

# Supporting Information

## DFT Calculations of Comparative Energetics and Mössbauer Properties for Two Protonation States of the Iron Dimer Cluster of Ribonucleotide Reductase Intermediate X

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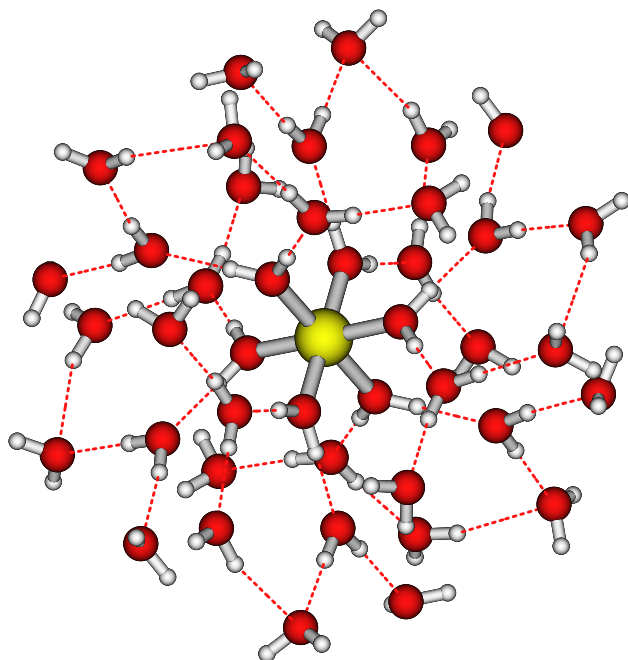
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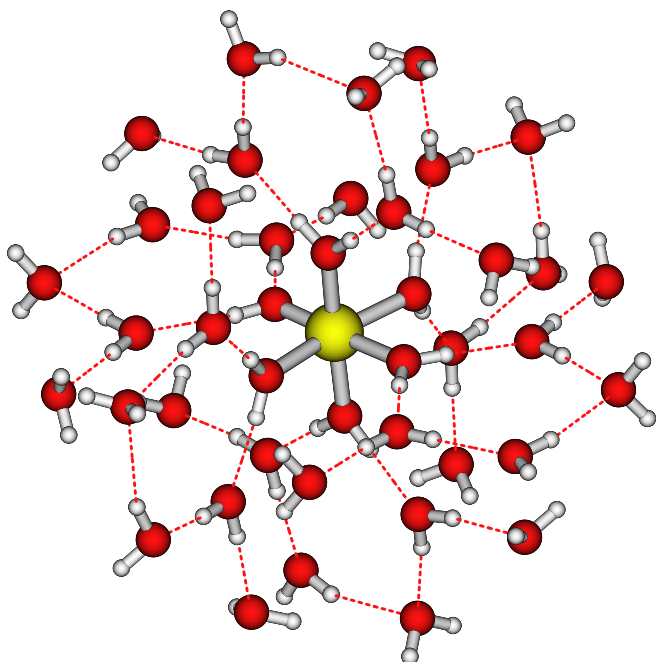
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## $pK_a$ Calculations for $Fe^{2+}$ and $Fe^{3+}$ in Water



**Figure S1.** Structure of  $Fe^{2+}$  with 3 shells (6 + 12 + 24 = 42) of water molecules optimized with DFT/OPBE method using all-electron TZP Slater-type basis sets in COSMO solvation model with  $\epsilon = 80$ .



**Figure S2.** Structure of  $Fe^{2+} - OH^-$  with 3 shells (5 + 12 + 24 = 41) of water molecules.

**Table S1.** COSMO and DFT/PB-SCRF calculated energies ( $E$ , eV) for  $\text{Fe}(\text{H}_2\text{O})_{42}^{2+}$ ,  $\text{Fe}(\text{OH})(\text{H}_2\text{O})_{41}^+$ ,  $\text{Fe}(\text{H}_2\text{O})_{42}^{3+}$ , and  $\text{Fe}(\text{OH})(\text{H}_2\text{O})_{41}^{2+}$  systems, and the calculated (cal) and experimental (exp)  $\text{p}K_a$ 's for the processes of  $\text{Fe}(\text{H}_2\text{O})_{42}^{2+} \rightarrow \text{Fe}(\text{OH})(\text{H}_2\text{O})_{41}^+ + \text{H}^+$ , and  $\text{Fe}(\text{H}_2\text{O})_{42}^{3+} \rightarrow \text{Fe}(\text{OH})(\text{H}_2\text{O})_{41}^{2+} + \text{H}^+$ .

	$\text{Fe}(\text{H}_2\text{O})_{42}^{2+}$		$\text{Fe}(\text{OH})(\text{H}_2\text{O})_{41}^+$		$\text{Fe}(\text{H}_2\text{O})_{42}^{3+}$		$\text{Fe}(\text{OH})(\text{H}_2\text{O})_{41}^{2+}$	
	COSMO	SCRF	COSMO	SCRF	COSMO	SCRF	COSMO	SCRF
$E$	-619.263	-618.664	-619.229	-618.653	-614.254	-613.768	-614.780	-614.295
$\text{p}K_a(\text{cal})^a$	10.91	10.52			1.04	1.02		
$\text{p}K_a(\text{exp})$	9.5 <sup>b</sup>	9.5 <sup>b</sup>			2.2 <sup>c</sup>	2.2 <sup>c</sup>		

<sup>a</sup> See section 3.5. The  $\Delta\text{ZPE}$  terms are  $-7.1 \text{ kcal mol}^{-1}$  for  $\text{Fe}(\text{H}_2\text{O})_{42}^{2+} \rightarrow \text{Fe}(\text{OH})(\text{H}_2\text{O})_{41}^+ + \text{H}^+$ , and  $-7.7 \text{ kcal mol}^{-1}$  for  $\text{Fe}(\text{H}_2\text{O})_{42}^{3+} \rightarrow \text{Fe}(\text{OH})(\text{H}_2\text{O})_{41}^{2+} + \text{H}^+$ , taken from "Li, J.; Fisher, C. L.; Chen, J. L.; Bashford, D.; Noodleman, L. *Inorg. Chem.* **1996**, *35*, 4694."

<sup>b</sup> In alkaline solution. Taken from "Baes, C. J.; Mesmer, R. E. *The hydrolysis of Cations*; Krieger: Malabar, India, 1986".

<sup>c</sup> Ionic strength = 0. Taken from "Flynn, C. M., Jr. *Chem. Rev.* **1984**, *84*, 31".

