8177	-2.4450	1.3407
52O	-5.7570	2.4928	-1.3372
53O	8.1238	-1.4614	-0.0026
54O	-8.0866	1.5379	0.0029
55O	5.8177	-2.4394	-1.3500
56O	-5.7571	2.4871	1.3474
57O	4.1897	-4.3899	-2.8271
58O	-4.1128	4.3987	2.8183
59O	2.1554	-2.9803	-1.4583
60O	-2.0766	2.9861	1.4212
61O	-1.5520	-4.4481	2.4792
62O	1.3963	4.4056	-2.3349
63O	2.9833	-0.2411	5.3504
64O	-2.9604	0.2299	-5.3412
65O	4.7223	0.9953	3.4155
66O	-4.7385	-0.9568	-3.4146
67O	1.3710	-0.5285	3.0356
68O	-1.3451	0.4793	-3.0262
69O	2.1554	-2.9864	1.4469
70O	-2.0766	2.9920	-1.4088
71O	0.3098	-4.2106	-0.0086
72O	-0.2166	4.6530	0.0095
73O	4.1898	-4.4015	2.8099
74O	-4.1127	4.4107	-2.8001
75O	3.8306	-1.5465	-2.9662
76O	-3.7653	1.5556	2.9415
77P	2.8654	-0.0890	0.0000
78P	-2.8741	0.0500	-0.0001
79W	3.0365	0.0383	-3.6277
80W	-3.0139	-0.0674	3.6214
81W	3.9420	-3.0675	1.7104
82W	-3.8988	3.0658	-1.7127
83W	2.1140	2.8615	1.8916
84W	-2.1487	-2.9217	-1.8878
85W	5.4467	1.8785	1.8697
86W	-5.4650	-1.8476	-1.8745
87W	3.0363	0.0234	3.6283
88W	-3.0133	-0.0517	-3.6221
89W	2.1141	2.8693	-1.8793
90W	-2.1491	-2.9299	1.8748
91W	6.3959	-1.2456	-0.0022
92W	-6.3664	1.2772	0.0025
93W	5.4468	1.8860	-1.8614
94W	-5.4653	-1.8557	1.8659
95W	3.9420	-3.0604	-1.7222
96W	-3.8988	3.0585	1.7253

bs1Fe4-SK-OH_-6_20

Energy (POTENTIAL) = -6999.52672386 Eh

Atom	X	Y	Z
1 Fe	-0.0792	-0.0335	-1.7958
2 Fe	0.0728	0.0139	1.9071
3 Fe	-0.8588	-2.6499	-0.0329
4 Fe	0.8584	2.6347	0.0095
5 H	-0.3028	4.9173	-0.7555
6 H	0.0747	-4.5722	-0.9266
7 H	-0.2807	4.9091	0.8305
8 O	-1.3084	-0.5141	3.0602
9 O	1.2974	0.4255	-2.9517
10O	0.4704	-1.9941	-1.2632
11O	-0.5511	1.8845	1.4272
12O	-5.5072	2.3007	0.0273
13O	5.5032	-2.3185	0.0203
14O	-2.2805	1.8308	3.5219
15O	2.1708	-1.9709	-3.3627
16O	-2.9855	-0.3527	5.3193
17O	2.8411	0.0844	-5.3047
18O	-3.1793	0.7986	1.3322
19O	3.1691	-0.8870	-1.2753
20O	-1.3425	-0.5739	-0.0410
21O	1.3254	0.5113	0.0538
22O	-3.2149	0.8612	-1.3305
23O	3.2348	-0.8085	1.3820
24O	-3.9144	-1.3332	-0.0644
25O	3.8719	1.3386	-0.0227
26O	-2.3396	3.2019	0.0550
27O	2.3384	-3.2365	0.1158
28O	-2.2698	1.9613	-3.4669
29O	2.3575	-1.8107	3.5916
30O	-3.8804	-1.4663	-3.0659
31O	3.8302	1.6217	2.9202
32O	-4.0699	-3.9220	-0.1345
33O	4.0909	3.9343	-0.0747
34O	-6.1337	0.1451	1.2501
35O	6.1265	-0.2067	-1.3228
36O	-6.8416	2.6123	2.5550
37O	6.8228	-2.7203	-2.4980
38O	-4.7182	0.8828	3.4001
39O	4.6405	-1.0789	-3.3889
40O	-4.0581	3.1222	2.1158
41O	4.0324	-3.2447	-2.0003
42O	-1.4105	4.4589	-2.2606
43O	1.5236	-4.3575	2.6337
44O	-0.5857	1.8879	-1.3556
45O	0.6070	-1.8680	1.5249
46O	-4.0504	3.2270	-2.0156
47O	4.0947	-3.1279	2.1492
48O	-6.8473	2.7706	-2.4664
49O	6.8860	-2.6313	2.5230
50O	-6.1700	0.2171	-1.3205
51O	6.1568	-0.1628	1.2340
52O	-5.7980	-2.4555	-1.3971
53O	5.7867	2.5011	1.2670
54O	-8.1087	-1.4876	-0.0584
55O	8.0881	1.5121	-0.0837
56O	-5.7787	-2.5020	1.2802
57O	5.7391	2.4359	-1.4160
58O	-4.1094	-4.4386	2.6309
59O	4.0813	4.3314	-2.8922
60O	-2.0415	-2.9190	1.2414
61O	2.0623	2.9551	-1.4310
62O	1.4324	-4.5036	-2.2316
63O	-1.4331	4.3858	2.4220
64O	-2.9647	-0.0780	-5.3906
65O	3.0797	0.3457	5.3770
66O	-4.7376	1.0918	-3.4214
67O	4.8023	-0.8994	3.4298
68O	-1.4127	-0.4638	-3.0370
69O	1.4077	0.5533	3.0950
70O	-2.1556	-2.8915	-1.6090
71O	2.1087	3.0113	1.3984
72O	-0.3891	-4.3464	-0.0868
73O	0.2252	4.6589	0.0307
74O	-4.1554	-4.3287	-2.9852
75O	4.1731	4.4585	2.7228
76O	-3.7132	-1.6298	2.8371
77O	3.7209	1.4844	-2.9572
78P	-2.8751	-0.0686	-0.0230
79P	2.8638	0.0482	0.0370
80W	-2.9975	-0.0330	3.6089
81W	2.9444	-0.1359	-3.5814
82W	-3.9277	-2.9996	-1.8803
83W	3.9360	3.0942	1.6688
84W	-2.1324	2.9186	-1.8345
85W	2.1438	-2.8566	2.0103
86W	-5.4601	1.9270	-1.8515
87W	5.4752	-1.8351	1.8955
88W	-3.0477	0.1380	-3.6664
89W	3.0913	0.0249	3.6666
90W	-2.1237	2.8529	1.9321
91W	2.1536	-2.9799	-1.7603
92W	-6.3902	-1.2361	-0.0780
93W	6.3694	1.2608	-0.0507
94W	-5.4458	1.8191	1.8929
95W	5.4426	-1.8972	-1.8407
96W	-3.9649	-3.0727	1.5652
97W	3.8820	3.0174	-1.7688

bs1Fe4-SK-O_-8_19

Energy (POTENTIAL) = -6999.29953312 Eh

Atom	X	Y	Z
1 Fe	0.0021	-0.0323	1.8440
2 Fe	-0.0188	-0.0150	-1.8166
3 Fe	0.8110	-2.6731	0.0014
4 Fe	-0.8046	2.6826	0.0161
5 H	0.3898	4.9851	0.7888
6 H	0.3447	5.0018	-0.7798
7 O	1.3626	-0.4881	-3.0244
8 O	-1.3584	0.4844	3.0213
9 O	-0.5538	-1.9305	1.4160
10O	0.5933	1.8755	-1.3985
11O	5.5353	2.3158	0.0053
12O	-5.5279	-2.3647	-0.0071
13O	2.2920	1.8957	-3.4872
14O	-2.2895	-1.8833	3.4773
15O	2.9705	-0.2178	-5.3411
16O	-2.9920	0.2281	5.3218
17O	3.2167	0.8151	-1.3195
18O	-3.2332	-0.8327	1.3239
19O	1.3523	-0.5865	0.0121
20O	-1.3265	0.4861	0.0037
21O	3.2325	0.8021	1.3400
22O	-3.2342	-0.8331	-1.3308
23O	3.9202	-1.3658	-0.0036
24O	-3.8625	1.3773	-0.0108
25O	2.3507	3.2010	0.0215
26O	-2.3501	-3.2523	-0.0025
27O	2.3338	1.8690	3.5306
28O	-2.2795	-1.8748	-3.4813
29O	3.8391	-1.5751	2.9560
30O	-3.8183	1.5632	-2.9541
31O	4.1566	-3.9598	-0.0135
32O	-4.2144	3.9618	-0.0100
33O	6.1715	0.1861	-1.2868
34O	-6.1665	-0.2182	1.2628
35O	6.8551	2.6874	-2.5155
36O	-6.8601	-2.6952	2.5132
37O	4.7386	0.9874	-3.4088
38O	-4.7470	-0.9890	3.4072
39O	4.0656	3.1674	-2.0508
40O	-4.0710	-3.1829	2.0691
41O	1.4629	4.3943	2.3995
42O	-1.5269	-4.4221	-2.4997
43O	0.6262	1.8425	1.4644
44O	-0.5579	-1.9197	-1.4095
45O	4.0848	3.1474	2.0813
46O	-4.0652	-3.1819	-2.0806
47O	6.8759	2.6659	2.5210
48O	-6.8546	-2.7004	-2.5280

49O	6.1843	0.1770	1.2695
50O	-6.1722	-0.2191	-1.2800
51O	5.8259	-2.4761	1.3302
52O	-5.8370	2.4309	-1.3522
53O	8.1351	-1.5051	-0.0208
54O	-8.1429	1.4707	-0.0027
55O	5.8156	-2.4660	-1.3604
56O	-5.8251	2.4260	1.3443
57O	4.1721	-4.3962	-2.8356
58O	-4.2560	4.4011	2.8168
59O	2.1486	-2.9840	-1.4550
60O	-2.1607	3.1056	1.4660
61O	-1.5376	-4.4310	2.4938
62O	1.4504	4.4176	-2.3442
63O	3.0154	-0.2620	5.3557
64O	-2.9750	0.2285	-5.3282
65O	4.7739	0.9523	3.4162
66O	-4.7421	-0.9907	-3.4184
67O	1.3824	-0.5118	3.0542
68O	-1.3685	0.5019	-3.0041
69O	2.1586	-2.9957	1.4490
70O	-2.1749	3.1467	-1.5219
71O	0.3036	-4.1978	-0.0030
72O	-0.1836	4.8083	0.0186
73O	4.1927	-4.4159	2.8057
74O	-4.2879	4.4085	-2.8540
75O	3.8194	-1.5530	-2.9636
76O	-3.8035	1.5603	2.9315
77P	2.8824	-0.0953	0.0079
78P	-2.8682	0.0692	-0.0037
79W	3.0268	0.0433	-3.6158
80W	-3.0431	-0.0416	3.5970
81W	3.9444	-3.0777	1.7073
82W	-3.9407	3.1036	-1.7383
83W	2.1458	2.8524	1.9058
84W	-2.1369	-2.9090	-1.8865
85W	5.4799	1.8469	1.8754
86W	-5.4658	-1.8793	-1.8681
87W	3.0529	0.0177	3.6328
88W	-3.0428	-0.0376	-3.6034
89W	2.1343	2.8727	-1.8634
90W	-2.1404	-2.9146	1.8816
91W	6.4068	-1.2732	-0.0125
92W	-6.4104	1.2591	-0.0105
93W	5.4657	1.8631	-1.8628
94W	-5.4676	-1.8773	1.8567
95W	3.9329	-3.0669	-1.7245
96W	-3.9417	3.0897	1.7022

bs1Fe4-SK-OO_-7_22decoord

Energy (POTENTIAL) = -7074.29900807 Eh

	Atom	X	Y	Z
1	Fe	-0.0110	0.0348	-1.8378
2	Fe	0.0002	-0.1063	1.8308
3	Fe	0.7974	2.5772	0.1119
4	Fe	-0.8764	-2.6767	-0.1028
5	H	0.3029	-4.9102	-0.9715
6	H	0.2967	-4.9656	0.6125
7	O	1.3537	0.3392	3.0384
8	O	-1.3719	-0.4132	-3.0603
9	O	-0.6146	1.8994	-1.3959
10O		0.5303	-1.9990	1.3234
11O		5.4828	-2.4218	-0.0683
12O		-5.5310	2.2777	0.0827
13O		2.2306	-2.0673	3.4212
14O		-2.3308	1.9810	-3.4480
15O		2.9474	-0.0335	5.3568
16O		-2.9986	-0.0746	-5.3560
17O		3.2021	-0.9377	1.3137
18O		-3.2362	0.8532	-1.3029
19O		1.3096	0.4414	0.0244
20O		-1.3551	-0.5616	-0.0278
21O		3.2066	-0.8285	-1.3459
22O		-3.2255	0.7604	1.3515
23O		3.8451	1.3180	0.0838
24O		-3.8993	-1.3825	-0.0503
25O		2.3121	-3.2440	-0.1159
26O		-2.3091	3.2507	0.1098
27O		2.2577	-1.7914	-3.5482
28O		-2.3007	1.7298	3.5579
29O		3.7911	1.6338	-2.8516
30O		-3.7879	-1.6943	2.8750
31O		4.1997	3.9069	0.1898
32O		-4.1258	-3.9721	-0.1419
33O		6.1355	-0.3325	1.2919
34O		-6.1694	0.1915	-1.2675
35O		6.8120	-2.8675	2.4351
36O		-6.8643	2.7355	-2.4177
37O		4.7013	-1.1909	3.3959
38O		-4.7665	1.0531	-3.3757
39O		4.0137	-3.3198	1.9664
40O		-4.0786	3.2082	-1.9539
41O		1.4082	-4.3761	-2.5121
42O		-1.4920	4.2932	2.6346
43O		0.5332	-1.8941	-1.4680
44O		-0.5884	1.8063	1.4918
45O		4.0278	-3.1516	-2.1810
46O		-4.0661	3.0640	2.1738
47O		6.8276	-2.6581	-2.5938
48O		-6.8531	2.5575	2.6124
49O		6.1365	-0.2292	-1.2493
50O		-6.1641	0.1003	1.2908
51O		5.8011	2.4226	-1.2240
52O		-5.7908	-2.5514	1.2557
53O		8.1127	1.4055	0.0881
54O		-8.1166	-1.5366	-0.0469
55O		5.8063	2.3168	1.4696
56O		-5.7959	-2.4565	-1.4268
57O		4.2580	4.2464	3.0458
58O		-4.1710	-4.3270	-2.9661
59O		2.1522	3.0379	1.6500
60O		-2.1152	-2.9905	-1.5246
61O		-1.4959	4.4655	-2.3439
62O		1.3912	-4.5616	2.1744
63O		2.9917	0.4017	-5.3027
64O		-2.9769	-0.4463	5.3308
65O		4.7220	-0.9093	-3.4271
66O		-4.7445	0.8180	3.4410
67O		1.3546	0.5672	-2.9985
68O		-1.3610	-0.6370	3.0140
69O		2.1404	3.1120	-1.3071
70O		-2.1112	-3.0875	1.2992
71O		1.0777	6.6609	-0.5748
72O		-0.2319	-4.7102	-0.1740
73O		4.2329	4.4696	-2.6093
74O		-4.1599	-4.5267	2.6509
75O		3.7956	1.3969	3.0397
76O		-3.7970	-1.4870	-2.9901
77P		2.8508	0.0165	0.0202
78P		-2.8893	-0.0900	-0.0085
79W		3.0210	-0.2242	3.6248
80W		-3.0341	0.1560	-3.6280
81W		3.9249	3.1112	-1.5548
82W		-3.9341	-3.1490	1.6063
83W		2.1109	-2.8532	-1.9901
84W		-2.1294	2.8083	1.9805
85W		5.4390	-1.8607	-1.9105
86W		-5.4602	1.7652	1.9335
87W		3.0374	0.0666	-3.5917
88W		-3.0207	-0.1036	3.6218
89W		2.1018	-3.0032	1.7829
90W		-2.1334	2.9391	-1.7910
91W		6.3815	1.1991	0.0827
92W		-6.3939	-1.2874	-0.0417
93W		5.4305	-2.0126	1.8096
94W		-5.4673	1.8971	-1.8051
95W		3.9192	2.9853	1.8824
96W		-3.9398	-3.0255	-1.8292
97O		1.0711	6.1588	0.5307