### Cartesian coordinates of $\text{Fe}(\text{H}_2\text{O})_{42}^{2+}$

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(Using OPBE potential, optimized in COSMO solvation model with  $\epsilon = 80$ )

Fe	-0.001038164	-0.010090621	0.000666714
O	2.112100214	0.000469626	0.027312602
O	0.019370243	2.120316773	0.001577353
O	-0.041990131	0.010562614	-2.255024222
O	-2.115416916	0.022179515	-0.025777757
O	-0.010399715	-2.142210562	0.004247615
O	0.003544132	-0.057204517	2.239184787
O	3.886178488	-2.137209291	-0.118468352
O	3.833419531	2.171452985	-0.179132020
O	-0.036777451	3.861543162	2.197242440
O	0.144819069	3.849498473	-2.208504516
O	-2.376226454	0.029220615	-3.943388455
O	2.273284010	-0.087739619	-3.989443202
O	-3.900700514	-2.112138345	0.060133456
O	-3.755107779	2.249718433	0.223454955
O	-0.064063355	-3.832982190	2.255197151

O	0.115452055	-3.893083389	-2.207023267
O	-2.300595186	-0.044380365	3.916606585
O	2.260066089	-0.029125921	4.021116230
H	2.703161052	-0.780819663	-0.021826702
H	2.679036333	0.799810902	-0.029802954
H	-0.008556328	2.706542055	0.787440950
H	0.045862110	2.698096077	-0.790786451
H	-0.835191414	0.011542360	-2.820193461
H	0.734766476	-0.008778297	-2.841588908
H	-2.716805615	-0.751937338	0.005480101
H	-2.665629830	0.832410624	0.042339614
H	-0.023446386	-2.706848330	0.805857871
H	0.028341101	-2.733852587	-0.774817155
H	-0.794879005	-0.028625572	2.798380351
H	0.773519197	-0.032452684	2.834635595
H	3.740512603	-3.094241829	-0.032971572
H	4.848383332	-2.040306802	-0.031804128
H	3.677903649	3.117101280	-0.014037578
H	4.784236068	2.063181017	-0.015117170
H	-0.003454698	3.703653059	3.154692058
H	0.009363511	4.827717606	2.121667945
H	0.014732435	3.710173547	-3.162523592
H	0.030853311	4.806789058	-2.099819151
H	-3.344380482	0.031670257	-3.815591582
H	-2.267955148	0.015770773	-4.906047832
H	3.228132300	-0.009660658	-3.826842080
H	2.196315678	0.010050535	-4.950726296
H	-3.746435437	-3.069322549	0.000403331
H	-4.864683824	-2.028773809	-0.007132476
H	-3.612281576	3.203455699	0.063465243
H	-4.706097303	2.136813490	0.076406284
H	-0.004431298	-3.714785849	3.223823937
H	-0.009275490	-4.793274182	2.139274864
H	0.000214741	-3.728948456	-3.158778698
H	0.029175368	-4.855631586	-2.129018991
H	-3.262255387	-0.003993431	3.776136643
H	-2.206368116	-0.007465166	4.880160770
H	3.218964417	-0.016955261	3.864523096
H	2.182027215	-0.048588907	4.987511613
O	5.311967440	0.036153632	-3.689618556
H	5.666120467	0.809021606	-3.227741854
H	5.676361798	-0.709671893	-3.193698441
O	1.785328782	0.096082599	-7.053202957
H	1.935885418	0.846888141	-7.644890465
H	1.995416275	-0.662317475	-7.617003451
O	-1.800282376	-0.151197402	-6.980476077
H	-2.351688307	0.113895120	-7.731115426
H	-0.905418030	0.057537302	-7.282709886
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H	-5.638630801	-0.728779351	-3.235420261
H	-5.650935613	0.792657245	-3.232157214
O	-6.959616414	-1.712098994	-0.082948778
H	-7.494325815	-1.998659272	0.668027049
H	-7.469457966	-2.025887696	-0.840633815
O	-3.683682228	-5.182558236	-0.050429890
H	-3.301790380	-5.551671750	-0.858914251
H	-3.171164633	-5.604631452	0.653404167
O	-6.791210376	1.785622946	-0.111727837

H	-7.126770232	0.879025375	-0.083846666
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O	-3.628014930	5.144597437	-0.075501717
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H	-3.163180465	5.540899289	-0.826170387
O	0.051414202	6.935818024	1.796422064
H	0.801884179	7.426973881	2.159690104
H	-0.707624391	7.422812204	2.146257542
O	0.013540767	3.644571139	5.285267619
H	-0.725380835	3.170138078	5.692054154
H	0.791338947	3.207876033	5.659924510
O	-0.206755185	6.851639153	-1.663753041
H	-0.045354353	7.120775512	-0.748747678
H	0.004472893	7.651979116	-2.166885035
O	-0.059494787	3.680479639	-5.226953107
H	0.725142719	3.274439518	-5.620659735
H	-0.791769834	3.203453571	-5.641118690
O	6.942871477	-1.712307682	0.042847703
H	7.442184680	-2.063047701	-0.708869513
H	7.417089869	-2.085773850	0.799668042
O	3.698744097	-5.179224010	0.020868085
H	3.226080194	-5.582381973	0.763249005
H	3.274236107	-5.572641033	-0.754674808
O	6.823473543	1.719252658	0.326850119
H	7.130229521	0.822015343	0.137797589
H	7.568944858	2.269210225	0.044648305
O	3.668990274	5.196743725	0.089099839
H	3.170838429	5.623492249	-0.621930396
H	3.285549377	5.573610003	0.892280865
O	-0.095687445	-3.662276421	-5.250037455
H	-0.827980252	-3.173268498	-5.651794532
H	0.688342713	-3.240858304	-5.629657179
O	-0.033926069	-6.972799076	-1.790849998
H	-0.791204035	-7.523820747	-2.034698459
H	0.719012674	-7.528466064	-2.037552325
O	0.079424202	-6.865912591	1.736028972
H	0.034854050	-7.171308366	0.819578799
H	0.032650044	-7.687852633	2.244270184
O	1.759594858	-0.085154752	7.087612800
H	2.088876153	-0.830660227	7.611568856
H	2.044687457	0.679707562	7.609349857
O	5.304956931	0.010287274	3.697383946
H	5.664517878	-0.775584610	3.264512689
H	5.677644312	0.741387705	3.185428669
O	-1.720530745	0.148049015	6.952189411
H	-0.807640612	-0.041805178	7.209149931
H	-2.228596249	-0.142815043	7.724146679
O	-5.332994918	0.009334625	3.672806362
H	-5.715295583	0.706213010	3.121822149
H	-5.686500033	-0.803697168	3.287432039
O	0.043626680	-3.745900715	5.153807247
H	0.816132101	-3.330776672	5.562599812
H	-0.703975534	-3.295931999	5.572232013

## Cartesian coordinates of $\text{Fe}(\text{OH})(\text{H}_2\text{O})_{41}^+$

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Fe	0.001717368	0.175107618	-0.162075091
O	2.262570610	0.014238638	-0.018024147
O	-0.020109949	2.065045798	-0.351894409
O	0.040320602	-0.391455813	-2.347164754
O	-2.257175750	0.005858503	-0.190537038
O	0.025094977	-2.076792515	0.042534659
O	-0.002443247	0.146648024	2.129527077
O	4.090742725	-2.213597265	-0.003029855
O	3.938126869	2.308627665	-0.107782392
O	-0.034799782	4.003349151	2.292350990
O	0.236790457	3.686801947	-2.344816816
O	-2.374184562	0.166888979	-3.992075751
O	2.253315841	0.328505059	-4.052521957
O	-4.009288918	-2.206115821	0.238788742
O	-3.884311806	2.314922100	0.227799022
O	-0.069738040	-3.885385638	2.400661158
O	0.030231226	-4.097134030	-2.203394958
O	-2.359933285	0.085278326	4.023595147
O	2.327193143	-0.120064490	4.096922657
H	2.864882829	-0.751740944	-0.025441967
H	2.823383564	0.810191926	-0.081220254
H	-0.038117732	2.544344154	0.487286540
H	0.137076266	3.049222976	-1.543756162
H	-0.758081130	-0.154705240	-2.849584063
H	0.794134371	-0.091450570	-2.892709256
H	-2.830810860	-0.761068342	0.001611646
H	-2.793772742	0.802260302	-0.012552511
H	-0.011650199	-2.613141985	0.851081247
H	0.013805945	-2.702537097	-0.698668567
H	-0.782153320	0.086111032	2.702236607
H	0.765918257	0.036765203	2.709716909
H	3.950212722	-3.174970489	0.003618006
H	5.058843153	-2.114048946	0.002709709
H	3.804619677	3.267068007	0.006825438
H	4.892298928	2.193432615	0.021724940
H	-0.001907699	3.869423054	3.253658307
H	0.023057094	4.968350700	2.206573684
H	-0.070240034	3.632314969	-4.119753466
H	0.114093150	4.574209124	-1.978456255
H	-3.333752297	0.082981618	-3.848907611
H	-2.282399587	0.077043211	-4.952825863
H	3.191285299	0.139399664	-3.886546305
H	2.153512155	0.161992382	-5.003283149
H	-3.848376231	-3.147760183	0.061493078
H	-4.959631632	-2.097549628	0.062104861
H	-3.731732512	3.267300730	0.078853732
H	-4.836138524	2.212788407	0.074406511
H	-0.025005753	-3.789712412	3.371231287
H	-0.028970537	-4.844252115	2.267917275
H	-0.019387908	-3.947577268	-3.161351815
H	-0.000016305	-5.064744067	-2.118463390
H	-3.318848760	-0.013773653	3.898437138
H	-2.238303798	-0.064883164	4.974629939

H	3.286295861	-0.042197992	3.962119719
H	2.228230365	-0.070975447	5.061766348
O	5.325137090	0.014009169	-3.678136675
H	5.674003738	0.769161168	-3.184283174
H	5.671063115	-0.749096426	-3.195336742
O	1.652816756	0.019696800	-7.104131790
H	2.042280521	0.777080658	-7.563510362
H	2.062699565	-0.730961994	-7.556471625
O	-1.819449352	-0.186710600	-7.021019799
H	-2.331736950	0.227951619	-7.730663310
H	-0.905855296	0.017223344	-7.265196380
O	-5.348995899	0.037881091	-3.691100845
H	-5.648064851	-0.739870321	-3.199839538
H	-5.676634145	0.779337455	-3.162606887
O	-6.981149365	-1.667835535	-0.069730016
H	-7.451908017	-2.075534646	0.671106851
H	-7.383889491	-2.101666922	-0.835178332
O	-3.660176156	-5.272732946	-0.042533483
H	-3.234983005	-5.574059904	-0.857420404
H	-3.109656783	-5.657092733	0.654094574
O	-6.894806430	1.802914777	-0.244689978
H	-7.186157437	0.891288235	-0.105722175
H	-7.663821170	2.322478000	0.030756040
O	-3.638509263	5.229313109	-0.038164319
H	-3.178056137	5.595631040	0.729438418
H	-3.122286371	5.553502664	-0.789270035
O	0.079608577	7.108478467	1.802687819
H	0.830746521	7.567455906	2.204667105
H	-0.677910580	7.568293718	2.191657200
O	0.034442424	3.675178118	5.410361473
H	-0.692527281	3.136905618	5.753151276
H	0.822259374	3.226423134	5.747311085
O	-0.151117506	6.763988001	-1.586272370
H	-0.029754837	7.038753149	-0.666955855
H	0.041224933	7.575090764	-2.079608058
O	-0.154826723	3.710958837	-5.098081533
H	-0.942034877	3.187893584	-5.298401824
O	7.029403477	-1.720402866	0.040499629
H	7.456627648	-2.139474977	-0.719647990
H	7.431714290	-2.183250925	0.789045520
O	3.739451753	-5.281251115	0.010799674
H	3.215637074	-5.625630513	0.747575597
H	3.274295718	-5.611530380	-0.770257324
O	6.944751403	1.728564045	0.337817383
H	7.208483696	0.816223457	0.154462527
H	7.682623988	2.243688912	-0.018546035
O	3.717483666	5.296023713	0.127895333
H	3.164167646	5.622018378	-0.595579923
H	3.240423807	5.572594032	0.922102320
O	-0.075114042	-3.678014237	-5.295027178
H	-0.823948515	-3.158859467	-5.619851958
H	0.694028971	-3.193947048	-5.626625323
O	-0.007086034	-7.093275850	-1.684507497
H	-0.765649662	-7.528383784	-2.098944537
H	0.742724999	-7.524447594	-2.118554563
O	-0.134459820	-6.936248225	1.777891947
H	0.006546803	-7.209457657	0.860833641
H	0.116010894	-7.724949872	2.280220901