bs1Fe4-SK-OO_-7_20coord

Energy (POTENTIAL) = -7074.27646388 Eh

	Atom	X	Y	Z
1	Fe	-0.0115	0.0230	-1.8456
2	Fe	0.0163	-0.0304	1.8223
3	Fe	0.8330	2.6072	0.0465
4	Fe	-0.8655	-2.6569	-0.0501
5	H	0.2951	-4.9151	-0.8837
6	H	0.2948	-4.9424	0.7015
7	O	1.3754	0.4171	3.0219
8	O	-1.3706	-0.4622	-3.0543
9	O	-0.6055	1.9000	-1.4325
10O		0.5415	-1.9440	1.3544
11O		5.4811	-2.4245	-0.0401
12O		-5.5351	2.2824	0.0391
13O		2.2398	-1.9895	3.4525
14O		-2.3342	1.9175	-3.4890
15O		2.9676	0.0731	5.3483
16O		-3.0022	-0.1785	-5.3544
17O		3.2086	-0.9046	1.3199
18O		-3.2338	0.8362	-1.3215
19O		1.3242	0.4735	0.0100
20O		-1.3454	-0.5392	-0.0193
21O		3.2060	-0.8450	-1.3402
22O		-3.2170	0.8022	1.3346
23O		3.8693	1.3197	0.0468
24O		-3.8879	-1.3732	-0.0189
25O		2.3077	-3.2352	-0.0637
26O		-2.3109	3.2612	0.0383
27O		2.2508	-1.8443	-3.5226
28O		-2.2883	1.8197	3.5142
29O		3.7977	1.5860	-2.8898
30O		-3.7709	-1.6248	2.9118
31O		4.2295	3.9088	0.1073
32O		-4.1079	-3.9673	-0.0561
33O		6.1506	-0.3157	1.2801
34O		-6.1677	0.1655	-1.2648
35O		6.8149	-2.8329	2.4691
36O		-6.8741	2.6795	-2.4698
37O		4.7146	-1.1282	3.4020
38O		-4.7690	0.9868	-3.3939
39O		4.0129	-3.2782	2.0153
40O		-4.0891	3.1730	-2.0203
41O		1.3919	-4.4050	-2.4369
42O		-1.5123	4.3708	2.5403
43O		0.5352	-1.8980	-1.4344
44O		-0.5660	1.8895	1.4393
45O		4.0186	-3.1874	-2.1356
46O		-4.0714	3.1192	2.1080
47O		6.8188	-2.7158	-2.5652
48O		-6.8544	2.6080	2.5663
49O		6.1441	-0.2587	-1.2632
50O		-6.1549	0.1277	1.2950
51O		5.8197	2.3940	-1.2858
52O		-5.7742	-2.5220	1.3146
53O		8.1322	1.3898	0.0368
54O		-8.1064	-1.5439	-0.0041
55O		5.8357	2.3380	1.4091
56O		-5.7855	-2.4838	-1.3691
57O		4.2894	4.2981	2.9566

58O	-4.1561	-4.3829	-2.8720
59O	2.1876	3.0537	1.5789
60O	-2.1057	-3.0027	-1.4638
61O	-1.5160	4.4279	-2.4437
62O	1.3810	-4.4984	2.2550
63O	2.9891	0.3136	-5.3183
64O	-2.9517	-0.3241	5.3332
65O	4.7180	-0.9701	-3.4215
66O	-4.7301	0.8996	3.4254
67O	1.3570	0.5280	-3.0144
68O	-1.3459	-0.5474	3.0096
69O	2.1602	3.0929	-1.3583
70O	-2.0946	-3.0435	1.3633
71O	0.2821	4.7551	0.1297
72O	-0.2345	-4.6969	-0.0876
73O	4.2546	4.4197	-2.6989
74O	-4.1338	-4.4636	2.7474
75O	3.8283	1.4517	3.0042
76O	-3.7947	-1.5424	-2.9588
77P	2.8617	0.0276	0.0104
78P	-2.8824	-0.0769	-0.0072
79W	3.0384	-0.1510	3.6205
80W	-3.0373	0.0862	-3.6317
81W	3.9514	3.0809	-1.6199
82W	-3.9161	-3.1080	1.6735
83W	2.1036	-2.8770	-1.9443
84W	-2.1362	2.8668	1.9211
85W	5.4363	-1.8996	-1.8928
86W	-5.4599	1.8089	1.8998
87W	3.0359	0.0080	-3.6022
88W	-3.0070	-0.0180	3.6180
89W	2.1020	-2.9539	1.8301
90W	-2.1444	2.9117	-1.8570
91W	6.4011	1.1879	0.0417
92W	-6.3850	-1.2883	-0.0079
93W	5.4364	-1.9833	1.8311
94W	-5.4732	1.8610	-1.8406
95W	3.9561	3.0142	1.8175
96W	-3.9294	-3.0566	-1.7637
97O	0.9410	5.6666	-0.3480

bs1Fe4-SK-OO_-7_20decoord

Energy (POTENTIAL) = -7074.27375280 Eh

	Atom	X	Y	Z
1	Fe	0.0182	-0.2361	-1.7761
2	Fe	-0.0191	-0.0001	1.7811
3	Fe	0.7621	2.4680	-0.1473
4	Fe	-0.8809	-2.7443	0.2343
5	H	0.2994	-5.0402	-0.4670
6	H	0.3390	-4.9572	1.1098
7	O	1.3097	0.5858	3.1550
8	O	-1.3369	-0.7882	-2.9376
9	O	-0.5010	1.7538	-1.4399
10	O	0.5586	-2.0677	1.5333
11	O	5.5242	-2.3221	0.1230
12	O	-5.4477	2.3185	-0.1884
13	O	2.3122	-1.7799	3.6227
14	O	-2.1608	1.5927	-3.5575
15	O	3.0147	0.4979	5.3546
16	O	-2.8935	-0.6125	-5.2929
17	O	3.1840	-0.8279	1.3952
18	O	-3.1714	0.7254	-1.3679
19	O	1.2955	0.3491	-0.0318
20	O	-1.3360	-0.6219	0.0404
21	O	3.2137	-1.0139	-1.2732
22	O	-3.1591	0.8897	1.2807
23	O	3.7938	1.2843	-0.1008
24	O	-3.8967	-1.3653	0.0905
25	O	2.4143	-3.3106	0.2103
26	O	-2.2591	3.2717	-0.2209
27	O	2.2574	-2.2134	-3.3507
28	O	-2.2365	2.0837	3.3450
29	O	3.6755	1.3042	-3.0486
30	O	-3.8497	-1.3769	3.0392
31	O	3.9805	3.8946	-0.2833
32	O	-4.1789	-3.9452	0.2680
33	O	6.0972	-0.0936	1.2392
34	O	-6.1238	0.1135	-1.3394
35	O	6.8876	-2.4754	2.6573
36	O	-6.7655	2.5380	-2.7233
37	O	4.7401	-0.7801	3.4454
38	O	-4.6510	0.7537	-3.4807
39	O	4.1227	-3.0927	2.2556
40	O	-3.9685	3.0265	-2.3034
41	O	1.4705	-4.6908	-2.0241
42	O	-1.4467	4.5687	2.1953
43	O	0.5702	-2.1242	-1.2410
44	O	-0.5143	2.0176	1.2347
45	O	4.0853	-3.3660	-1.8928
46	O	-4.0070	3.3055	1.8150
47	O	6.8623	-2.8334	-2.3521
48	O	-6.8018	2.8774	2.2938
49	O	6.0986	-0.2628	-1.3158
50	O	-6.1340	0.2941	1.2159
51	O	5.6426	2.3708	-1.5339
52	O	-5.8357	-2.3586	1.4785
53	O	7.9973	1.5546	-0.1514
54	O	-8.1148	-1.4331	0.0436
55	O	5.6590	2.5502	1.1482
56	O	-5.7965	-2.5410	-1.1972
57	O	3.9851	4.5165	2.4808
58	O	-4.1914	-4.5964	-2.5072
59	O	1.9524	3.0388	1.1265
60	O	-2.1231	-3.1711	-1.1832
61	O	-1.3793	4.2045	-2.7515
62	O	1.5661	-4.4327	2.6476
63	O	2.9046	-0.2178	-5.3574
64	O	-3.0395	0.1266	5.3774
65	O	4.7028	-1.2425	-3.3681
66	O	-4.7217	1.2244	3.3107
67	O	1.3124	0.1765	-3.0417
68	O	-1.3863	-0.3944	3.1939
69	O	1.9580	2.8560	-1.5796
70	O	-2.1620	-2.9603	1.6322
71	O	1.0713	6.4151	-0.8055
72	O	-0.2155	-4.7713	0.3238
73	O	3.9512	4.1488	-3.1241
74	O	-4.2633	-4.2026	3.0995
75	O	3.6812	1.7039	2.7948
76	O	-3.7726	-1.7766	-2.8182
77P		2.8392	-0.0467	-0.0016
78P		-2.8551	-0.0989	0.0135
79W		2.9641	0.1282	3.6483
80W		-2.9663	-0.2251	-3.5941
81W		3.7591	2.8921	-1.9285
82W		-3.9947	-2.9404	1.9274
83W		2.1511	-3.1112	-1.6684
84W		-2.0710	3.0170	1.7047
85W		5.4478	-2.0143	-1.7531
86W		-5.4082	1.9973	1.7321
87W		2.9829	-0.3796	-3.6233
88W		-2.9946	0.2455	3.6351
89W		2.1603	-2.8780	2.0886
90W		-2.0648	2.7638	-2.0528
91W		6.2816	1.2585	-0.1270
92W		-6.3863	-1.2266	0.0460
93W		5.4530	-1.7509	1.9856
94W		-5.3924	1.7476	-2.0032
95W		3.7956	3.1031	1.4793
96W		-3.9387	-3.1942	-1.5017
97O		1.1585	6.6241	0.3873

bs1Fe4-SK-O-OH2_TS2-7_20

Energy (POTENTIAL) = -7151.96746490 Eh

	Atom	X	Y	Z
1	Fe	-0.0353	0.1127	1.8173
2	Fe	-0.0328	-0.0507	-1.8178
3	Fe	-0.8072	2.8067	-0.1345
4	Fe	0.8290	-2.6449	0.1052
5	H	-0.3125	-4.8976	0.9729
6	H	-0.3090	-4.9508	-0.6132
7	O	-1.3919	0.3724	-3.0237
8	O	1.3425	-0.3635	3.0275
9	O	0.6020	1.9894	1.3715
10	O	-0.5531	-1.9550	-1.3164
11	O	-5.4835	-2.4502	0.0921
12	O	5.5749	2.2042	-0.0927
13	O	-2.2487	-2.0473	-3.4113
14	O	2.3461	1.9995	3.4236
15	O	-2.9948	-0.0182	-5.3344
16	O	2.9563	-0.0735	5.3389
17	O	-3.2106	-0.9258	-1.2918
18	O	3.2311	0.8403	1.2969
19	O	-1.3363	0.5094	-0.0131
20	O	1.3313	-0.5353	0.0220
21	O	-3.2107	-0.8260	1.3656
22	O	3.2298	0.7370	-1.3602
23	O	-3.9136	1.2973	-0.0484
24	O	3.8644	-1.4091	0.0504
25	O	-2.3043	-3.2360	0.1247
26	O	2.4125	3.1916	-0.1201
27	O	-2.2505	-1.7886	3.5650
28	O	2.3319	1.7276	-3.5651
29	O	-3.8660	1.5985	2.9054
30	O	3.7488	-1.7385	-2.8811
31	O	-4.2677	3.8807	-0.1441
32	O	4.0453	-4.0123	0.1496
33	O	-6.1754	-0.3684	-1.2583
34	O	6.1613	0.1124	1.2690
35	O	-6.8198	-2.9051	-2.4088
36	O	6.9081	2.6457	2.4142
37	O	-4.7286	-1.2045	-3.3687
38	O	4.7620	1.0108	3.3675
39	O	-4.0140	-3.3228	-1.9488
40	O	4.1392	3.1706	1.9402
41	O	-1.3733	-4.3525	2.5128
42	O	1.5604	4.3137	-2.5789
43	O	-0.5539	-1.8444	1.4665
44	O	0.6220	1.8429	-1.4975
45	O	-4.0109	-3.1684	2.1946
46	O	4.1266	3.0140	-2.1877
47	O	-6.8168	-2.7220	2.6202
48	O	6.9008	2.4526	-2.6277
49	O	-6.1736	-0.2757	1.2865
50	O	6.1628	0.0150	-1.2938
51	O	-5.8772	2.3836	1.2632
52	O	5.7356	-2.6250	-1.2490
53	O	-8.1725	1.3369	-0.0438
54	O	8.0808	-1.6495	0.0540
55	O	-5.8798	2.2822	-1.4303
56	O	5.7394	-2.5230	1.4328
57	O	-4.3322	4.2243	-2.9896
58	O	4.0814	-4.3635	2.9747
59	O	-2.2298	2.9721	-1.6114
60	O	2.0585	-2.9803	1.5312
61	O	1.6565	4.5303	2.2987
62	O	-1.3808	-4.5317	-2.1737
63	O	-3.0009	0.3769	5.3310
64	O	2.9481	-0.4780	-5.3293
65	O	-4.7300	-0.9516	3.4539

66	O	4.7508	0.7519	-3.4453
67	O	-1.3906	0.5964	3.0052
68	O	1.3362	-0.6066	-3.0049
69	O	-2.2237	3.0506	1.3690
70	O	2.0561	-3.0824	-1.3000
71	O	-0.3719	4.5395	0.0324
72	O	0.2186	-4.6943	0.1735
73	O	-4.3007	4.4325	2.6648
74	O	4.0709	-4.5779	-2.6413
75	O	-3.8664	1.3815	-3.0115
76	O	3.7527	-1.5134	2.9954
77	P	-2.8654	0.0353	0.0027
78	P	2.8742	-0.1024	0.0040
79	W	-3.0576	-0.2160	-3.6025
80	W	3.0162	0.1411	3.6097
81	W	-3.9930	3.0756	1.6037
82	W	3.8727	-3.1922	-1.6020
83	W	-2.1033	-2.8390	1.9985
84	W	2.1841	2.7789	-1.9840
85	W	-5.4445	-1.8979	1.9361
86	W	5.4927	1.6918	-1.9448
87	W	-3.0590	0.0516	3.6183
88	W	3.0086	-0.1393	-3.6204
89	W	-2.1099	-2.9837	-1.7730
90	W	2.1828	2.9436	1.7765
91	W	-6.4387	1.1536	-0.0380
92	W	6.3634	-1.3675	0.0449
93	W	-5.4481	-2.0330	-1.7857
94	W	5.4955	1.8371	1.7978
95	W	-4.0048	2.9554	-1.8316
96	W	3.8780	-3.0610	1.8340
97	O	0.0125	5.7883	-1.0900
98	H	0.6117	6.2664	-0.4071
99	H	0.6083	5.2883	-1.7228
100	O	1.3658	6.8084	0.8173
101	H	2.2689	7.1052	0.6401
102	H	1.4491	6.0246	1.4096