O	1.747336076	-0.052894513	7.146600928
H	2.148002777	-0.802513743	7.609782059
H	2.117109478	0.705609139	7.620490352
O	5.380772574	0.026512484	3.716270749
H	5.697745121	-0.768308772	3.265022730
H	5.711297380	0.746257361	3.160885505
O	-1.739720649	-0.436556820	7.024024130
H	-0.816984415	-0.215643389	7.213728663
H	-2.223694401	0.098167128	7.669218833
O	-5.411294244	-0.097356810	3.700673017
H	-5.759515862	0.711998684	3.301116786
H	-5.721303269	-0.793310890	3.105335083
O	0.017620439	-3.731165155	5.316852039
H	0.816952123	-3.303582631	5.654332262
H	-0.700952695	-3.209474343	5.700612929

### Cartesian coordinates of $\text{Fe}(\text{H}_2\text{O})_{42}^{3+}$

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Fe	-0.003106604	-0.000060459	-0.005589307
O	2.025363831	0.013858980	-0.002408877
O	-0.000770733	2.032653934	-0.017070964
O	-0.009507577	-0.002296448	-2.046282726
O	-2.029228638	0.011665061	-0.012595419
O	0.001609294	-2.031226694	0.003788348
O	-0.008087128	0.014032151	2.037924196
O	3.703021348	-2.016787600	0.007768522
O	3.655442248	2.085417874	-0.027045156
O	-0.002319878	3.711082225	2.036405684
O	0.009748611	3.666366185	-2.091755108
O	-2.094734983	-0.025889901	-3.701767069
O	2.022418187	-0.014397925	-3.740703403
O	-3.706600075	-2.010881447	0.048507464
O	-3.655171473	2.083388049	0.098260374
O	-0.009846169	-3.676357644	2.077065957
O	0.005324250	-3.691470731	-2.045541769
O	-2.113993963	0.031058993	3.678430521
O	2.034729201	-0.014049226	3.734483188
H	2.623492065	-0.787927229	0.000293540
H	2.600684204	0.832554588	-0.002972942
H	0.002757305	2.625669298	0.785903409
H	-0.003372964	2.608113020	-0.834630844
H	-0.823102020	-0.002677945	-2.622211380
H	0.790681018	-0.001580400	-2.642625375
H	-2.626885827	-0.791678888	-0.007077970
H	-2.605112243	0.830196172	0.003451920
H	0.002104980	-2.611761824	0.816869709
H	-0.001319872	-2.621098302	-0.803436231
H	-0.824039479	0.010261671	2.608512311
H	0.790279016	0.002943718	2.636148682
H	3.558148648	-2.976478332	0.013559987
H	4.667461218	-1.916227276	-0.002181603
H	3.520284692	3.049204608	0.026103816



H	4.617111934	1.974495031	0.016244254
H	0.019292048	3.560900945	2.995986900
H	0.011866027	4.675349796	1.942948547
H	-0.016193694	3.532198087	-3.056567549
H	-0.014673350	4.627805044	-1.978372572
H	-3.055082088	0.009145972	-3.547557725
H	-2.005661437	0.010890016	-4.665665747
H	2.981117501	0.010246787	-3.590563553
H	1.925488371	0.002196569	-4.704881223
H	-3.559529230	-2.966533894	-0.045787024
H	-4.667052607	-1.905153284	-0.028489345
H	-3.503777702	3.038153596	-0.022865323
H	-4.612735018	1.978810500	-0.009629213
H	0.017076499	-3.535410237	3.040332585
H	0.011309027	-4.639621061	1.973056263
H	-0.022369884	-3.552254915	-3.007579405
H	-0.013444987	-4.654272405	-1.938304230
H	-3.074801843	-0.003086812	3.528029216
H	-2.023062020	-0.003774998	4.642375499
H	2.995574126	-0.018659196	3.585493285
H	1.941579536	-0.012371606	4.698625593
O	5.029918397	0.031836251	-3.509675250
H	5.636011909	0.754769611	-3.300303305
H	5.593091293	-0.752788487	-3.454407235
O	1.886644135	0.010056671	-6.798473881
H	1.900314329	0.774705707	-7.390268018
H	1.836763278	-0.738068670	-7.408921246
O	-1.820480071	0.042055724	-6.774763302
H	-2.405626577	0.029533897	-7.545503467
H	-0.937681498	0.036864408	-7.168941219
O	-5.077454276	0.020521866	-3.620845193
H	-5.573469621	-0.732906685	-3.271855089
H	-5.584371840	0.785183249	-3.314205751
O	-6.754436063	-1.844366338	-0.061432236
H	-7.370138769	-1.894646009	0.682588160
H	-7.337114630	-1.916432830	-0.829628912
O	-3.643100314	-5.039943435	-0.064740184
H	-3.377470161	-5.541853659	-0.847886460
H	-3.264070446	-5.550917753	0.664487478
O	-6.695880709	1.777260453	-0.100530859
H	-7.090160238	0.894507901	-0.106348328
H	-7.464901219	2.363515978	-0.070770284
O	-3.627715192	5.029799235	-0.070167335
H	-3.256735660	5.529882218	0.669752633
H	-3.325013902	5.520217220	-0.846800610
O	0.024287079	6.782982867	1.883751515
H	0.785862099	7.365844513	2.010436821
H	-0.726660589	7.378854420	2.012374185
O	0.027960616	3.609945540	5.086851385
H	-0.730159708	3.274489868	5.586265073
H	0.787292473	3.300176092	5.600344788
O	0.010895788	6.721808007	-1.674747410
H	-0.022103773	7.048359924	-0.765368970
H	-0.021023888	7.532953581	-2.201278218
O	-0.028947417	3.643751214	-5.040128310
H	0.726843962	3.311052002	-5.543796020
H	-0.791934648	3.336648027	-5.549526817
O	6.763939989	-1.795663906	0.022487711