bs1Fe4-SK-O-OH2_TS1T-7_20

Energy (POTENTIAL) = -7075.51289733 Eh

	Atom	X	Y	Z
1	Fe	-0.0120	-0.1555	1.8206
2	Fe	-0.0279	0.2639	-1.7877
3	Fe	-0.8125	2.8070	0.3443
4	Fe	0.8547	-2.5996	-0.3075
5	H	-0.2788	-4.9604	0.2061
6	H	-0.2846	-4.7680	-1.3695
7	O	-1.3881	0.8629	-2.9159
8	O	1.3579	-0.8199	2.9466
9	O	0.6094	1.7644	1.6859
10	O	-0.5361	-1.6993	-1.5991
11	O	-5.4611	-2.4219	-0.2780
12	O	5.5678	2.2442	0.2732
13	O	-2.2343	-1.4718	-3.6824
14	O	2.3553	1.4493	3.7215
15	O	-2.9858	0.8311	-5.2631
16	O	2.9801	-0.9034	5.2694
17	O	-3.1971	-0.6969	-1.4126
18	O	3.2449	0.6574	1.4290
19	O	-1.3259	0.5255	0.0750
20	O	1.3465	-0.4995	-0.0508
21	O	-3.1952	-1.0112	1.2282
22	O	3.2332	0.9948	-1.2092
23	O	-3.9058	1.3042	0.1616
24	O	3.8830	-1.3517	-0.1729
25	O	-2.2828	-3.1948	-0.3742
26	O	2.4096	3.2122	0.4071
27	O	-2.2267	-2.3003	3.2477
28	O	2.3228	2.3184	-3.2194
29	O	-3.8474	1.1493	3.1224
30	O	3.7599	-1.2016	-3.1130
31	O	-4.2738	3.8720	0.4662
32	O	4.0763	-3.9360	-0.4918
33	O	-6.1676	-0.1625	-1.2917
34	O	6.1742	-0.0345	1.2758
35	O	-6.7988	-2.4971	-2.8170
36	O	6.9078	2.2816	2.8169
37	O	-4.7171	-0.6555	-3.5059
38	O	4.7768	0.5004	3.4978
39	O	-3.9923	-2.9671	-2.4323
40	O	4.1371	2.8658	2.4445
41	O	-1.3468	-4.6710	1.8072
42	O	1.5241	4.7089	-1.8514
43	O	-0.5304	-2.0315	1.1646
44	O	0.6196	2.0901	-1.1647
45	O	-3.9868	-3.4563	1.6852
46	O	4.1107	3.3791	-1.6624
47	O	-6.7917	-3.0889	2.1780
48	O	6.8889	2.9140	-2.1848
49	O	-6.1586	-0.4643	1.2380
50	O	6.1697	0.2850	-1.2702
51	O	-5.8700	2.1657	1.6285
52	O	5.7561	-2.3317	-1.6501
53	O	-8.1659	1.3238	0.1795
54	O	8.0984	-1.5655	-0.2135
55	O	-5.8822	2.4854	-1.0466
56	O	5.7671	-2.6645	1.0120
57	O	-4.3406	4.6512	-2.2976
58	O	4.1235	-4.7343	2.2463
59	O	-2.2366	3.2112	-1.1262
60	O	2.0876	-3.1533	1.0419
61	O	1.6153	4.0990	3.0390
62	O	-1.3523	-4.1136	-2.8454
63	O	-2.9813	-0.4323	5.3279
64	O	2.9446	0.4349	-5.3223
65	O	-4.7089	-1.4603	3.2747
66	O	4.7491	1.3540	-3.2702
67	O	-1.3742	0.1458	3.0619
68	O	1.3447	-0.0806	-3.0426
69	O	-2.2196	2.8377	1.8298
70	O	2.0770	-2.7990	-1.7684
71	O	-0.2784	4.5425	0.6062
72	O	0.2473	-4.6351	-0.5555
73	O	-4.3135	3.9806	3.3232
74	O	4.1016	-4.0388	-3.3383
75	O	-3.8678	1.8473	-2.7560
76	O	3.7767	-1.9294	2.7155
77	P	-2.8542	0.0526	0.0155
78	P	2.8873	-0.0598	0.0002
79	W	-3.0500	0.3641	-3.5837
80	W	3.0311	-0.4031	3.5994
81	W	-3.9962	2.8081	2.0653
82	W	3.8946	-2.8427	-2.0869
83	W	-2.0789	-3.0962	1.5381
84	W	2.1735	3.1059	-1.4882
85	W	-5.4223	-2.1641	1.6301
86	W	5.4874	2.0410	-1.6358
87	W	-3.0383	-0.4901	3.5855
88	W	3.0110	0.4943	-3.5812
89	W	-2.0887	-2.6503	-2.2090
90	W	2.1797	2.6549	2.2475
91	W	-6.4315	1.1500	0.1494
92	W	6.3796	-1.2945	-0.1710
93	W	-5.4303	-1.7232	-2.0696
94	W	5.4957	1.5769	2.0827
95	W	-4.0051	3.2207	-1.3475
96	W	3.9096	-3.2698	1.3248
97	O	-0.4138	5.7085	-0.6097
98	H	-0.1181	6.4756	-0.0886
99	H	0.3851	5.4079	-1.1850

bs1Fe4-SK-O-OH2_TS1B-7_20

Energy (POTENTIAL) = -7075.50721626 Eh

	Atom	X	Y	Z
1	Fe	0.0116	-0.1373	1.8424
2	Fe	-0.0204	0.2406	-1.7834
3	Fe	-0.8300	2.7395	0.3338
4	Fe	0.8879	-2.6046	-0.2573
5	H	-0.2248	-4.9699	0.2986
6	H	-0.2387	-4.8012	-1.2796
7	O	-1.4155	0.8033	-2.9068
8	O	1.3822	-0.7613	2.9721
9	O	0.6001	1.7807	1.6642
10	O	-0.5307	-1.7345	-1.5568
11	O	-5.4419	-2.4879	-0.1910
12	O	5.5488	2.2964	0.2107
13	O	-2.2499	-1.5490	-3.6330
14	O	2.3587	1.5419	3.6817
15	O	-3.0338	0.7276	-5.2319
16	O	3.0200	-0.7596	5.2866
17	O	-3.1979	-0.7533	-1.3669
18	O	3.2458	0.7151	1.4051
19	O	-1.3321	0.5150	0.0851
20	O	1.3523	-0.4943	-0.0386
21	O	-3.1778	-1.0282	1.2752
22	O	3.2204	0.9854	-1.2401
23	O	-3.9119	1.2707	0.1759
24	O	3.8961	-1.3288	-0.1475
25	O	-2.2553	-3.2310	-0.2996
26	O	2.3497	3.2622	0.3386
27	O	-2.1854	-2.2842	3.3069
28	O	2.2873	2.2519	-3.2805
29	O	-3.8487	1.1458	3.1414
30	O	3.7584	-1.2408	-3.0900
31	O	-4.3382	3.8237	0.4533
32	O	4.1135	-3.9126	-0.4154
33	O	-6.1792	-0.2524	-1.2243
34	O	6.1839	0.0457	1.2627
35	O	-6.7889	-2.6101	-2.7260
36	O	6.8979	2.4073	2.7432
37	O	-4.7366	-0.7429	-3.4402
38	O	4.7903	0.6191	3.4736
39	O	-3.9791	-3.0410	-2.3498
40	O	4.1158	2.9527	2.3689
41	O	-1.2800	-4.6626	1.8988
42	O	1.5497	4.6743	-2.0498
43	O	-0.5037	-2.0251	1.2091
44	O	0.5611	2.0811	-1.2139
45	O	-3.9377	-3.4862	1.7726
46	O	4.0749	3.3723	-1.7413
47	O	-6.7392	-3.1579	2.2846
48	O	6.8509	2.9193	-2.2705
49	O	-6.1587	-0.5297	1.3119
50	O	6.1574	0.3083	-1.2894
51	O	-5.8898	2.1129	1.6510
52	O	5.7761	-2.3193	-1.6151
53	O	-8.1973	1.2096	0.2529
54	O	8.1148	-1.4966	-0.2055
55	O	-5.9377	2.3853	-1.0203
56	O	5.7991	-2.5932	1.0532
57	O	-4.5393	4.5587	-2.3048
58	O	4.1785	-4.6465	2.3404
59	O	-2.3128	3.2971	-1.1562
60	O	2.1223	-3.1170	1.1057
61	O	1.5775	4.1658	2.9554
62	O	-1.3287	-4.1705	-2.7637
63	O	-2.9471	-0.3953	5.3639
64	O	2.9215	0.3324	-5.3355
65	O	-4.6739	-1.4744	3.3358
66	O	4.7236	1.3187	-3.3132

67O	-1.3628	0.1685	3.0793
68O	1.3280	-0.1462	-3.0393
69O	-2.2439	2.8275	1.8100
70O	2.0994	-2.8251	-1.7124
71O	-0.3360	4.5014	0.4338
72O	0.2936	-4.6487	-0.4699
73O	-4.3345	3.9737	3.3051
74O	4.1350	-4.0774	-3.2602
75O	-3.8973	1.7746	-2.7206
76O	3.8088	-1.8366	2.7487
77P	-2.8550	0.0213	0.0463
78P	2.8912	-0.0394	-0.0053
79W	-3.0694	0.2757	-3.5484
80W	3.0549	-0.2954	3.6059
81W	-4.0184	2.7844	2.0638
82W	3.9202	-2.8572	-2.0335
83W	-2.0312	-3.1010	1.6092
84W	2.1275	3.1055	-1.5721
85W	-5.3881	-2.2213	1.7138
86W	5.4555	2.0514	-1.6964
87W	-3.0122	-0.4771	3.6230
88W	2.9906	0.4391	-3.5963
89W	-2.0703	-2.7055	-2.1393
90W	2.1662	2.7226	2.1781
91W	-6.4627	1.0522	0.2113
92W	6.3934	-1.2420	-0.1608
93W	-5.4250	-1.8139	-1.9946
94W	5.4923	1.6690	2.0299
95W	-4.1188	3.1526	-1.3607
96W	3.9471	-3.2047	1.3877
97O	-1.2898	5.5353	-0.5603
98H	-1.7994	4.7462	-0.9680
99H	-1.8668	5.9054	0.1313

Co_4-SK species.

Co_4-SK species. Large basis sets BS2

Co4-SK-OH_-10_10

Energy (POTENTIAL) = -7087.40541058 Eh

	Atom	X	Y	Z
1	Co	0.0031	0.0530	-1.6794
2	Co	-0.0096	-0.0120	1.6898
3	Co	-0.8249	-2.5550	-0.0585
4	Co	0.8558	2.6781	0.0546
5	H	-0.3995	4.9107	-0.6867
6	H	-0.0804	-4.4919	-1.0015
7	H	-0.4035	4.8798	0.8740
8	O	-1.3882	-0.5248	3.0945
9	O	1.3986	0.5709	-3.0445
10	O	0.5217	-1.9885	-1.3627
11	O	-0.6204	1.9890	1.4434
12	O	-5.5636	2.3220	0.0237
13	O	5.4869	-2.4203	-0.0186
14	O	-2.3598	1.8825	3.5247
15	O	2.2505	-1.8599	-3.4590
16	O	-3.0510	-0.2795	5.3081
17	O	3.0221	0.2555	-5.2748
18	O	-3.2161	0.8038	1.3017
19	O	3.2039	-0.8154	-1.2883
20	O	-1.3624	-0.5387	-0.0087
21	O	1.3675	0.5438	0.0196
22	O	-3.2017	0.8578	-1.2908
23	O	3.1939	-0.8540	1.2958
24	O	-3.8952	-1.2838	-0.0446
25	O	3.8954	1.2929	0.0370
26	O	-2.4549	3.2988	0.0592
27	O	2.3936	-3.3199	-0.0340
28	O	-2.3256	2.0285	-3.4608
29	O	2.2321	-1.9634	3.4281
30	O	-3.8314	-1.4576	-3.0127
31	O	3.8833	1.4748	2.9926
32	O	-4.1303	-3.9140	-0.1058
33	O	4.2815	3.8932	0.0793
34	O	-6.1979	0.1513	1.2651
35	O	6.1914	-0.2695	-1.2720
36	O	-6.8807	2.6141	2.5282
37	O	6.7921	-2.7399	-2.5268
38	O	-4.8000	0.9232	3.3957
39	O	4.7417	-1.0016	-3.3912
40	O	-4.1410	3.1530	2.1044
41	O	4.0400	-3.2054	-2.0985
42	O	-1.5384	4.5195	-2.2740
43	O	1.5191	-4.4811	2.4445
44	O	-0.6075	2.0445	-1.3627
45	O	0.5004	-2.0516	1.3198
46	O	-4.1202	3.2403	-2.0055
47	O	4.0296	-3.2669	2.0333
48	O	-6.8561	2.7229	-2.4790
49	O	6.7721	-2.8178	2.4918
50	O	-6.1870	0.2079	-1.3154
51	O	6.1764	-0.3109	1.3013
52	O	-5.7829	-2.4231	-1.4248
53	O	5.8884	2.3304	1.4047
54	O	-8.0798	-1.5142	-0.0730
55	O	8.1432	1.3363	0.0553
56	O	-5.7987	-2.4830	1.2618
57	O	5.8977	2.3718	-1.2809
58	O	-4.1210	-4.3817	2.6754
59	O	4.3649	4.3565	-2.7128
60	O	-2.1188	-2.9531	1.3182
61	O	2.2285	3.1079	-1.4251
62	O	1.4859	-4.4006	-2.4881
63	O	-1.5618	4.4214	2.4500
64	O	-2.9952	-0.0554	-5.3400
65	O	2.9889	0.0939	5.3079
66	O	-4.7663	1.0681	-3.3949
67	O	4.7237	-1.0991	3.3967
68	O	-1.3634	-0.3993	-3.1143
69	O	1.3746	0.4741	3.0804
70	O	-2.0981	-2.8832	-1.4676
71	O	2.2186	3.0673	1.5489
72	O	-0.3758	-4.3293	-0.0924
73	O	0.1757	4.7768	0.0930
74	O	-4.0861	-4.2624	-2.8995
75	O	4.3487	4.2738	2.8854
76	O	-3.8557	-1.5821	2.9089
77	O	3.9064	1.5616	-2.9108
78	P	-2.8926	-0.0419	-0.0110
79	P	2.8895	0.0500	0.0170
80	W	-3.0227	-0.0029	3.5973
81	W	3.0134	0.0003	-3.5599
82	W	-3.8804	-2.9604	-1.7749
83	W	3.9969	2.9903	1.7747
84	W	-2.1497	2.9539	-1.8126
85	W	2.0655	-2.9641	1.8307
86	W	-5.4627	1.9118	-1.8579
87	W	5.4015	-1.9743	1.8601
88	W	-2.9888	0.1486	-3.6189
89	W	2.9887	-0.1093	3.5859
90	W	-2.1672	2.8764	1.9182
91	W	2.0985	-2.8963	-1.8843
92	W	-6.3727	-1.2495	-0.0579
93	W	6.4238	1.1546	0.0461
94	W	-5.4801	1.8308	1.8880
95	W	5.4230	-1.9108	-1.8745
96	W	-3.8991	-3.0327	1.6108
97	W	4.0079	3.0398	-1.6434

Co4-SK-OH-11_13

Energy (POTENTIAL) = -7087.57591789 Eh

	Atom	X	Y	Z
1	Co	-0.0060	-0.0638	-1.6642
2	Co	-0.0137	-0.1250	1.6823
3	Co	-0.8594	-2.8912	-0.0686
4	Co	0.8461	2.5925	0.0519
5	H	-0.3869	4.8677	-0.6486
6	H	0.0370	-4.9097	-1.0253
7	H	-0.3863	4.8186	0.9106
8	O	-1.4483	-0.5909	3.0624
9	O	1.4072	0.4818	-3.0389
10	O	0.6461	-2.0400	-1.4400
11	O	-0.6123	1.9112	1.4590
12	O	-5.5481	2.4264	0.0330
13	O	5.6240	-2.3351	0.0026
14	O	-2.3554	1.8309	3.5324
15	O	2.4056	-1.9156	-3.4851
16	O	-3.1085	-0.3290	5.2761
17	O	3.0499	0.2236	-5.2729
18	O	-3.2414	0.7864	1.3007
19	O	3.2689	-0.8237	-1.2802
20	O	-1.3953	-0.5899	-0.0094
21	O	1.3849	0.4831	0.0182
22	O	-3.2255	0.8517	-1.2864
23	O	3.2614	-0.8421	1.3047
24	O	-3.9462	-1.2931	-0.0539
25	O	3.8918	1.3169	0.0301
26	O	-2.4009	3.2745	0.0773
27	O	2.4970	-3.3346	-0.0036
28	O	-2.3077	2.0145	-3.4497
29	O	2.3958	-1.9586	3.4913
30	O	-3.9595	-1.4184	-3.0382
31	O	3.8801	1.5227	2.9773
32	O	-4.3352	-3.8791	-0.1401
33	O	4.2235	3.9279	0.0537
34	O	-6.2620	0.2669	1.2549
35	O	6.2537	-0.1781	-1.2679
36	O	-6.8485	2.7255	2.5480
37	O	6.9196	-2.6468	-2.5133
38	O	-4.8204	0.9525	3.3887
39	O	4.8368	-0.9491	-3.3758
40	O	-4.0954	3.1718	2.1204
41	O	4.1881	-3.1778	-2.0648
42	O	-1.4563	4.4746	-2.2542
43	O	1.6985	-4.4817	2.5095
44	O	-0.5988	1.9650	-1.3524
45	O	0.6239	-2.0977	1.4361
46	O	-4.0651	3.2798	-1.9888
47	O	4.1874	-3.2051	2.0560
48	O	-6.8165	2.8668	-2.4777
49	O	6.9138	-2.6806	2.5204
50	O	-6.2523	0.3408	-1.3154
51	O	6.2509	-0.1983	1.3025
52	O	-5.9562	-2.2927	-1.4442
53	O	5.8737	2.4223	1.3834
54	O	-8.2180	-1.3231	-0.0860
55	O	8.1618	1.4937	0.0321
56	O	-5.9764	-2.3747	1.2397
57	O	5.8712	2.4463	-1.3005
58	O	-4.4716	-4.3831	2.6507
59	O	4.2848	4.3634	-2.7517
60	O	-2.3050	-3.1424	1.4323
61	O	2.1864	3.0915	-1.4292
62	O	1.6586	-4.4500	-2.4779
63	O	-1.4916	4.3577	2.4839
64	O	-3.0315	-0.0353	-5.3255
65	O	3.0295	0.1532	5.3091
66	O	-4.7794	1.1430	-3.3907
67	O	4.8273	-0.9944	3.4000
68	O	-1.4255	-0.4439	-3.0899
69	O	1.3972	0.4345	3.0676
70	O	-2.2826	-2.9877	-1.6358
71	O	2.1892	3.0710	1.5398
72	O	-0.4204	-4.7740	-0.1836
73	O	0.1960	4.7495	0.1279
74	O	-4.4041	-4.2230	-2.9495
75	O	4.2985	4.3297	2.8607
76	O	-3.9732	-1.5889	2.8906
77	O	3.8816	1.5605	-2.9093
78	P	-2.9082	-0.0729	-0.0133
79	P	2.9235	0.0432	0.0180
80	W	-3.0770	-0.0430	3.5641
81	W	3.0393	-0.0453	-3.5568
82	W	-4.0500	-2.9472	-1.8237
83	W	3.9693	3.0307	1.7562
84	W	-2.1126	2.9219	-1.7965
85	W	2.1913	-2.9521	1.8656
86	W	-5.4594	1.9957	-1.8486
87	W	5.5157	-1.8822	1.8811
88	W	-3.0339	0.1521	-3.5995
89	W	3.0292	-0.0895	3.5888
90	W	-2.1335	2.8283	1.9362
91	W	2.2015	-2.9198	-1.8614
92	W	-6.4953	-1.1457	-0.0697
93	W	6.4469	1.2495	0.0308
94	W	-5.4798	1.8960	1.8883
95	W	5.5221	-1.8549	-1.8652
96	W	-4.0739	-3.0563	1.6019
97	W	3.9632	3.0481	-1.6652

Co4-SK-O-10_11

Energy (POTENTIAL) = -7086.73266461 Eh

	Atom	X	Y	Z
1	Co	-0.0025	0.0000	1.6889
2	Co	-0.0020	0.0082	-1.6890

3 Co	0.7668	-2.5427	-0.0055
4 Co	-0.8386	2.6903	0.0057
5 H	0.4409	4.8959	0.7903
6 H	0.4404	4.8999	-0.7699
7 O	1.3625	-0.4423	-3.1172
8 O	-1.3875	0.5555	3.0576
9 O	-0.5306	-1.9976	1.3399
10O	0.6296	2.0307	-1.4036
11O	5.5918	2.2691	0.0056
12O	-5.4998	-2.3793	-0.0054
13O	2.3678	1.9559	-3.4919
14O	-2.2468	-1.8850	3.4358
15O	3.0247	-0.1779	-5.3276
16O	-3.0021	0.1958	5.2883
17O	3.2126	0.8122	-1.2956
18O	-3.2084	-0.8088	1.2876
19O	1.3482	-0.5305	-0.0009
20O	-1.3686	0.5644	0.0012
21O	3.2136	0.8060	1.2992
22O	-3.2082	-0.8034	-1.2914
23O	3.8686	-1.3161	-0.0034
24O	-3.8911	1.3293	0.0026
25O	2.4912	3.2791	0.0067
26O	-2.3511	-3.3518	-0.0074
27O	2.3659	1.9396	3.4995
28O	-2.2464	-1.8693	-3.4442
29O	3.8095	-1.5597	2.9552
30O	-3.8941	1.5576	-2.9438
31O	4.0683	-3.9558	-0.0090
32O	-4.2646	3.9309	0.0089
33O	6.1837	0.1191	-1.2899
34O	-6.1886	-0.2463	1.2856
35O	6.8970	2.6045	-2.4981
36O	-6.7922	-2.7345	2.5024
37O	4.7923	0.9574	-3.3935
38O	-4.7346	-1.0257	3.3908
39O	4.1679	3.1678	-2.0478
40O	-4.0444	-3.2066	2.0446
41O	1.5982	4.4634	2.3688
42O	-1.5467	-4.4124	-2.5281
43O	0.6298	2.0237	1.4113
44O	-0.5308	-1.9912	-1.3479
45O	4.1670	3.1571	2.0623
46O	-4.0442	-3.1974	-2.0590
47O	6.8964	2.5914	2.5116
48O	-6.7921	-2.7230	-2.5148
49O	6.1826	0.1126	1.2916
50O	-6.1884	-0.2402	-1.2871
51O	5.7462	-2.5157	1.3374
52O	-5.8863	2.4019	-1.3379
53O	8.0478	-1.6011	-0.0035
54O	-8.1399	1.3969	0.0033
55O	5.7468	-2.5095	-1.3489
56O	-5.8860	2.3956	1.3489
57O	4.0388	-4.3547	-2.7975
58O	-4.3329	4.3458	2.8092
59O	2.0610	-2.9330	-1.3937
60O	-2.2077	3.1109	1.4926
61O	-1.5476	-4.4246	2.5085
62O	1.5984	4.4737	-2.3512
63O	3.0213	-0.2002	5.3276
64O	-3.0016	0.2200	-5.2874
65O	4.7906	0.9417	3.3988
66O	-4.7341	-1.0106	-3.3955
67O	1.3608	-0.4582	3.1154
68O	-1.3875	0.5695	-3.0546
69O	2.0621	-2.9381	1.3792
70O	-2.2081	3.1175	-1.4789
71O	0.2774	-4.2388	-0.0080
72O	-0.1377	4.7826	0.0100
73O	4.0390	-4.3655	2.7792
74O	-4.3334	4.3583	-2.7898
75O	3.8105	-1.5478	-2.9620
76O	-3.8938	1.5445	2.9509
77P	2.8862	-0.0580	0.0000
78P	-2.8915	0.0793	0.0000
79W	3.0055	0.0611	-3.6116
80W	-2.9979	-0.0286	3.5687
81W	3.8433	-3.0348	1.6868
82W	-3.9864	3.0550	-1.7013
83W	2.1837	2.8990	1.8710
84W	-2.1033	-2.9168	-1.8741
85W	5.4874	1.8177	1.8781
86W	-5.4233	-1.8884	-1.8692
87W	3.0024	0.0472	3.6128
88W	-2.9978	-0.0122	-3.5688
89W	2.1834	2.9068	-1.8610
90W	-2.1031	-2.9256	1.8611
91W	6.3446	-1.3112	-0.0038
92W	-6.4214	1.2102	0.0028
93W	5.4876	1.8280	-1.8688
94W	-5.4234	-1.8969	1.8607
95W	3.8427	-3.0298	-1.6981
96W	-3.9860	3.0472	1.7151

Co4-SK-OH2-10_13
Energy (POTENTIAL) = -7088.07035289 Eh

Atom	X	Y	Z
1 Co	0.0000	0.0000	1.6735
2 Co	0.0000	0.0000	-1.6735
3 Co	2.6906	0.8192	0.0000
4 Co	-2.6906	-0.8192	0.0000
5 H	-4.9177	0.4374	0.7801
6 H	4.9177	-0.4374	-0.7801
7 H	4.9177	-0.4374	0.7801
8 H	-4.9177	0.4374	-0.7801
9 O	0.4722	1.3923	-3.0353
10O	-0.4722	-1.3923	3.0353
11O	2.0541	-0.6248	1.4102
12O	-2.0541	0.6248	-1.4102
13O	-2.3482	5.5912	0.0000
14O	2.3482	-5.5912	0.0000
15O	-1.9436	2.3562	-3.4843
16O	1.9436	-2.3562	3.4843
17O	0.1851	3.0069	-5.2870
18O	-0.1851	-3.0069	5.2870
19O	-0.8227	3.2264	-1.2916
20O	0.8227	-3.2264	1.2916
21O	0.5199	1.3464	0.0000
22O	-0.5199	-1.3464	0.0000
23O	-0.8227	3.2264	1.2916
24O	0.8227	-3.2264	-1.2916
25O	1.3222	3.8591	0.0000
26O	-1.3222	-3.8591	0.0000
27O	-3.3061	2.4855	0.0000
28O	3.3061	-2.4855	0.0000
29O	-1.9436	2.3562	3.4843
30O	1.9436	-2.3562	-3.4843
31O	1.5480	3.8656	2.9509
32O	-1.5480	-3.8656	-2.9509
33O	3.9304	4.2087	0.0000
34O	-3.9304	-4.2087	0.0000
35O	-0.1990	6.2187	-1.2848
36O	0.1990	-6.2187	1.2848
37O	-2.6698	6.8858	-2.5182
38O	2.6698	-6.8858	2.5182
39O	-0.9781	4.7931	-3.3867
40O	0.9781	-4.7931	3.3867
41O	-3.1943	4.1539	-2.0648
42O	3.1943	-4.1539	2.0648
43O	-4.4865	1.5886	2.3700
44O	4.4865	-1.5886	-2.3700
45O	-2.0541	0.6248	1.4102
46O	2.0541	-0.6248	-1.4102
47O	-3.1943	4.1539	2.0648
48O	3.1943	-4.1539	-2.0648
49O	-2.6698	6.8858	2.5182
50O	2.6698	-6.8858	-2.5182
51O	-0.1990	6.2187	1.2848
52O	0.1990	-6.2187	-1.2848
53O	2.4259	5.8507	1.3415
54O	-2.4259	-5.8507	-1.3415
55O	1.4784	8.1364	0.0000
56O	-1.4784	-8.1364	0.0000
57O	2.4259	5.8507	-1.3415
58O	-2.4259	-5.8507	1.3415
59O	4.3533	4.2842	-2.8028
60O	-4.3533	-4.2842	2.8028
61O	3.0922	2.1713	-1.4919
62O	-3.0922	-2.1713	1.4919
63O	4.4865	-1.5886	2.3700
64O	-4.4865	1.5886	-2.3700
65O	0.1851	3.0069	5.2870
66O	-0.1851	-3.0069	-5.2870
67O	-0.9781	4.7931	3.3867
68O	0.9781	-4.7931	-3.3867
69O	0.4722	1.3923	3.0353
70O	-0.4722	-1.3923	-3.0353
71O	3.0922	2.1713	1.4919
72O	-3.0922	-2.1713	-1.4919
73O	4.8043	0.1412	0.0000
74O	-4.8043	-0.1412	0.0000
75O	4.3533	4.2842	2.8028
76O	-4.3533	-4.2842	-2.8028
77O	1.5480	3.8656	-2.9509
78O	-1.5480	-3.8656	2.9509
79P	0.0548	2.8875	0.0000
80P	-0.0548	-2.8875	0.0000
81W	-0.0580	3.0241	-3.5709
82W	0.0580	-3.0241	3.5709
83W	3.0475	3.9514	1.7114
84W	-3.0475	-3.9514	-1.7114
85W	-2.9220	2.1732	1.8655
86W	2.9220	-2.1732	-1.8655
87W	-1.8763	5.4932	1.8696
88W	1.8763	-5.4932	-1.8696
89W	-0.0580	3.0241	3.5709
90W	0.0580	-3.0241	-3.5709
91W	-2.9220	2.1732	-1.8655
92W	2.9220	-2.1732	1.8655
93W	1.2438	6.4226	0.0000
94W	-1.2438	-6.4226	0.0000
95W	-1.8763	5.4932	-1.8696
96W	1.8763	-5.4932	1.8696
97W	3.0475	3.9514	-1.7114
98W	-3.0475	-3.9514	1.7114

Co_4-SK species. Small basis sets BS1
bs1Co4-SK-O-OH2+H2O_TS2-10_11
Energy (POTENTIAL) = -7238.99736427 Eh

Atom	X	Y	Z
1 Co	-0.0094	-0.0252	1.7250
2 Co	-0.0071	-0.0720	-1.7210
3 Co	-0.8679	2.5947	-0.0399
4 Co	0.8206	-2.7398	0.0520
5 H	-0.3983	-4.9626	0.8685
6 H	-0.3935	-4.9862	-0.7010
7 O	-1.4121	0.3913	-3.1050
8 O	1.3924	-0.4702	3.1110

9	O	0.5888	1.9926	1.3893
10	O	-0.6250	-2.0574	-1.3832
11	O	-5.5752	-2.3827	0.0361
12	O	5.5601	2.2751	-0.0557
13	O	-2.3544	-2.0279	-3.4761
14	O	2.3382	1.9522	3.4527
15	O	-3.0528	0.0922	-5.3515
16	O	3.0303	-0.1417	5.3557
17	O	-3.2512	-0.9069	-1.3196
18	O	3.2286	0.8181	1.3154
19	O	-1.3884	0.5046	-0.0134
20	O	1.3584	-0.5890	0.0217
21	O	-3.2504	-0.8669	1.3455
22	O	3.2285	0.7508	-1.3435
23	O	-3.9495	1.2974	-0.0175
24	O	3.9101	-1.4127	0.0372
25	O	-2.4332	-3.3075	0.0478
26	O	2.3981	3.2311	-0.0707
27	O	-2.3509	-1.9251	3.5331
28	O	2.3175	1.7689	-3.5275
29	O	-3.8954	1.5357	2.9437
30	O	3.8612	-1.6846	-2.9111
31	O	-4.2332	3.8880	-0.0426
32	O	4.2091	-4.0024	0.0960
33	O	-6.2262	-0.2763	-1.2733
34	O	6.2052	0.1783	1.2723
35	O	-6.9044	-2.7935	-2.4793
36	O	6.8905	2.7033	2.4557
37	O	-4.8023	-1.0889	-3.3844
38	O	4.7838	1.0153	3.3792
39	O	-4.1283	-3.2752	-2.0196
40	O	4.1146	3.1832	1.9849
41	O	-1.5150	-4.4879	2.4210
42	O	1.5431	4.3446	-2.5627
43	O	-0.6271	-2.0046	1.4459
44	O	0.5904	1.9077	-1.4405
45	O	-4.1261	-3.2157	2.1137
46	O	4.0989	3.0814	-2.1319
47	O	-6.9052	-2.7259	2.5613
48	O	6.8771	2.5834	-2.5870
49	O	-6.2308	-0.2423	1.2870
50	O	6.2007	0.1149	-1.2854
51	O	-5.8865	2.4050	1.3140
52	O	5.8574	-2.5329	-1.2823
53	O	-8.1920	1.4080	-0.0220
54	O	8.1661	-1.5259	0.0367
55	O	-5.8782	2.3724	-1.3716
56	O	5.8543	-2.4659	1.4031
57	O	-4.2907	4.2961	-2.8791
58	O	4.2681	-4.3786	2.9363
59	O	-2.2047	3.0066	-1.5003
60	O	2.1782	-3.1032	1.5593
61	O	1.5797	4.4936	2.3408
62	O	-1.5180	-4.5605	-2.2925
63	O	-3.0442	0.2333	5.3565
64	O	3.0157	-0.4025	-5.3383
65	O	-4.8026	-1.0008	3.4214
66	O	4.7711	0.8544	-3.4250
67	O	-1.4226	0.4948	3.0876
68	O	1.3928	-0.6373	-3.0694
69	O	-2.2149	2.9950	1.4459
70	O	2.1832	-3.1792	-1.4205
71	O	-0.3865	4.4316	0.0539
72	O	0.1684	-4.8203	0.0828
73	O	-4.2842	4.3698	2.7764
74	O	4.2786	-4.5196	-2.7238
75	O	-3.8714	1.4638	-2.9654
76	O	3.8544	-1.5408	2.9902
77	P	-2.9078	0.0212	-0.0007
78	P	2.8785	-0.1270	0.0088
79	W	-3.0398	-0.1443	-3.6110
80	W	3.0209	0.0719	3.6115
81	W	-3.9941	3.0212	1.6877
82	W	3.9596	-3.1664	-1.6481
83	W	-2.1607	-2.9222	1.9168
84	W	2.1346	2.8050	-1.9373
85	W	-5.5005	-1.9092	1.9085
86	W	5.4745	1.7744	-1.9188
87	W	-3.0410	-0.0434	3.6213
88	W	3.0145	-0.1106	-3.6049
89	W	-2.1576	-2.9787	-1.8341
90	W	2.1421	2.9056	1.8123
91	W	-6.4550	1.1831	-0.0149
92	W	6.4280	-1.3037	0.0314
93	W	-5.4978	-1.9631	-1.8480
94	W	5.4828	1.8673	1.8322
95	W	-3.9870	2.9823	-1.7541
96	W	3.9530	-3.0779	1.7965
97	O	-0.0380	6.1641	-1.3316
98	H	0.4986	6.4237	-0.5405
99	H	0.5262	5.5222	-1.8231
100	O	1.3822	6.8037	0.9169
101	H	2.3017	7.0302	0.7250
102	H	1.4300	5.9815	1.4587

Fe-K species.