H	7.348696858	-1.930052920	-0.736068329
H	7.344515375	-1.972043186	0.775497622
O	3.626726180	-5.038638560	0.018721465
H	3.330507859	-5.552774276	0.783424307
H	3.314268572	-5.559475448	-0.734209685
O	6.703819920	1.733363983	0.104513945
H	7.040484882	0.827023376	0.102042449
H	7.508693461	2.269363821	0.076670018
O	3.633670009	5.025606767	0.049279878
H	3.249821671	5.544385581	-0.671764876
H	3.354673636	5.504447028	0.842228423
O	-0.041448521	-3.682863634	-5.060495671
H	-0.797866588	-3.330513384	-5.550172531
H	0.718749828	-3.323656203	-5.539341677
O	-0.031167609	-6.767931169	-1.859417849
H	-0.795401661	-7.356116636	-1.932253507
H	0.717348819	-7.374491032	-1.943079523
O	0.027751706	-6.729539813	1.756511839
H	0.039290281	-7.109288706	0.867476791
H	0.029753855	-7.508749446	2.330104306
O	1.926787350	-0.017319331	6.823245685
H	1.998615555	-0.778638821	7.415462609
H	1.971871709	0.733989017	7.430703487
O	5.054028299	-0.004350940	3.662989999
H	5.567180652	-0.754062820	3.330428884
H	5.528625289	0.762220439	3.311651134
O	-1.745715418	-0.067915284	6.757005833
H	-0.837087703	-0.046226349	7.086893279
H	-2.273378213	-0.031632976	7.567564915
O	-5.111306573	-0.040509134	3.628642968
H	-5.608550943	0.744195110	3.356976163
H	-5.587720795	-0.765024532	3.200544642
O	0.025568364	-3.655238694	5.043670408
H	0.793051986	-3.341128278	5.541941460
H	-0.724263003	-3.299150475	5.540718975

### Cartesian coordinates of $\text{Fe}(\text{OH})(\text{H}_2\text{O})_{41}^{2+}$

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TIME:

0.18000

Fe	-0.020557456	0.170297938	-0.020815064
O	2.046956346	0.004491490	-0.003115910
O	-0.023384977	2.008086737	-0.058481547
O	0.014844562	-0.040735334	-2.110329749
O	-2.079783370	0.007184876	-0.026253732
O	-0.025202930	-2.010211533	0.025663416
O	0.009062018	0.007368352	2.094125685
O	3.753983354	-2.109717967	0.015750022
O	3.746387069	2.104816786	-0.021450458
O	-0.050404708	3.758689117	2.191065090
O	0.121184669	3.772749899	-2.272157685
O	-2.151112051	-0.056503221	-3.790645171
O	2.121931919	-0.000414465	-3.812749295
O	-3.764326949	-2.114967466	0.029314745

O	-3.753059290	2.117547967	0.062713683
O	0.088407350	-3.740246314	2.165711924
O	0.018387997	-3.791461793	-2.103835490
O	-2.170281134	0.014172536	3.786087198
O	2.115458837	-0.043489450	3.830595911
H	2.611849777	-0.806633461	0.002640540
H	2.641624998	0.793953764	-0.007079833
H	-0.021250242	2.506019830	0.785567986
H	0.047856810	3.211191394	-1.472806337
H	-0.784242246	-0.019619932	-2.685844750
H	0.811652200	-0.012937975	-2.693215816
H	-2.643095201	-0.806607669	-0.010498598
H	-2.671471349	0.799926681	-0.010358817
H	0.008604026	-2.571941986	0.831239850
H	-0.005800851	-2.610408431	-0.750990596
H	-0.789479789	0.005459308	2.668509934
H	0.800860156	-0.008603953	2.681265413
H	3.621412920	-3.073939735	0.002045386
H	4.717584757	-2.003568890	0.010833658
H	3.591984760	3.064918940	0.020093437
H	4.710801393	2.017493416	0.019555260
H	0.002064666	3.647103884	3.154508349
H	0.002626728	4.719060372	2.070452145
H	-0.032400208	3.569418499	-4.165600264
H	0.025624431	4.686646571	-1.967698990
H	-3.107420010	-0.005351280	-3.622853990
H	-2.081691507	-0.005232977	-4.755885695
H	3.081172171	0.004469394	-3.659106566
H	2.030202314	0.000362401	-4.777931198
H	-3.627255994	-3.078395076	-0.018611706
H	-4.726946644	-2.009326986	-0.015948125
H	-3.596125831	3.075773159	-0.007767625
H	-4.715657416	2.029975126	-0.012055695
H	0.034859611	-3.679173662	3.137759643
H	-0.069457469	-4.679309691	1.984390990
H	-0.013689547	-3.655869968	-3.067349966
H	-0.004441270	-4.755352250	-2.004842036
H	-3.128430092	-0.023388300	3.622312985
H	-2.100917997	-0.020965141	4.751828483
H	3.075928370	-0.035986235	3.679067077
H	2.030543143	-0.033313195	4.795996232
O	5.145101169	0.016439123	-3.637136011
H	5.631829651	0.786060445	-3.310586709
H	5.627905997	-0.729871944	-3.256063800
O	1.908811009	-0.008916141	-6.856015170
H	1.899197068	0.770322129	-7.428328653
H	1.878157208	-0.744151722	-7.482712920
O	-1.869397330	0.042063261	-6.835601003
H	-2.417452563	0.023940934	-7.632824757
H	-0.968446273	0.043115029	-7.186404583
O	-5.144337253	0.017052262	-3.613090096
H	-5.639992094	-0.734877660	-3.261139644
H	-5.641978170	0.783149485	-3.296400554
O	-6.803270811	-1.915176722	-0.062656434
H	-7.418663998	-1.923567665	0.682850678
H	-7.389209245	-1.971346675	-0.829685506
O	-3.639543496	-5.075619928	-0.051951085
H	-3.347372923	-5.550409283	-0.842450664

H	-3.255237130	-5.588800805	0.672635219
O	-6.766171374	1.802363363	-0.067916592
H	-7.121492766	0.904479224	-0.114570016
H	-7.559293848	2.356509553	-0.070254575
O	-3.637098967	5.069420908	-0.045682150
H	-3.280940143	5.579573255	0.695239200
H	-3.331955579	5.557350488	-0.823482040
O	0.019792055	6.823626665	1.908949497
H	0.777126992	7.408324910	2.050250165
H	-0.735402770	7.410483252	2.053105306
O	0.008140779	3.617124526	5.212608717
H	-0.748147885	3.233791685	5.678799330
H	0.769643646	3.269110463	5.696870378
O	0.006033523	6.757865081	-1.683916128
H	-0.018567234	7.062513980	-0.767051564
H	-0.026257552	7.579893956	-2.192454036
O	-0.055028025	3.592578860	-5.141211475
H	-0.957887365	3.311588557	-5.342429286
O	6.798399570	-1.844851395	0.035119689
H	7.410980231	-1.977920513	-0.698026744
H	7.362525415	-1.977987662	0.809919590
O	3.649780692	-5.088409741	0.019607052
H	3.316718610	-5.575439927	0.786549862
H	3.295563812	-5.583850618	-0.731805652
O	6.757323261	1.748670322	0.099763282
H	7.065771989	0.832601753	0.102593195
H	7.578446586	2.260114637	0.093442378
O	3.635846684	5.072052684	0.061169453
H	3.240983044	5.574289900	-0.665465735
H	3.340983127	5.547423105	0.850158497
O	-0.041413542	-3.663941213	-5.097210902
H	-0.793261816	-3.299755354	-5.584970607
H	0.723579423	-3.302319281	-5.565481435
O	-0.018828411	-6.838241490	-1.909808310
H	-0.783450982	-7.429552368	-1.936226859
H	0.730542059	-7.448555831	-1.935901102
O	-0.055848663	-6.794059329	1.780333903
H	0.041411604	-7.141013138	0.883171201
H	0.032043896	-7.584916727	2.331740770
O	1.980516016	-0.031721083	6.880209910
H	1.982854543	-0.793846373	7.475302203
H	1.970665900	0.720289604	7.487899047
O	5.117763934	-0.015759499	3.674061824
H	5.620261545	-0.764420660	3.323361379
H	5.584606954	0.753659831	3.318285520
O	-1.797791591	-0.077203592	6.830652494
H	-0.876209558	-0.065630618	7.122236256
H	-2.290909631	-0.048861544	7.662983307
O	-5.157212463	-0.034273238	3.624948203
H	-5.651501657	0.701383422	3.238135466
H	-5.652302546	-0.813101263	3.336666086
O	0.004905449	-3.683087879	5.126866554
H	0.778564114	-3.335881400	5.590524867
H	-0.739393165	-3.287822561	5.600674340

## Cartesian coordinates of Model-I with three explicit water molecules around site O2:

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(Using OPBE potential, optimized in COSMO solvation model with  $\epsilon = 4$ )

Fe	-0.007942423	0.365008027	0.474242346
Fe	-1.076012740	0.046576972	3.027751066
O	0.003812919	-0.826600156	1.996915360
O	-1.425928948	1.055597217	1.628157292
O	-1.247417967	-0.994652125	-0.560490200
H	-2.017959053	-1.235689604	0.047924467
H	-1.607364061	-0.452139768	-1.310333364
C	-1.044040105	2.922194892	-3.026577216
C	-1.083516728	1.642323206	-2.216177220
O	-1.833438308	0.689010150	-2.589757136
O	-0.318824354	1.623408205	-1.200505623
C	3.531695486	3.392348460	1.385686625
C	2.697330154	2.982863145	2.586507326
C	1.570103402	1.978966278	2.341451040
O	1.394028457	1.628394638	1.113799515
O	0.918487036	1.586726559	3.329744172
C	2.911483252	0.409583940	-2.337362737
C	2.744923772	-0.793379342	-1.475100205
N	1.753351467	-0.919834409	-0.519276931
C	3.493741274	-1.949518173	-1.491744706
C	1.911211042	-2.121626036	0.011253260
N	2.946210598	-2.774329347	-0.542683859
C	1.369111556	0.962448536	-9.722462641
C	0.472638275	0.482216493	-8.617385886
C	0.036255062	-0.849276771	-8.577562574
C	0.070044531	1.322732637	-7.576161593
C	-0.751619714	-1.331999177	-7.538751078
C	-0.720179308	0.857628253	-6.527880445
C	-1.123864453	-0.478316712	-6.495701395
O	-1.884262651	-0.996835917	-5.482692435
C	-5.399641180	1.141298276	4.247399009
C	-4.123355233	1.749893371	3.678131618
C	-2.972877433	1.835638510	4.664271099
O	-3.101427509	2.490087140	5.728922701
O	-1.853053082	1.254449127	4.396132252
C	-3.268244692	-4.547419741	2.510300354
C	-4.041152208	-3.237027703	2.651432723
C	-3.226242240	-2.050469234	2.136153126
O	-3.175827362	-1.892742119	0.890092148
O	-2.663730836	-1.336244237	3.030435153
C	-2.148816713	-1.418622925	6.420853304
C	-0.764967293	-1.607009318	5.910038747
N	-0.265820767	-1.092458001	4.723443808
C	0.240105654	-2.312485574	6.525535302
C	0.997226505	-1.485321442	4.645112036
N	1.338208339	-2.219407479	5.712544815
C	8.663600394	-8.834038825	-2.015985944
C	7.432304029	-7.993696227	-2.151460457
C	6.699729594	-7.485302019	-1.104783743
C	6.797447941	-7.508796042	-3.343982414
N	5.648850706	-6.737417770	-1.568743666
C	5.675303203	-6.728051308	-2.937942552

C	7.060529863	-7.636078787	-4.721330978
C	4.828468515	-6.095343373	-3.850969536
C	6.222381816	-7.005971026	-5.631004871
C	5.117099336	-6.243986360	-5.201598631
C	1.990358620	-5.243272036	2.464743585
C	3.241549430	-5.923063047	1.918470625
O	3.688771347	-6.915130893	2.575164445
O	3.757060264	-5.456315499	0.855054619
C	6.456706094	-3.642192412	6.925478525
C	5.215516417	-3.873502941	6.099122075
O	4.134899007	-3.326025225	6.369875139
N	5.352335538	-4.730539270	5.069731061
C	4.057111330	2.013678664	8.144098780
C	2.626032579	2.413062297	7.987111452
C	1.809675971	2.086348149	6.929289393
C	1.813170200	3.190901770	8.882069832
N	0.553973799	2.604512290	7.110972654
C	0.517413171	3.286210798	8.297234332
C	2.038987521	3.821029853	10.120337799
C	-0.531861744	3.981497890	8.906869925
C	0.997529514	4.511113740	10.729364747
C	-0.274917545	4.590363071	10.128314001
O	-4.381502278	1.251926521	8.351353093
H	-1.147302002	3.786364440	-2.362400209
H	-0.060481002	3.005524245	-3.504810330
H	-1.821059847	2.952776739	-3.793006256
H	4.051341469	2.534307248	0.944033172
H	2.912244212	3.838380868	0.599624478
H	4.289108975	4.129679474	1.682357003
H	2.225003712	3.860954088	3.049112792
H	3.330762836	2.551451625	3.373704803
H	3.827537735	0.327984897	-2.930436575
H	2.069857675	0.518879543	-3.031221562
H	2.958912120	1.325117363	-1.739370801
H	4.346311740	-2.245434753	-2.091281274
H	1.292818727	-2.546338098	0.787640280
H	3.256581844	-3.698450327	-0.249952259
H	2.198000000	0.260000000	-9.844000000
H	0.843367276	1.022073467	-10.685198486
H	1.785087417	1.951847229	-9.505887383
H	0.333146950	-1.536416631	-9.371764136
H	0.383870443	2.367424346	-7.571211946
H	-1.068011858	-2.373957798	-7.515967371
H	-1.020733194	1.536604763	-5.733780025
H	-1.887830695	-0.368951953	-4.741754465
H	-6.179212204	1.132531950	3.475275315
H	-5.239136966	0.105789943	4.570854618
H	-5.779336064	1.713198105	5.100471937
H	-4.327827145	2.779456539	3.356366516
H	-3.803811207	1.195427410	2.794776655
H	-2.340055089	-4.526373354	3.095756516
H	-3.871669545	-5.392993554	2.865164673
H	-3.002051793	-4.737761935	1.463240516
H	-4.311585614	-3.070002366	3.699804640
H	-4.965396925	-3.291578123	2.061585740
H	-2.301215532	-2.040639022	7.308337853
H	-2.326560007	-0.377901965	6.704412471
H	-2.892298112	-1.688030303	5.666494170