Fe-K species. Large basis sets BS2

Fe-O_-5_5

Energy (POTENTIAL) = -3888.10764665 Eh

	Atom	X	Y	Z
1	O	0.0324	0.9458	-1.4630
2	Fe	0.0055	0.2829	-3.5807
3	O	-1.3453	1.7712	-3.5286
4	W	-1.6292	2.6699	-1.9780
5	O	0.1223	3.4885	-2.0647
6	W	1.8124	2.5479	-1.9820
7	O	1.4608	1.6723	-3.5312
8	P	0.0001	0.0117	-0.1759
9	O	1.2590	-0.9508	-0.1890
10	W	3.5780	-0.2232	-0.1428
11	O	3.4021	-1.5822	-1.4726
12	W	1.7477	-2.5134	-1.9933
13	O	1.9925	-3.4324	-0.2099
14	W	1.7801	-2.6713	1.4912
15	O	-0.1075	-3.0542	1.4370
16	W	-1.9628	-2.5368	1.4964
17	O	-2.2324	-3.2820	-0.2036
18	W	-1.9292	-2.3829	-1.9888
19	O	-0.1103	-3.0021	-1.8239
20	O	-2.6543	3.9648	-2.4649
21	O	-1.5252	3.0339	-0.0098
22	W	-1.6321	2.5399	1.7911
23	O	-1.2676	1.4153	3.3409
24	W	0.0041	-0.0232	3.4459
25	O	1.3743	1.3215	3.3381
26	W	1.8151	2.4174	1.7872
27	O	0.1210	3.2947	2.1103
28	O	-2.9095	1.3216	-1.3669
29	W	-3.5848	0.0328	-0.1337
30	O	-3.4802	-1.3903	1.1811
31	O	-2.6420	3.7489	2.4814
32	O	0.0330	0.8856	1.1472
33	O	-2.9041	1.2103	1.2354
34	O	2.9119	3.5491	2.4760
35	O	2.9851	0.9980	1.2295
36	O	1.7402	2.9181	-0.0135
37	O	-5.2655	0.3885	-0.1055
38	O	-1.3241	-0.8590	-0.1852
39	O	-3.5116	-1.3369	-1.4619
40	O	5.2802	0.0094	-0.1177
41	O	2.9967	1.1132	-1.3729
42	O	3.3750	-1.6362	1.1713
43	O	2.9235	3.7688	-2.4713
44	O	2.3745	-3.9046	2.5306
45	O	1.2568	-1.2910	2.7571
46	O	2.3732	-3.7420	-3.0284
47	O	1.3074	-1.1717	-3.1138
48	O	-2.6428	-3.5640	-3.0222
49	O	-1.3986	-1.0759	-3.1107
50	O	-2.6413	-3.7248	2.5368
51	O	-1.3374	-1.1996	2.7629
52	O	-0.0064	-0.3750	5.1283
53	O	-0.0034	0.0614	-5.1805

Fe-OH2_-4_6

Energy (POTENTIAL) = -3889.23530695 Eh

	Atom	X	Y	Z
1	O	-1.3990	0.9658	0.0000
2	W	-1.9542	2.6174	1.7225
3	O	-2.4642	3.8691	2.7832
4	O	0.0062	2.9741	1.6381
5	W	1.8130	2.4725	1.7260
6	O	2.5039	3.6405	2.7781
7	O	1.1893	0.8718	0.0000
8	W	1.8130	2.4725	-1.7260
9	O	2.5039	3.6405	-2.7781
10	O	1.2460	1.0954	2.9458
11	W	-0.1296	-0.0910	3.5854
12	O	-0.1052	0.1966	5.2767
13	O	-0.1743	-0.9046	1.2923
14	P	-0.1333	0.0058	0.0000
15	O	-0.1743	-0.9046	-1.2923
16	W	-0.1296	-0.0910	-3.5854
17	O	-0.1052	0.1966	-5.2767
18	O	1.2460	1.0954	-2.9458
19	O	-1.3558	1.2247	-2.9578
20	W	-1.9542	2.6174	-1.7225
21	O	-2.4642	3.8691	-2.7832
22	O	1.1646	-1.5286	-3.4312
23	W	1.4912	-2.6085	-1.8710
24	O	2.5142	-3.8315	-2.5066
25	O	-1.4780	-1.4499	-3.4461
26	W	-1.9868	-2.4541	-1.8488
27	O	-3.0365	-3.6424	-2.5106
28	O	-1.3558	1.2247	2.9578
29	O	-1.4780	-1.4499	3.4461
30	W	-1.9868	-2.4541	1.8488
31	O	-3.0365	-3.6424	2.5106
32	O	1.1646	-1.5286	3.4312
33	W	1.4912	-2.6085	1.8710
34	O	2.5142	-3.8315	2.5066
35	O	0.0062	2.9741	-1.6381
36	O	-2.0465	3.4916	0.0000
37	O	-3.4948	1.6964	-1.3826
38	O	-5.5839	0.1323	0.0000
39	O	-3.1249	-1.1059	1.3401
40	O	-3.1249	-1.1059	-1.3401
41	O	-3.4948	1.6964	1.3826
42	O	2.1272	3.2856	0.0000
43	O	3.3589	1.3566	1.3233
44	W	3.4578	-0.0348	0.0000
45	O	5.1354	-0.3983	0.0000
46	O	2.7602	-1.2611	-1.2978
47	O	2.7602	-1.2611	1.2978
48	O	3.3589	1.3566	-1.3233
49	O	1.4189	-3.0573	0.0000
50	O	-0.2293	-3.3563	2.1057
51	O	-1.8462	-2.9808	0.0000
52	O	-0.2293	-3.3563	-2.1057
53	H	-5.9520	0.5861	-0.7750
54	Fe	-3.4489	0.2557	0.0000
55	H	-5.9520	0.5861	0.7750

Fe-O-OH2-OH2_TS2-5_5

Energy (POTENTIAL) = -4040.95656769 Eh

	Atom	X	Y	Z
1	O	1.4318	-0.62620.9352	
2	Fe	1.7896	-0.10423.2518	
3	O	2.1168	-2.18103.0296	
4	W	1.9712	-2.94461.4193	
5	O	3.5796	-2.06560.7515	
6	W	3.7642	-0.17380.4756	
7	O	3.6148	0.2004	2.2469
8	P	0.2099	-0.10520.0784	
9	O	0.1941	1.4840	0.0479
10	W	1.9598	2.8645	-0.8406
11	O	1.3865	3.6316	0.8084
12	W	-0.00652.9422	2.0303	
13	O	-1.24933.5929	0.5578	
14	W	-1.47072.8903	-1.1593	
15	O	-2.77541.6400	-0.4708	
16	W	-3.4278-0.1360	-0.1492	
17	O	-3.42930.1750	1.6950	
18	W	-1.8871-0.07792.9937		
19	O	-1.41941.7468	2.5174	
20	O	2.5479	-4.54851.6938	
21	O	1.5031	-3.1509-0.5577	
22	W	0.3692	-3.0060-2.0157	
23	O	-0.9006-2.0987	-3.2091	
24	W	-1.3030-0.2280	-3.2227	
25	O	0.4746	0.0552	-3.9133
26	W	2.1391	-0.1986-2.9345	
27	O	1.7337	-2.0941-3.0353	
28	O	0.0348	-3.15771.5819	
29	W	-1.7724-2.92711.0163		
30	O	-3.2922-2.02720.2236		
31	O	0.4147	-4.5748-2.7254	
32	O	0.2974	-0.6476-1.4167	
33	O	-1.0955-3.1655	-0.7680	
34	O	3.2972	-0.0478-4.2001	
35	O	1.9756	1.6082	-2.3167
36	O	3.1869	-0.5103-1.4164	
37	O	-2.4549-4.46981.3517		
38	O	-1.1559-0.60650.7198		
39	O	-2.1926-1.97912.6318		
40	O	3.0564	4.0671	-1.3982
41	O	3.1112	1.6346	0.0308
42	O	0.2896	3.5196	-1.5997
43	O	5.4591	-0.02060.1993	
44	O	-2.46454.0699	-1.9224	
45	O	-1.26651.5707	-2.5692	
46	O	-0.21384.2775	3.1039	
47	O	1.2242	1.9250	2.8647
48	O	-2.76190.1301	4.4661	
49	O	-0.2038-0.38043.5339		
50	O	-5.09350.0074	-0.5561	
51	O	-2.6255-0.5318	-1.8784	
52	O	-2.2502-0.0862	-4.6528	
53	O	2.4237	-0.06205.0083	
54	O	2.9779	1.3119	5.7449
55	H	3.7182	0.9248	6.2420
56	H	3.3829	1.8354	4.8987
57	O	3.7415	2.4554	3.6836
58	H	2.8349	2.6166	3.3289
59	H	4.0077	1.6863	3.1202

Fe-OH_-5_6

Energy (POTENTIAL) = -3888.78109162 Eh

	Atom	X	Y	Z
1	O	-0.4290	-0.8646	1.4196
2	Fe	-0.0892	-0.1639	3.7040
3	O	-1.9979	-0.8594	3.5465
4	W	-2.6740	-1.5419	2.0144
5	O	-1.5304	-3.1004	2.1209
6	W	0.4001	-3.0428	2.0221
7	O	0.5154	-2.0822	3.5599
8	P	-0.0105	-0.0244	0.1505
9	O	1.5559	0.2353	0.1567
10	W	3.2543	-1.4953	0.1233
11	O	3.7584	-0.1957	1.4323
12	W	2.7449	1.4075	1.9430
13	O	3.3753	2.0794	0.1400
14	W	2.8202	1.4845	-1.5483
15	O	1.3423	2.7196	-1.5028
16	W	-0.5358	3.1372	-1.5445
17	O	-0.4091	3.9377	0.1466
18	W	-0.5553	3.0295	1.9484
19	O	1.3365	2.7145	1.7694
20	O	-4.1880	-2.1962	2.5138
21	O	-2.7806	-1.9487	0.0412
22	W	-2.6572	-1.4916	-1.7632
23	O	-1.8176	-0.6967	-3.3374
24	W	-0.0154	-0.0369	-3.4560
25	O	0.5606	-1.8675	-3.3322

26W	0.4331	-3.0152	-1.7562
27O	-1.4742	-2.9934	-2.0737
28O	-3.1844	0.2337	1.3726
29W	-3.1706	1.6673	0.1195
30O	-2.4158	2.8567	-1.2092
31O	-4.1270	-2.0844	-2.4332
32O	-0.3964	-0.8058	-1.1787
33O	-3.1424	0.2944	-1.2333
34O	0.8611	-4.5427	-2.4225
35O	2.1454	-2.3133	-1.2219
36O	0.1493	-3.3886	0.0517
37O	-4.8179	2.1572	0.1009
38O	-0.7595	1.3749	0.1597
39O	-2.4416	2.8462	1.4411
40O	4.6411	-2.5108	0.1077
41O	2.1193	-2.3655	1.3856
42O	3.7401	-0.1769	-1.2130
43O	0.8087	-4.6368	2.5320
44O	3.9209	2.2764	-2.6055
45O	1.6969	0.5023	-2.7940
46O	3.8874	2.2132	2.9520
47O	1.7353	0.4590	3.0950
48O	-0.6153	4.4307	2.9493
49O	-0.6822	1.6556	3.1205
50O	-0.5814	4.4946	-2.5987
51O	-0.6339	1.6484	-2.7910
52O	0.1306	0.2563	-5.1444
53O	0.0312	0.0730	5.5341
54H	0.2583	-0.7356	6.0157

Fe-O-OH2_TS1B2-5_5

Energy (POTENTIAL) = -3964.50559556 Eh

Atom	X	Y	Z
1 O	-0.4566	-0.6262	1.5316
2 W	-2.4740	-0.0968	2.7708
3 O	-3.9437	0.0882	3.6562
4 O	-3.2977	-0.2306	0.9002
5 W	-3.4371	0.2333	-0.8850
6 O	-5.1176	0.5454	-1.0950
7 O	-1.0829	-0.3861	-0.9888
8 W	-1.6968	-2.6471	-1.6263
9 O	-2.3143	-4.1180	-2.2743
10O	-2.7578	1.9698	-0.3896
11W	-1.7102	3.0387	0.8208
12O	-2.8006	4.3103	1.2106
13O	0.1057	1.5533	0.2337
14P	-0.0155	-0.0285	0.1367
15O	1.4006	-0.6131	-0.2844
16W	1.8733	-2.9457	-0.6584
17O	2.4851	-4.5215	-0.9755
18O	0.2008	-2.9681	-1.6213
19O	0.8305	-3.2229	0.8974
20W	-0.7700	-2.9781	2.0279
21O	-1.1460	-4.5988	2.4835
22O	2.5910	-1.9716	-2.1836
23W	2.5966	-0.0643	-2.4105
24O	3.6108	0.1203	-3.7875
25O	3.3253	-2.1903	0.3476
26W	3.5310	-0.3393	0.9581
27O	5.1758	-0.2881	1.4587
28O	-2.1314	1.7267	2.1340
29O	-0.1508	3.5818	1.7935
30W	1.6105	2.7168	1.7651
31O	2.5585	3.8674	2.6337
32O	-0.8399	3.7783	-0.7518
33W	0.7404	3.0819	-1.6033
34O	1.1200	4.3484	-2.7042
35O	-1.6524	-2.9628	0.2095
36O	-2.3339	-2.0279	2.6453
37O	0.2440	-2.3939	3.3931
38O	1.7274	-0.4656	5.1598
39O	1.1132	1.5314	3.0127
40O	2.6739	-0.7583	2.5254
41O	-1.2190	0.0141	4.0439
42O	-3.3296	-1.6227	-1.4193
43O	-2.7661	0.6191	-2.6962
44W	-1.0065	0.2679	-3.3480
45O	-1.1858	0.5797	-5.0308
46O	0.8485	-0.2226	-3.2155
47O	-0.4422	1.9630	-2.6699
48O	-1.4329	-1.6045	-3.2565
49O	2.0580	1.7485	-2.0496
50O	1.7233	3.5536	-0.0828
51O	2.9585	1.4819	1.1026
52O	3.8270	0.0352	-0.9873
53Fe	0.7846	-0.4154	3.5404
54O	3.3542	-0.7602	4.8753
55H	3.2370	-0.7825	3.8127
56H	3.7116	0.1145	5.1059

Fe-O-OH2_TS1B1-5_5

Energy (POTENTIAL) = -3964.50559768 Eh

Atom	X	Y	Z
1 O	1.1672	-0.2115	1.1937
2 Fe	1.0251	0.5747	3.4570
3 O	1.6405	-1.3931	3.5324
4 W	1.9033	-2.3558	2.0380
5 O	3.4749	-1.3292	1.5330
6 W	3.4753	0.5349	1.0429
7 O	3.0408	1.0543	2.7444
8 P	0.0419	0.0144	0.1078
9 O	-0.1744	1.5695	-0.1383
10W	1.5323	3.0970	-0.9132
11O	0.6148	3.9214	0.5410
12W	-0.8554	3.1467	1.6074
13O	-1.9225	3.4810	-0.0884
14W	-1.7744	2.5831	-1.7235
15O	-3.0048	1.2370	-1.1071
16W	-3.4744	-0.5774	-0.6593
17O	-3.8382	-0.0836	1.0933
18W	-2.5256	0.0487	2.6721
19O	-2.2114	1.8383	2.0256
20O	2.6271	-3.8058	2.6291
21O	1.8056	-2.8495	0.0738
22W	0.9114	-3.0349	-1.5474
23O	-0.2255	-2.4488	-3.0303
24W	-0.8569	-0.6617	-3.3353
25O	0.9662	-0.2025	-3.7750
26W	2.4600	-0.1217	-2.5325
27O	2.3179	-2.0466	-2.4480
28O	0.0089	-2.8424	1.9417
29W	-1.6949	-2.9455	1.0973
30O	-3.1522	-2.3783	-0.0453
31O	1.2824	-4.6443	-2.0350
32O	0.4495	-0.6668	-1.2726
33O	-0.6968	-3.2788	-0.5256
34O	3.7863	0.0661	-3.6142
35O	1.9649	1.7043	-2.1773
36O	3.2690	-0.1036	-0.8431
37O	-2.2155	-4.5292	1.5206
38O	-1.3320	-0.6084	0.6074
39O	-2.5070	-1.9104	2.4855
40O	2.5472	4.3808	-1.4421
41O	2.6795	2.1483	0.2904
42O	-0.0548	3.4255	-1.9732
43O	5.1606	0.8785	0.9852
44O	-2.7666	3.5299	-2.7625
45O	-1.1547	1.1836	-2.9192
46O	-1.3634	4.5256	2.5121
47O	0.3130	2.3218	2.6877
48O	-3.7069	0.2754	3.9106
49O	-0.9798	0.0429	3.5690
50O	-5.0445	-0.7272	-1.3476
51O	-2.3297	-1.0157	-2.1837
52O	-1.5564	-0.8062	-4.9013
53O	1.5813	1.1287	5.1642
54O	3.1513	1.6890	5.0961
55H	3.5883	0.9896	5.6117
56H	3.2887	1.4561	4.0617

Fe-K species. Small basis sets BS1

bs1Fe-O_-5_5

Energy (POTENTIAL) = -3887.71527097 Eh

Atom	X	Y	Z
1 O	0.0324	0.9411	-1.4619
2 Fe	0.0084	0.2832	-3.5850
3 O	-1.3481	1.7711	-3.5231
4 W	-1.6504	2.6817	-1.9900
5 O	0.1216	3.4744	-2.0715
6 W	1.8335	2.5596	-1.9907
7 O	1.4682	1.6720	-3.5230
8 P	0.0004	0.0182	-0.1826
9 O	1.2974	-0.9786	-0.1790
10W	3.6049	-0.2220	-0.1361
11O	3.4167	-1.5839	-1.4700
12W	1.7621	-2.5208	-2.0068
13O	2.0025	-3.4346	-0.2153
14W	1.7886	-2.6829	1.5008
15O	-0.1064	-3.0449	1.4390
16W	-1.9709	-2.5506	1.5017
17O	-2.2399	-3.2859	-0.2134
18W	-1.9367	-2.3913	-2.0055
19O	-0.1058	-2.9840	-1.8408
20O	-2.6856	3.9928	-2.4955
21O	-1.5387	3.0212	-0.0185
22W	-1.6475	2.5532	1.7986
23O	-1.2715	1.4245	3.3472
24W	0.0001	-0.0238	3.4618
25O	1.3697	1.3325	3.3475
26W	1.8241	2.4309	1.7981
27O	0.1169	3.3015	2.1101
28O	-2.9153	1.3250	-1.3590
29W	-3.6123	0.0314	-0.1335
30O	-3.4943	-1.4010	1.1768
31O	-2.6750	3.7799	2.4894
32O	0.0325	0.9077	1.1919
33O	-2.9038	1.2116	1.2241
34O	2.9359	3.5827	2.4871
35O	2.9834	1.0047	1.2233
36O	1.7464	2.9049	-0.0189
37O	-5.3144	0.3984	-0.1036
38O	-1.3628	-0.8858	-0.1779
39O	-3.5216	-1.3410	-1.4670
40O	5.3287	0.0241	-0.1084
41O	3.0006	1.1171	-1.3612
42O	3.3886	-1.6435	1.1736
43O	2.9593	3.7946	-2.4945
44O	2.3863	-3.9357	2.5538
45O	1.2452	-1.2946	2.7529
46O	2.3922	-3.7590	-3.0676
47O	1.3170	-1.1705	-3.1089
48O	-2.6504	-3.5840	-3.0655
49O	-1.3997	-1.0763	-3.1089
50O	-2.6518	-3.7576	2.5576
51O	-1.3310	-1.2038	2.7533
52O	-0.0130	-0.3890	5.1650
53O	0.0009	0.0629	-5.1815

bs1Fe-OH2_-4_6

Energy (POTENTIAL) = -

3888.83701969 Eh

	Atom	X	Y	Z
1	O	-0.9373	-1.4189	0.0000
2	W	-2.5885	-2.0148	1.7428
3	O	-3.8439	-2.5701	2.8150
4	O	-2.9653	-0.0576	1.6534
5	W	-2.5228	1.7735	1.7388
6	O	-3.7215	2.4458	2.8064
7	O	-0.9223	1.2128	0.0000
8	W	-2.5228	1.7735	-1.7388
9	O	-3.7215	2.4458	-2.8064
10	O	-1.1254	1.2150	2.9450
11	W	0.0935	-0.1231	3.6134
12	O	-0.2088	-0.1028	5.3260
13	O	0.9334	-0.1483	1.3303
14	P	-0.0131	-0.1434	0.0000
15	O	0.9334	-0.1483	-1.3303
16	W	0.0935	-0.1231	-3.6134
17	O	-0.2088	-0.1028	-5.3260
18	O	-1.1254	1.2150	-2.9450
19	O	-1.2006	-1.3703	-2.9605
20	W	-2.5885	-2.0148	-1.7428
21	O	-3.8439	-2.5701	-2.8150
22	O	1.5123	1.1944	-3.4443
23	W	2.5917	1.5500	-1.8792
24	O	3.8117	2.6116	-2.5210
25	O	1.4800	-1.4484	-3.4595
26	W	2.4937	-1.9544	-1.8572
27	O	3.7112	-3.0084	-2.5228
28	O	-1.2006	-1.3703	2.9605
29	O	1.4800	-1.4484	3.4595
30	W	2.4937	-1.9544	1.8572
31	O	3.7112	-3.0084	2.5228
32	O	1.5123	1.1944	3.4443
33	W	2.5917	1.5500	1.8792
34	O	3.8117	2.6116	2.5210
35	O	-2.9653	-0.0576	-1.6534
36	O	-3.4375	-2.1178	0.0000
37	O	-1.6298	-3.5219	-1.3832
38	O	0.0200	-5.5897	0.0000
39	O	1.1563	-3.0933	1.3437
40	O	1.1563	-3.0933	-1.3437
41	O	-1.6298	-3.5219	1.3832
42	O	-3.3346	2.0618	0.0000
43	O	-1.4335	3.3393	1.3226
44	W	-0.0332	3.4742	0.0000
45	O	0.3110	5.1796	0.0000
46	O	1.2086	2.7769	-1.2885
47	O	1.2086	2.7769	1.2885
48	O	-1.4335	3.3393	-1.3226
49	O	3.0213	1.4858	0.0000
50	O	3.3604	-0.1698	2.1131
51	O	2.9970	-1.8061	0.0000
52	O	3.3604	-0.1698	-2.1131
53	H	-0.3775	-6.0140	-0.7772
54	Fe	-0.1946	-3.4872	0.0000
55	H	-0.3775	-6.0140	0.7772

bs1Fe-OH_-5_6

Energy (POTENTIAL) = -3888.39010681 Eh

	Atom	X	Y	Z
1	O	-0.4246	-0.8578	1.4229
2	Fe	-0.0884	-0.1661	3.7145
3	O	-2.0027	-0.8599	3.5393
4	W	-2.6995	-1.5441	2.0245
5	O	-1.5240	-3.0894	2.1295
6	W	0.4133	-3.0640	2.0312
7	O	0.5193	-2.0889	3.5530
8	P	-0.0117	-0.0299	0.1588
9	O	1.6044	0.2402	0.1480
10	W	3.2780	-1.5067	0.1197
11	O	3.7699	-0.2005	1.4341
12	W	2.7600	1.4115	1.9567
13	O	3.3880	2.0769	0.1460
14	W	2.8329	1.4911	-1.5562
15	O	1.3357	2.7065	-1.5013
16	W	-0.5393	3.1497	-1.5518
17	O	-0.4170	3.9462	0.1528
18	W	-0.5599	3.0410	1.9608
19	O	1.3309	2.7014	1.7823
20	O	-4.2320	-2.2072	2.5384
21	O	-2.7788	-1.9320	0.0500
22	W	-2.6716	-1.4974	-1.7720
23	O	-1.8238	-0.7051	-3.3464
24	W	-0.0152	-0.0365	-3.4728
25	O	0.5533	-1.8774	-3.3427
26	W	0.4387	-3.0319	-1.7665
27	O	-1.4774	-2.9998	-2.0736
28	O	-3.1905	0.2329	1.3654
29	W	-3.1961	1.6796	0.1183
30	O	-2.4259	2.8700	-1.2094
31	O	-4.1674	-2.0964	-2.4383
32	O	-0.4066	-0.8253	-1.2209
33	O	-3.1410	0.2886	-1.2200
34	O	0.8776	-4.5836	-2.4297
35	O	2.1400	-2.3105	-1.2165
36	O	0.1604	-3.3809	0.0574
37	O	-4.8690	2.1658	0.0966
38	O	-0.7788	1.4182	0.1491
39	O	-2.4519	2.8558	1.4396
40	O	4.6773	-2.5445	0.1002
41	O	2.1200	-2.3695	1.3731
42	O	3.7567	-0.1756	-1.2126
43	O	0.8307	-4.6759	2.5569
44	O	3.9433	2.2982	-2.6300
45	O	1.6911	0.5070	-2.7883
46	O	3.9113	2.2273	2.9888
47	O	1.7431	0.4603	3.0931
48	O	-0.6177	4.4495	2.9930
49	O	-0.6884	1.6542	3.1094
50	O	-0.5731	4.5232	-2.6240
51	O	-0.6253	1.6476	-2.7876
52	O	0.1336	0.2685	-5.1822
53	O	0.0266	0.0737	5.5315
54	H	0.2515	-0.7201	6.0386

bs1Fe-O-OH2-OH2_TS2-5_5

Energy (POTENTIAL) = -4040.56912036 Eh

	Atom	X	Y	Z
1	O	0.7894	-1.1400	0.9233
2	Fe	2.5291	-0.6796	2.5247
3	O	1.1977	-2.0592	3.4200
4	W	-0.2199	-2.6925	2.5414
5	O	0.9070	-3.6961	1.2984
6	W	2.1392	-2.9651	0.0025
7	O	3.1918	-2.2566	1.2910
8	P	0.0324	-0.0551	0.0802
9	O	1.0788	0.7932	-0.8571
10	W	2.4803	-0.1877	-2.5497
11	O	3.5296	1.0396	-1.5217
12	W	2.9603	2.1084	0.0488
13	O	1.9509	3.1588	-1.3733
14	W	0.4658	2.6244	-2.3930
15	O	-0.7201	3.1905	-0.9755
16	W	-2.0940	2.9210	0.3464
17	O	-0.9237	3.4761	1.7109
18	W	0.4223	2.3503	2.7392
19	O	1.6489	2.7627	1.2924
20	O	-0.8252	-3.9496	3.5970
21	O	-1.6238	-2.8023	1.0756
22	W	-2.9143	-2.1193	-0.0872
23	O	-3.6036	-0.8638	-1.4291
24	W	-2.5863	0.4346	-2.4232
25	O	-1.7956	-1.0652	-3.3538
26	W	-0.5493	-2.3719	-2.6120
27	O	-2.0751	-3.0141	-1.5932
28	O	-1.3260	-1.1412	3.0100
29	W	-2.4500	0.3624	2.6603
30	O	-3.0773	1.9216	1.6803
31	O	-4.3074	-3.1329	0.1897
32	O	-1.0949	-0.7370	-0.9048
33	O	-3.1453	-0.7146	1.2162
34	O	-0.4669	-3.5492	-3.8969
35	O	0.8812	-1.1623	-3.0489
36	O	0.6177	-3.0502	-1.3063
37	O	-3.6872	0.2053	3.8779
38	O	-0.7382	1.0035	1.0692
39	O	-1.2068	1.5504	3.5140
40	O	3.5916	-0.6223	-3.8210
41	O	2.7259	-1.5863	-1.2771
42	O	1.6185	1.3841	-3.3193
43	O	3.0375	-4.3733	-0.5108
44	O	0.3059	3.9098	-3.5610
45	O	-1.0245	1.4596	-2.8485
46	O	4.3176	3.1935	0.2580
47	O	3.3475	0.7310	1.1321
48	O	0.8672	3.5053	3.9757
49	O	1.3853	0.8946	3.1345
50	O	-3.1193	4.3132	0.1187
51	O	-2.7915	1.6696	-0.9755
52	O	-3.7568	1.0011	-3.5856
53	O	3.7958	-0.7839	3.8641
54	O	5.3917	-0.3357	3.6605
55	H	5.8029	-1.0121	4.2252
56	H	5.5392	-0.6205	2.6463
57	O	5.5421	-0.9149	1.2409
58	H	4.9928	-0.1654	0.9224
59	H	4.8962	-1.6559	1.1648

bs1Fe-O-OH2_TS1B1-5_5

Energy (POTENTIAL) = -3964.11737706 Eh

	Atom	X	Y	Z
1	O	-0.7456	-0.2147	1.4985
2	W	-2.8566	0.7767	2.2804
3	O	-4.4119	1.2968	2.8898
4	O	-3.3851	0.3543	0.3604
5	W	-3.2439	0.4542	-1.4967
6	O	-4.8478	0.8998	-2.0201
7	O	-1.0143	-0.4418	-1.1316
8	W	-1.8217	-2.7084	-1.3981
9	O	-2.5471	-4.2296	-1.8494
10	O	-2.4026	2.1661	-1.2024
11	W	-1.4021	3.3672	-0.0689
12	O	-2.3731	4.8145	-0.1033
13	O	0.2784	1.6275	-0.0883
14	P	-0.0522	0.0340	0.1140
15	O	1.3605	-0.7944	0.0209
16	W	1.5304	-3.1890	0.1703
17	O	1.9574	-4.8772	0.2504
18	O	0.0011	-3.2024	-1.0144
19	O	0.2410	-3.0154	1.5576
20	W	-1.4477	-2.3973	2.3725
21	O	-2.1031	-3.8582	3.0752
22	O	2.5744	-2.6103	-1.3712
23	W	2.8792	-0.7908	-1.9405
24	O	4.1038	-0.9919	-3.1655
25	O	2.9150	-2.3926	1.2449
26	W	3.2845	-0.4831	1.5530
27	O	4.8567	-0.5032	2.3103
28	O	-2.1696	2.3796	1.3717