H	0.260724843	-2.860067611	7.459091867
H	1.673906538	-1.254471029	3.836558858
H	2.249700282	-2.630808427	5.882613412
H	9.468000000	-8.258000000	-1.545000000
H	8.488733475	-9.716638642	-1.386844650
H	9.026421825	-9.188398510	-2.984915053
H	6.858016880	-7.599958498	-0.039117793
H	4.956659837	-6.299639728	-0.974623719
H	7.912806694	-8.216649477	-5.074361752
H	3.977625836	-5.501683795	-3.516340540
H	6.424683173	-7.095391473	-6.697792189
H	4.480836215	-5.757125170	-5.939194049
H	1.606000000	-5.719000000	3.376000000
H	2.201598420	-4.189758171	2.678098514
H	1.206365101	-5.257723421	1.698510049
H	6.513000000	-4.433000000	7.686000000
H	7.373114941	-3.682965680	6.327244848
H	6.382972496	-2.676055444	7.429116439
H	6.226583947	-5.199003621	4.890662710
H	4.541160535	-5.039017407	4.555023389
H	4.382000000	1.434000000	7.275000000
H	4.722105816	2.883289175	8.235403910
H	4.215291374	1.395393704	9.038644009
H	2.032593284	1.519901104	6.034177359
H	-0.218768066	2.480609808	6.471257193
H	3.015652655	3.766606410	10.602311199
H	-1.512375016	4.044835660	8.436629379
H	1.163650668	4.996987163	11.690489764
H	-1.072986261	5.138632824	10.627817584
H	-3.962122292	1.608717770	7.552079799
H	-5.079605089	1.895060296	8.533742578
C	2.674274874	-11.456208583	1.971832925
H	3.196575117	-10.568840069	1.616468207
H	2.053849178	-11.861340700	1.163336277
H	2.028166000	-11.148234000	2.797858000
N	3.610833121	-12.458696615	2.441463716
H	3.208204839	-13.269066398	2.889824680
C	4.906050771	-12.547734467	2.142089209
N	5.563053879	-11.553511805	1.556127614
H	6.546999436	-11.680133458	1.376846119
H	5.212730399	-10.582306602	1.550489919
N	5.557993409	-13.707556089	2.386429929
H	6.553044818	-13.646944552	2.549263461
H	5.089259254	-14.403980286	2.946647843
O	-4.840982131	4.689440202	6.189716055
H	-4.254476109	3.934343909	5.962926366
H	-4.476160094	5.413350011	5.663304688
O	8.620564876	-5.595047484	2.629620382
H	9.359055324	-4.977688877	2.539984396
H	7.898396466	-5.140161879	2.150198512
O	4.905184581	-8.872151476	1.366869646
H	4.461506578	-8.080925559	1.821347375
H	4.743438819	-8.714334805	0.429565423
O	6.504671250	-4.245107718	1.202639635
H	6.312105349	-3.381358965	1.590771185
H	5.632780366	-4.680643495	1.168325558
O	-2.552383326	3.587888010	1.103707306
O	-5.277075182	2.658740901	-0.216341585

O	-4.484440940	1.662284105	-3.162878466
H	-1.943272399	3.921707061	0.432808137
H	-2.150784033	2.724465662	1.345493190
H	-4.415191018	2.877979757	0.175096196
H	-5.040967026	2.291064588	-1.082948521
H	-4.983717052	0.938818025	-3.567696654
H	-3.599590771	1.271719778	-3.006086756

## Cartesian coordinates of Model-II with three explicit water molecules around site O2:

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(Using OPBE potential, optimized in COSMO solvation model with  $\epsilon = 4$ )

Fe	0.023048954	0.231649848	0.361418785
Fe	-1.146469860	-0.002190177	3.040548275
O	-0.157236488	-0.858959079	1.941948669
O	-1.593234370	0.984484412	1.462180286
O	-1.312078990	-1.040721312	-0.638638185
H	-2.047500583	-1.301781519	-0.002822673
H	-1.688285020	-0.465465523	-1.355561669
C	-0.948719256	2.975037188	-2.887570196
C	-1.025426656	1.644789575	-2.174336190
O	-1.832600693	0.752516699	-2.558396396
O	-0.214812494	1.518667835	-1.193238274
C	3.441308583	3.258433198	1.553213597
C	2.559576280	2.812189133	2.705705678
C	1.399568771	1.886850049	2.366767213
O	1.311647143	1.515676467	1.137998961
O	0.622309646	1.555919657	3.290322615
C	2.808161161	0.249658700	-2.320059963
C	2.642939780	-0.916026156	-1.409519518
N	1.644136101	-1.026085237	-0.455024354
C	3.399220230	-2.065247611	-1.370172593
C	1.809634573	-2.211683705	0.119172420
N	2.851471342	-2.866815146	-0.401342726
C	1.569182321	1.071884147	-9.480630924
C	0.675527955	0.555592287	-8.391380828
C	0.215449011	-0.767626541	-8.407126958
C	0.271247295	1.366154953	-7.327030034
C	-0.606241704	-1.271664697	-7.404459749
C	-0.553052500	0.880268799	-6.316219840
C	-0.989616270	-0.446174075	-6.344678781
O	-1.792013798	-0.981231716	-5.372351653
C	-5.509514473	0.846661629	4.322740591
C	-4.332417200	1.534132351	3.637576386
C	-3.143164932	1.758841419	4.546447127
O	-3.226701981	2.497864165	5.541414215
O	-1.998000576	1.187720049	4.280238321
C	-3.155041779	-4.653301797	2.565947331
C	-3.930515073	-3.349899281	2.747784862
C	-3.171940727	-2.151329197	2.187075545
O	-3.105698887	-2.030596741	0.943875747
O	-2.671990591	-1.357115279	3.064591305
C	-1.969892786	-1.369698049	6.501511802
C	-0.623951783	-1.550337159	5.897365380