29O	0.0772	3.9142	1.0243
30W	1.7032	2.8785	1.4488
31O	2.6779	4.0843	2.2591
32O	-0.2213	3.6645	-1.5917
33W	1.3551	2.6437	-2.0444
34O	2.0666	3.6210	-3.3013
35O	-2.0489	-2.6359	0.4600
36O	-2.9262	-1.1526	2.5367
37O	-0.5617	-1.6377	3.7332
38O	0.8876	0.4535	5.3442
39O	0.8666	2.0215	2.7763
40O	2.1615	-0.4804	2.9863
41O	-1.7666	0.9990	3.6783
42O	-3.3099	-1.4817	-1.6405
43O	-2.2793	0.3802	-3.2073
44W	-0.4975	-0.2818	-3.5020
45O	-0.3949	-0.2967	-5.2429
46O	1.2349	-0.9118	-2.9627
47O	0.1943	1.4463	-3.0479
48O	-1.1996	-2.0407	-3.1298
49O	2.5159	1.1012	-2.0064
50O	2.1694	3.3063	-0.4819
51O	2.9297	1.3817	1.2594
52O	3.8930	-0.5441	-0.3697
53Fe	0.2113	0.2704	3.6157
54O	2.4706	-0.0936	5.4271
55H	2.5398	-0.3146	4.4113
56H	2.9265	0.7548	5.5682

bs1Fe-O-OH2_TS1B2-5_5

Energy (POTENTIAL) = -3964.11738995 Eh

	Atom	X	Y	Z
1	O	1.2083	-0.3235	1.1340
2	Fe	1.2090	0.3433	3.4357
3	O	1.7517	-1.6538	3.3707
4	W	1.9119	-2.5647	1.8363
5	O	3.4842	-1.5370	1.3066
6	W	3.5673	0.3550	0.9111
7	O	3.2076	0.7928	2.6388
8	P	0.0570	-0.0090	0.1162
9	O	-0.1288	1.6116	-0.0589
10	W	1.6191	3.0915	-0.8302
11	O	0.7892	3.8648	0.7108
12	W	-0.6619	3.0911	1.8179
13	O	-1.7892	3.5452	0.1867
14	W	-1.7580	2.7270	-1.5076
15	O	-2.9900	1.3743	-0.8994
16	W	-3.5302	-0.4423	-0.5279
17	O	-3.7856	-0.0291	1.2796
18	W	-2.4069	-0.0193	2.7986
19	O	-2.0284	1.7886	2.2320
20	O	2.6165	-4.0849	2.3360
21	O	1.6838	-2.9257	-0.1383
22	W	0.7276	-3.0113	-1.7469
23	O	-0.4475	-2.2991	-3.1420
24	W	-1.0325	-0.4695	-3.3366
25	O	0.7941	-0.0642	-3.8321
26	W	2.3528	-0.0866	-2.6580
27	O	2.1346	-2.0139	-2.6494
28	O	-0.0086	-2.9642	1.7926
29	W	-1.7624	-2.9784	1.0363
30	O	-3.2460	-2.2853	-0.0117
31	O	1.0216	-4.6304	-2.3270
32	O	0.3760	-0.6448	-1.3660
33	O	-0.8341	-3.2345	-0.6452
34	O	3.6557	0.1152	-3.8006
35	O	1.9288	1.7286	-2.1678
36	O	3.2239	-0.1695	-0.9950
37	O	-2.3228	-4.5884	1.4015
38	O	-1.3666	-0.6293	0.6459
39	O	-2.4739	-1.9758	2.5056
40	O	2.6727	4.3779	-1.3530
41	O	2.7770	2.0221	0.2610
42	O	-0.0150	3.5236	-1.7899
43	O	5.2840	0.6456	0.7958
44	O	-2.7803	3.7668	-2.4641
45	O	-1.2420	1.3536	-2.7869
46	O	-1.0753	4.4478	2.8429
47	O	0.5241	2.1574	2.7776
48	O	-3.5130	0.1890	4.1396
49	O	-0.8093	-0.1385	3.5825
50	O	-5.1560	-0.4941	-1.1573
51	O	-2.4589	-0.8226	-2.1168
52	O	-1.8261	-0.5050	-4.8894
53	O	1.8452	0.7847	5.1362
54	O	3.4271	1.3143	5.0511
55	H	3.8665	0.5823	5.5186
56	H	3.5405	1.1425	4.0278

Co-K species.

Co-K species. Large basis sets BS2

Co-O-OH2_TS1B-5_2
Energy (POTENTIAL) = -3986.09675476 Eh

	Atom	X	Y	Z
1	O	-0.6835	-0.2645	1.5733
2	W	-2.8738	0.7016	2.3257
3	O	-4.4145	1.2042	2.9175
4	O	-3.4003	0.3316	0.3921
5	W	-3.2128	0.4920	-1.4413
6	O	-4.7829	0.9597	-1.9708
7	O	-0.9844	-0.4334	-1.0185
8	W	-1.8343	-2.6740	-1.4020
9	O	-2.5684	-4.1518	-1.8925
10	O	-2.3541	2.1829	-1.1275
11	W	-1.3365	3.3123	0.0674
12	O	-2.2573	4.7640	0.0657
13	O	0.3205	1.5382	0.0132
14	P	-0.0034	-0.0056	0.1506
15	O	1.3448	-0.8305	0.0433
16	W	1.5015	-3.2303	0.1323
17	O	1.8975	-4.9030	0.1713
18	O	-0.0225	-3.2171	-1.0527
19	O	0.2358	-3.0750	1.5390
20	W	-1.4522	-2.4498	2.3543
21	O	-2.0939	-3.8975	3.0336
22	O	2.5387	-2.6465	-1.4160
23	W	2.8748	-0.8293	-1.9334
24	O	4.0649	-1.0155	-3.1612
25	O	2.9169	-2.5002	1.1941
26	W	3.3071	-0.6015	1.5340
27	O	4.8599	-0.6531	2.2786
28	O	-2.1548	2.3232	1.4633
29	O	0.1423	3.8010	1.1863
30	W	1.7712	2.7583	1.5379
31	O	2.7496	3.9237	2.3486
32	O	-0.1582	3.6421	-1.4432
33	W	1.3969	2.6147	-1.9306
34	O	2.0996	3.6079	-3.1464
35	O	-2.0754	-2.6592	0.4483
36	O	-2.9423	-1.2251	2.5246
37	O	-0.5684	-1.7065	3.7372
38	O	0.6382	0.3271	5.0772
39	O	0.9831	1.8614	2.8940
40	O	2.1785	-0.6168	2.9461
41	O	-1.8008	0.9157	3.7267
42	O	-3.3019	-1.4371	-1.6318
43	O	-2.2480	0.4422	-3.1497
44	W	-0.4887	-0.2329	-3.4582
45	O	-0.3970	-0.2103	-5.1755
46	O	1.2341	-0.9003	-2.9592
47	O	0.2111	1.4820	-2.9711
48	O	-1.1953	-1.9836	-3.1167
49	O	2.5514	1.0770	-1.9383
50	O	2.2247	3.2440	-0.3649
51	O	3.0035	1.2811	1.2679
52	O	3.9174	-0.6302	-0.3906
53	Co	0.1693	0.1110	3.4066
54	O	2.3724	0.8000	5.0485
55	H	2.5328	0.1560	4.2735
56	H	2.1651	1.6337	4.5744

Co-O-OH2_TS1B2-5_2
Energy (POTENTIAL) = -3986.09758094 Eh

	Atom	X	Y	Z
1	O	1.2150	-0.1854	1.2084
2	Co	1.2175	0.4530	3.1720
3	O	1.8927	-1.4126	3.4235
4	W	2.0064	-2.3938	1.8863
5	O	3.5556	-1.3784	1.3062
6	W	3.6170	0.5079	0.8773
7	O	3.2885	0.9750	2.5885
8	P	0.0491	0.0625	0.1459
9	O	-0.1366	1.6223	-0.0558
10	W	1.5689	3.1350	-0.8975
11	O	0.7540	3.9262	0.6313
12	W	-0.6761	3.1538	1.7611
13	O	-1.8291	3.5638	0.1317
14	W	-1.7964	2.6947	-1.5226
15	O	-3.0099	1.3496	-0.8782
16	W	-3.4955	-0.4778	-0.4701
17	O	-3.7765	-0.0177	1.3093
18	W	-2.3852	0.0774	2.8144
19	O	-2.0625	1.8749	2.1936
20	O	2.7309	-3.8554	2.4338
21	O	1.7916	-2.8355	-0.0503
22	W	0.7966	-2.9659	-1.6358
23	O	-0.4084	-2.3251	-3.0254
24	W	-1.0199	-0.5158	-3.2765
25	O	0.7810	-0.0909	-3.7901
26	W	2.3555	-0.0556	-2.6370
27	O	2.1658	-1.9833	-2.5845
28	O	0.0980	-2.8062	1.9193
29	W	-1.6633	-2.8953	1.1601
30	O	-3.1635	-2.2951	0.0817
31	O	1.1095	-4.5708	-2.1733
32	O	0.4160	-0.5992	-1.2468
33	O	-0.7402	-3.2031	-0.5161
34	O	3.6136	0.1293	-3.7974
35	O	1.9043	1.7646	-2.2203
36	O	3.2597	-0.1025	-1.0121
37	O	-2.1629	-4.4887	1.5686
38	O	-1.3048	-0.5572	0.6876
39	O	-2.4164	-1.8995	2.5856
40	O	2.5678	4.4175	-1.4562
41	O	2.7793	2.1345	0.2019
42	O	-0.0711	3.5067	-1.8545
43	O	5.3058	0.8053	0.7183
44	O	-2.8244	3.6824	-2.4852
45	O	-1.2648	1.3141	-2.7918
46	O	-1.0926	4.5179	2.7330
47	O	0.5187	2.2635	2.7512
48	O	-3.4659	0.2950	4.1445
49	O	-0.7859	-0.0309	3.5692
50	O	-5.0975	-0.5829	-1.0890
51	O	-2.4347	-0.8817	-2.0556
52	O	-1.8027	-0.6175	-4.8048
53	O	1.5947	0.8514	4.8388
54	O	3.2523	0.1907	5.0327
55	H	2.9455	-0.7023	4.7249
56	H	3.5439	0.5993	4.1542

Co-O-OH2_TS2-5_2
Energy (POTENTIAL) = -4062.54338266 Eh

	Atom	X	Y	Z
1	O	-0.8301	1.0041	0.9908
2	Co	-2.2559	0.3034	2.5869
3	O	-1.1951	1.7182	3.4905
4	W	0.0868	2.5872	2.5716
5	O	-1.2234	3.5233	1.4752
6	W	-2.4525	2.6496	0.2825
7	O	-3.2809	1.7673	1.6415
8	P	-0.0124	0.0262	0.0589
9	O	-1.0098	-0.8837	-0.7741
10	W	-2.6781	-0.0568	-2.3275
11	O	-3.4857	-1.4094	-1.2530
12	W	-2.6448	-2.4174	0.2214
13	O	-1.6707	-3.3316	-1.3036
14	W	-0.3554	-2.5975	-2.4175
15	O	0.9982	-3.0745	-1.1253
16	W	2.4254	-2.6510	0.0888
17	O	1.4599	-3.3696	1.5193
18	W	0.0864	-2.4123	2.6788
19	O	-1.1700	-2.9759	1.3080
20	O	0.5696	3.8384	3.6552
21	O	1.3499	2.9558	1.0326
22	W	2.6033	2.4474	-0.2493
23	O	3.3332	1.3168	-1.6708
24	W	2.3941	-0.0658	-2.6175
25	O	1.3599	1.3394	-3.4389
26	W	0.0389	2.4666	-2.5531
27	O	1.5535	3.2716	-1.6462
28	O	1.4157	1.2023	2.9335
29	W	2.6813	-0.1293	2.4243
30	O	3.4069	-1.5700	1.3560
31	O	3.8676	3.6000	-0.0607
32	O	0.8956	0.8591	-0.9426
33	O	3.1345	1.0593	0.9802
34	O	-0.2724	3.6393	-3.7738
35	O	-1.2657	1.1136	-2.9423
36	O	-1.0815	2.9899	-1.1488
37	O	3.9684	0.1410	3.5316
38	O	0.9165	-0.9069	0.9446
39	O	1.6656	-1.4664	3.3487
40	O	-3.9217	0.2562	-3.4730
41	O	-2.9993	1.2638	-1.0004
42	O	-1.7112	-1.4910	-3.2170
43	O	-3.5599	3.9196	-0.0787
44	O	-0.1572	-3.8157	-3.6159
45	O	0.9434	-1.2642	-2.9755
46	O	-3.8413	-3.6238	0.5190
47	O	-3.0658	-1.1046	1.3893
48	O	-0.1142	-3.6201	3.8946
49	O	-1.0273	-1.1016	3.1832
50	O	3.5703	-3.8887	-0.2522
51	O	2.8810	-1.2998	-1.2440
52	O	3.5089	-0.4442	-3.8723
53	O	-3.3650	0.0478	4.0606
54	O	-5.1439	0.0680	4.1687
55	H	-5.2231	0.9752	4.5039
56	H	-5.3469	0.1144	3.1559
57	O	-5.4614	0.1921	1.6416
58	H	-4.8149	-0.5112	1.4108
59	H	-4.8848	0.9813	1.5130

Co-OH2_-5_4
Energy (POTENTIAL) = -3911.03918881 Eh

	Atom	X	Y	Z
1	O	-1.4352	0.9489	0.0000
2	W	-2.0385	2.5713	1.7194
3	O	-2.4937	3.8416	2.7956
4	O	-0.0414	2.9658	1.6226
5	W	1.7540	2.5010	1.7221
6	O	2.4249	3.6815	2.7829
7	O	1.1686	0.8859	0.0000
8	W	1.7540	2.5010	-1.7221
9	O	2.4249	3.6815	-2.7829
10	O	1.2261	1.1093	2.9432
11	W	-0.1335	-0.1091	3.5699
12	O	-0.1136	0.1829	5.2657
13	O	-0.1754	-0.9120	1.2898
14	P	-0.1580	0.0126	0.0000
15	O	-0.1754	-0.9120	-1.2898
16	W	-0.1335	-0.1091	-3.5699
17	O	-0.1136	0.1829	-5.2657
18	O	1.2261	1.1093	-2.9432
19	O	-1.3808	1.1859	-2.9500
20	W	-2.0385	2.5713	-1.7194
21	O	-2.4937	3.8416	-2.7956

22O	1.2093	-1.5048	-3.4275
23W	1.5471	-2.5937	-1.8722
24O	2.6124	-3.7837	-2.5153
25O	-1.4362	-1.5053	-3.4514
26W	-1.9648	-2.5120	-1.8437
27O	-2.9210	-3.7787	-2.5234
28O	-1.3808	1.1859	2.9500
29O	-1.4362	-1.5053	3.4514
30W	-1.9648	-2.5120	1.8437
31O	-2.9210	-3.7787	2.5234
32O	1.2093	-1.5048	3.4275
33W	1.5471	-2.5937	1.8722
34O	2.6124	-3.7837	2.5153
35O	-0.0414	2.9658	-1.6226
36O	-2.1197	3.4604	0.0000
37O	-3.5766	1.6911	-1.4495
38O	-5.6731	0.2165	0.0000
39O	-3.1703	-1.2646	1.3990
40O	-3.1703	-1.2646	-1.3990
41O	-3.5766	1.6911	1.4495
42O	2.0859	3.3227	0.0000
43O	3.3343	1.4127	1.3252
44W	3.4560	0.0277	0.0000
45O	5.1464	-0.3020	0.0000
46O	2.7911	-1.2096	-1.2986
47O	2.7911	-1.2096	1.2986
48O	3.3343	1.4127	-1.3252
49O	1.5146	-3.0480	0.0000
50O	-0.1308	-3.3765	2.1032
51O	-1.7706	-3.0512	0.0000
52O	-0.1308	-3.3765	-2.1032
53H	-5.8823	0.7692	-0.7694
54Co	-3.5137	0.1706	0.0000
55H	-5.8823	0.7692	0.7694

Co-OH_-5_1

Energy (POTENTIAL) = -3910.37073060 Eh

Atom	X	Y	Z
1 O	-1.4379	0.9330	0.0022
2 W	-2.0140	2.5704	1.7176
3 O	-2.5818	3.7974	2.7828
4 O	-0.0549	2.9792	1.6486
5 W	1.7554	2.4985	1.7280
6 O	2.4357	3.6792	2.7763
7 O	1.1487	0.8942	-0.0002
8 W	1.7529	2.4997	-1.7285
9 O	2.4305	3.6796	-2.7795
10O	1.2191	1.1180	2.9505
11W	-0.1385	-0.0968	3.5944
12O	-0.1127	0.1965	5.2869
13O	-0.1724	-0.9103	1.2930
14P	-0.1533	-0.0021	-0.0011
15O	-0.1694	-0.9099	-1.2958
16W	-0.1396	-0.0965	-3.5968
17O	-0.1163	0.2028	-5.2885
18O	1.2152	1.1184	-2.9505
19O	-1.3886	1.1970	-2.9588
20W	-2.0169	2.5647	-1.7113
21O	-2.5883	3.7883	-2.7766
22O	1.1844	-1.5034	-3.4386
23W	1.5001	-2.5930	-1.8760
24O	2.5482	-3.7993	-2.5095
25O	-1.4611	-1.4626	-3.4648
26W	-1.9806	-2.4379	-1.8325
27O	-3.0361	-3.6283	-2.4987
28O	-1.3827	1.2025	2.9660
29O	-1.4634	-1.4612	3.4575
30W	-1.9884	-2.4377	1.8289
31O	-3.0353	-3.6347	2.4961
32O	1.1835	-1.5055	3.4338
33W	1.4965	-2.5940	1.8707
34O	2.5429	-3.8015	2.5040
35O	-0.0615	2.9764	-1.6507
36O	-2.0901	3.4642	-0.0008
37O	-3.5317	1.6147	-1.3343
38O	-5.1908	-0.0450	-0.0070
39O	-3.0987	-1.1203	1.3113
40O	-3.0758	-1.1079	-1.3172
41O	-3.5166	1.6214	1.3431
42O	2.0541	3.3174	-0.0016
43O	3.3163	1.4061	1.3187
44W	3.4314	0.0091	-0.0023
45O	5.1172	-0.3267	-0.0031
46O	2.7559	-1.2192	-1.3015
47O	2.7573	-1.2210	1.2946
48O	3.3138	1.4061	-1.3249
49O	1.4464	-3.0412	-0.0033
50O	-0.1998	-3.3525	2.1142
51O	-1.7843	-3.0158	-0.0013
52O	-0.1975	-3.3522	-2.1229
53H	-5.4944	0.5463	-0.7129
54Co	-3.3910	0.2588	-0.0027

Co-OH_-6_4

Energy (POTENTIAL) = -3910.55270933 Eh

Atom	X	Y	Z
1 O	-1.4381	0.9818	-0.0242
2 W	-2.0348	2.5864	1.6792
3 O	-2.4502	3.8735	2.7587
4 O	-0.0098	2.9786	1.6033
5 W	1.7693	2.5015	1.7176
6 O	2.4461	3.6771	2.7852
7 O	1.1783	0.8896	-0.0048
8 W	1.7938	2.4998	-1.7209
9 O	2.4869	3.6725	-2.7812
10O	1.2276	1.1138	2.9406
11W	-0.1464	-0.0963	3.5500
12O	-0.1388	0.2014	5.2475
13O	-0.1885	-0.8957	1.2756
14P	-0.1710	0.0384	-0.0138
15O	-0.1691	-0.8983	-1.3014
16W	-0.0935	-0.1035	-3.5762
17O	-0.0611	0.1918	-5.2738
18O	1.2706	1.1085	-2.9482
19O	-1.3408	1.1976	-2.9635
20W	-2.0105	2.5827	-1.7396
21O	-2.4096	3.8677	-2.8277
22O	1.2410	-1.5046	-3.4292
23W	1.5556	-2.6023	-1.8705
24O	2.6262	-3.7943	-2.5080
25O	-1.4060	-1.4887	-3.4760
26W	-1.9613	-2.4765	-1.8592
27O	-2.9120	-3.7486	-2.5480
28O	-1.3835	1.2036	2.9171
29O	-1.4564	-1.4826	3.4327
30W	-1.9885	-2.4736	1.8100
31O	-2.9477	-3.7454	2.4877
32O	1.1912	-1.4977	3.4246
33W	1.5283	-2.5981	1.8736
34O	2.5901	-3.7887	2.5285
35O	0.0137	2.9781	-1.6345
36O	-2.0771	3.4954	-0.0311
37O	-3.5714	1.7659	-1.4983
38O	-5.6854	-0.1024	-0.0545
39O	-3.1783	-1.2399	1.3570
40O	-3.1556	-1.2405	-1.4248
41O	-3.5913	1.7667	1.4183
42O	2.1365	3.3212	0.0003
43O	3.3480	1.3948	1.3370
44W	3.4649	0.0125	0.0120
45O	5.1550	-0.3321	0.0248
46O	2.8036	-1.2215	-1.2902
47O	2.7846	-1.2195	1.3063
48O	3.3677	1.3939	-1.3147
49O	1.5147	-3.0577	0.0013
50O	-0.1439	-3.3697	2.0977
51O	-1.7589	-3.0350	-0.0224
52O	-0.1137	-3.3733	-2.1185
53H	-6.1604	0.7390	-0.0661
54Co	-3.7986	0.2159	-0.0404

Co-O_-5_2

Energy (POTENTIAL) = -3909.69572417 Eh

Atom	X	Y	Z
1 O	-1.4284	0.9347	0.0000
2 W	-2.0041	2.5691	1.7136
3 O	-2.5752	3.7944	2.7780
4 O	-0.0478	2.9759	1.6475
5 W	1.7653	2.4988	1.7277
6 O	2.4442	3.6798	2.7763
7 O	1.1593	0.8930	0.0000
8 W	1.7653	2.4988	-1.7277
9 O	2.4442	3.6798	-2.7763
10O	1.2288	1.1179	2.9511
11W	-0.1296	-0.0942	3.5966
12O	-0.1040	0.2008	5.2887
13O	-0.1644	-0.9083	1.2946
14P	-0.1446	-0.0006	0.0000
15O	-0.1644	-0.9083	-1.2946
16W	-0.1296	-0.0942	-3.5966
17O	-0.1040	0.2008	-5.2887
18O	1.2288	1.1179	-2.9511
19O	-1.3735	1.2023	-2.9636
20W	-2.0041	2.5691	-1.7136
21O	-2.5752	3.7944	-2.7780
22O	1.1886	-1.5062	-3.4367
23W	1.5030	-2.5937	-1.8730
24O	2.5470	-3.8029	-2.5070
25O	-1.4570	-1.4586	-3.4600
26W	-1.9779	-2.4339	-1.8320
27O	-3.0273	-3.6292	-2.4971
28O	-1.3735	1.2023	2.9636
29O	-1.4570	-1.4586	3.4600
30W	-1.9779	-2.4339	1.8320
31O	-3.0273	-3.6292	2.4971
32O	1.1886	-1.5062	3.4367
33W	1.5030	-2.5937	1.8730
34O	2.5470	-3.8029	2.5070
35O	-0.0478	2.9759	-1.6475
36O	-2.0807	3.4657	0.0000
37O	-3.5114	1.6158	-1.3409
38O	-5.1259	-0.0375	0.0000
39O	-3.0878	-1.1098	1.3154
40O	-3.0878	-1.1098	-1.3154
41O	-3.5114	1.6158	1.3409
42O	2.0636	3.3179	0.0000
43O	3.3254	1.4054	1.3206
44W	3.4387	0.0069	0.0000
45O	5.1236	-0.3321	0.0000
46O	2.7615	-1.2222	-1.2983
47O	2.7615	-1.2222	1.2983
48O	3.3254	1.4054	-1.3206
49O	1.4499	-3.0398	0.0000
50O	-0.1968	-3.3510	2.1151
51O	-1.7811	-3.0062	0.0000
52O	-0.1968	-3.3510	-2.1151
53Co	-3.3873	0.2553	0.0000

Co-OH2_-4_1

Energy (POTENTIAL) = -3910.83437402 Eh

	Atom	X	Y	Z
1	O	-1.4580	0.9106	0.0000
2	W	-2.0065	2.5816	1.7256
3	O	-2.6091	3.7932	2.7808
4	O	-0.0746	2.9879	1.6560
5	W	1.7493	2.5007	1.7312
6	O	2.4296	3.6797	2.7766
7	O	1.1174	0.9006	0.0000
8	W	1.7493	2.5007	-1.7312
9	O	2.4296	3.6797	-2.7766
10	O	1.2010	1.1228	2.9473
11	W	-0.1483	-0.0968	3.6025
12	O	-0.1237	0.2015	5.2914
13	O	-0.1790	-0.9190	1.2958
14	P	-0.1544	-0.0256	0.0000
15	O	-0.1790	-0.9190	-1.2958
16	W	-0.1483	-0.0968	-3.6025
17	O	-0.1237	0.2015	-5.2914
18	O	1.2010	1.1228	-2.9473
19	O	-1.3954	1.2021	-2.9598
20	W	-2.0065	2.5816	-1.7256
21	O	-2.6091	3.7932	-2.7808
22	O	1.1713	-1.5039	-3.4350
23	W	1.4912	-2.5951	-1.8745
24	O	2.5335	-3.8023	-2.5078
25	O	-1.4722	-1.4597	-3.4605
26	W	-1.9849	-2.4438	-1.8339
27	O	-3.0546	-3.6176	-2.4963
28	O	-1.3954	1.2021	2.9598
29	O	-1.4722	-1.4597	3.4605
30	W	-1.9849	-2.4438	1.8339
31	O	-3.0546	-3.6176	2.4963
32	O	1.1713	-1.5039	3.4350
33	W	1.4912	-2.5951	1.8745
34	O	2.5335	-3.8023	2.5078
35	O	-0.0746	2.9879	-1.6560
36	O	-2.0968	3.4526	0.0000
37	O	-3.5153	1.6009	-1.3236
38	O	-5.2123	-0.0090	0.0000
39	O	-3.0763	-1.0946	1.3089
40	O	-3.0763	-1.0946	-1.3089
41	O	-3.5153	1.6009	1.3236
42	O	2.0296	3.3161	0.0000
43	O	3.2984	1.4075	1.3175
44	W	3.4245	0.0049	0.0000
45	O	5.1076	-0.3279	0.0000
46	O	2.7441	-1.2201	-1.2978
47	O	2.7441	-1.2201	1.2978
48	O	3.2984	1.4075	-1.3175
49	O	1.4313	-3.0368	0.0000
50	O	-0.2143	-3.3531	2.1187
51	O	-1.7995	-3.0136	0.0000
52	O	-0.2143	-3.3531	-2.1187
53	H	-5.5275	0.4885	-0.7757
54	Co	-3.2818	0.2753	0.0000
55	H	-5.5275	0.4885	0.7757

Co-K species. Small basis sets BS1

bs1Co-O-OH2_TS2-5_2

Energy (POTENTIAL) = -4062.15306424 Eh

	Atom	X	Y	Z
1	O	-0.8360	0.9932	0.9959
2	Co	-2.2834	0.3030	2.5697
3	O	-1.2103	1.7076	3.4904
4	W	0.0836	2.5885	2.6104
5	O	-1.2242	3.5079	1.4899
6	W	-2.4624	2.6712	0.2639
7	O	-3.2833	1.7792	1.6112
8	P	-0.0167	0.0305	0.0680
9	O	-1.0285	-0.9028	-0.8193
10	W	-2.6675	-0.0314	-2.3769
11	O	-3.4878	-1.3895	-1.3069
12	W	-2.6761	-2.4130	0.1815
13	O	-1.6834	-3.3217	-1.3399
14	W	-0.3392	-2.5963	-2.4411
15	O	0.9957	-3.0578	-1.1229
16	W	2.4255	-2.6739	0.1077
17	O	1.4309	-3.3886	1.5347
18	W	0.0437	-2.4367	2.6852
19	O	-1.2043	-2.9565	1.2898
20	O	0.5601	3.8454	3.7271
21	O	1.3558	2.9266	1.0783
22	W	2.6368	2.4453	-0.2028
23	O	3.3660	1.3188	-1.6309
24	W	2.4361	-0.0667	-2.6001
25	O	1.4113	1.3584	-3.4194
26	W	0.0811	2.4911	-2.5503
27	O	1.5899	3.2778	-1.6070
28	O	1.4041	1.1848	2.9563
29	W	2.6770	-0.1554	2.4746
30	O	3.3970	-1.6021	1.3981
31	O	3.9149	3.6106	0.0200
32	O	0.9392	0.8816	-0.9564
33	O	3.1248	1.0406	1.0281
34	O	-0.2246	3.6922	-3.7772
35	O	-1.2333	1.1407	-2.9413
36	O	-1.0586	2.9822	-1.1379
37	O	3.9723	0.1127	3.6086
38	O	0.9381	-0.9466	0.9715
39	O	1.6313	-1.4944	3.3700
40	O	-3.9115	0.3057	-3.5497
41	O	-2.9773	1.2852	-1.0317
42	O	-1.6897	-1.4739	-3.2489
43	O	-3.5766	3.9653	-0.1036
44	O	-0.1186	-3.8286	-3.6547
45	O	0.9760	-1.2573	-2.9583
46	O	-3.9004	-3.6261	0.4802
47	O	-3.0863	-1.0953	1.3392
48	O	-0.1931	-3.6598	3.9130
49	O	-1.0593	-1.1129	3.1693
50	O	3.5755	-3.9376	-0.2391
51	O	2.8812	-1.3114	-1.2165
52	O	3.5766	-0.4545	-3.8604
53	O	-3.3999	0.0558	4.0034
54	O	-5.2063	0.0537	4.0950
55	H	-5.2906	0.9552	4.4443
56	H	-5.4002	0.1167	3.0873
57	O	-5.5104	0.2227	1.5519
58	H	-4.8747	-0.4817	1.3071
59	H	-4.9376	1.0120	1.4340

bs1Co-O-OH2_TS1B2-5_2

Energy (POTENTIAL) = -3985.70594238 Eh

	Atom	X	Y	Z
1	O	1.1187	-0.4250	1.2080
2	Co	0.9146	-0.3803	3.2727
3	O	1.7914	-2.1881	3.0409
4	W	2.1578	-2.6741	1.3295
5	O	3.5731	-1.3403	1.2239
6	W	3.4424	0.5952	1.3377
7	O	2.8956	0.5027	3.0495
8	P	0.0220	-0.0179	0.1400
9	O	-0.3817	1.5526	0.3460
10	W	1.1889	3.3985	0.1382
11	O	0.1572	3.6210	1.7289
12	W	-1.2339	2.4058	2.4646
13	O	-2.3105	3.1334	0.8898
14	W	-2.0533	2.7862	-0.9385
15	O	-3.0965	1.1698	-0.8149
16	W	-3.3854	-0.7366	-0.9803
17	O	-3.8341	-0.8465	0.8347
18	W	-2.5769	-1.0424	2.4411
19	O	-2.4289	0.8863	2.3791
20	O	3.0484	-4.1613	1.5250
21	O	2.1134	-2.5309	-0.6629
22	W	1.2847	-2.3224	-2.3406
23	O	0.1108	-1.4300	-3.6154
24	W	-0.7291	0.3036	-3.4260
25	O	1.0423	1.0421	-3.6037
26	W	2.5189	0.9241	-2.3267
27	O	2.5783	-0.9543	-2.8167
28	O	0.3192	-3.2665	1.0214
29	W	-1.3654	-3.3378	0.0957
30	O	-2.8587	-2.5986	-0.9116
31	O	1.8609	-3.6845	-3.2650
32	O	0.5770	-0.2081	-1.3894
33	O	-0.2847	-3.0266	-1.4841
34	O	3.8416	1.5798	-3.2555
35	O	1.7904	2.4779	-1.4563
36	O	3.2894	0.5234	-0.6680
37	O	-1.6824	-5.0479	-0.0139
38	O	-1.3159	-0.9401	0.3307
39	O	-2.3323	-2.8629	1.6661
40	O	2.0639	4.9028	0.0553
41	O	2.4306	2.2412	1.0339
42	O	-0.4279	3.8394	-0.8462
43	O	5.1039	1.1133	1.4771
44	O	-3.1559	3.8966	-1.7074
45	O	-1.2547	1.8715	-2.4680
46	O	-1.9068	3.3850	3.7498
47	O	0.0090	1.4145	3.2743
48	O	-3.7617	-1.3354	3.6971
49	O	-1.0178	-1.1769	3.2708
50	O	-4.9345	-0.8221	-1.7764
51	O	-2.1547	-0.5444	-2.4801
52	O	-1.3985	0.5634	-5.0141
53	O	1.1072	-0.4368	4.9875
54	O	2.8189	-0.9808	5.1847
55	H	2.6637	-1.7743	4.6119
56	H	3.1457	-0.3077	4.5177