N	-0.207528352	-1.057209368	4.668955506
C	0.430126316	-2.232060508	6.454362199
C	1.054167551	-1.440519898	4.511792613
N	1.469205053	-2.146153012	5.568577732
C	8.603505970	-8.824141838	-1.907388116
C	7.398226026	-7.939851821	-1.963277675
C	6.731687962	-7.434944256	-0.872106437
C	6.736305487	-7.393392038	-3.113751057
N	5.692204373	-6.632861850	-1.269609912
C	5.665501449	-6.581871509	-2.637891707
C	6.938249149	-7.488585211	-4.504025406
C	4.806063823	-5.892062184	-3.496422923
C	6.089156184	-6.799273127	-5.359586684
C	5.032115915	-6.010352093	-4.862273546
C	1.978931754	-5.184011270	2.491851896
C	3.317053123	-5.715022771	1.982182622
O	3.900247194	-6.597507284	2.675780144
O	3.774715785	-5.230067790	0.892594809
C	6.475502218	-3.652662426	6.914758890
C	5.316737524	-3.934912879	5.987691206
O	4.253780216	-3.294097758	6.051042723
N	5.507165633	-4.938930696	5.114058019
C	3.994830717	1.987560916	8.136326677
C	2.568798042	2.370149504	7.905758734
C	1.817603969	2.036067106	6.804080421
C	1.695541549	3.135186886	8.754528580
N	0.547059902	2.538717494	6.912033617
C	0.434093721	3.216158592	8.097295540
C	1.841250892	3.764715790	10.004657847
C	-0.657317647	3.894921687	8.645492422
C	0.757737318	4.440063852	10.552810494
C	-0.478727682	4.505319986	9.880348312
O	-4.470900209	1.525470787	8.534742841
H	-1.075157437	3.784857672	-2.160724346
H	0.052896623	3.094692958	-3.316832366
H	-1.697613776	3.070345768	-3.675551540
H	3.933463107	2.408647765	1.067593950
H	2.865673165	3.788734713	0.786271267
H	4.221523098	3.936503464	1.920844978
H	2.124015822	3.674726109	3.227716062
H	3.154518575	2.288526237	3.466969753
H	3.743552406	0.157054037	-2.879616952
H	1.989822754	0.305502840	-3.047611396
H	2.822237031	1.194835435	-1.768296132
H	4.261902656	-2.366304681	-1.951959565
H	1.184404868	-2.617560850	0.898051732
H	3.186774834	-3.773709386	-0.032343997
H	2.198000000	0.259999000	-9.844000000
H	0.993978044	1.455005511	-10.335104795
H	2.216080520	1.882587775	-9.128378585
H	0.513883846	-1.430725234	-9.220480433
H	0.609866850	2.401904862	-7.275548218
H	-0.947022031	-2.305819481	-7.427607177
H	-0.855713174	1.536191295	-5.504906946
H	-1.833104680	-0.356980383	-4.631005660
H	-6.337977866	0.743308216	3.611629094
H	-5.241556328	-0.156880147	4.670860259
H	-5.871336840	1.425692972	5.179888136

H	-4.644735943	2.528588084	3.298482152
H	-4.027386239	0.968625663	2.755442087
H	-2.197093577	-4.627963149	3.101435991
H	-3.735485911	-5.497843392	2.957898385
H	-2.947035603	-4.847306635	1.507050796
H	-4.147024352	-3.181637435	3.807804938
H	-4.885232437	-3.413982143	2.208955652
H	-2.033154091	-1.953705494	7.424306967
H	-2.157105061	-0.321794548	6.753169709
H	-2.763517416	-1.698587831	5.825904661
H	0.519976335	-2.760146853	7.394749130
H	1.677802033	-1.218384920	3.659878987
H	2.392585005	-2.552280404	5.684113206
H	9.467999000	-8.258000000	-1.545000000
H	8.460032679	-9.667301361	-1.219763579
H	8.856625510	-9.237217623	-2.888166614
H	6.931153361	-7.588223757	0.181960498
H	5.046734188	-6.173947638	-0.636309175
H	7.752792600	-8.088857093	-4.909494475
H	3.990422291	-5.280816905	-3.110114128
H	6.245450125	-6.861447080	-6.436014696
H	4.384966230	-5.477448813	-5.557583356
H	1.606000000	-5.719000000	3.376000000
H	2.084650462	-4.125630939	2.754529258
H	1.230264230	-5.244133465	1.693879544
H	6.513000000	-4.432999000	7.686000000
H	7.434416718	-3.664030778	6.384652070
H	6.329346526	-2.684199994	7.396490887
H	6.385146103	-5.432379376	5.072316150
H	4.776297897	-5.237677199	4.482269360
H	4.382000000	1.434002000	7.274999000
H	4.637804280	2.865097265	8.287246088
H	4.111388157	1.350753063	9.024139885
H	2.102106842	1.465605047	5.930741803
H	-0.185625181	2.410956437	6.228781106
H	2.788782145	3.720820753	10.542128867
H	-1.610596398	3.946379915	8.121238961
H	0.862053860	4.926567574	11.522166198
H	-1.311322710	5.041831048	10.333628105
H	-4.096103000	1.815383374	7.691270519
H	-5.303529388	2.014889036	8.580654901
C	2.705647099	-11.464227350	2.002426682
H	3.220501220	-10.571648059	1.648238924
H	2.123519652	-11.904256434	1.183729755
H	2.028166000	-11.148234000	2.797858000
N	3.639278935	-12.429605995	2.547990334
H	3.243839281	-13.172956759	3.105539021
C	4.927544914	-12.560619406	2.234429650
N	5.565871798	-11.637240051	1.510625532
H	6.562200718	-11.746182093	1.396382975
H	5.228829004	-10.673465820	1.513351208
N	5.592199219	-13.643537165	2.663833364
H	6.563212121	-13.762290992	2.424072969
H	5.088904418	-14.466408413	2.955666893
O	-4.610030363	5.306469813	5.463849173
H	-4.180161286	4.435490320	5.477239994
H	-4.029011923	5.822797950	4.888139017
O	8.694099020	-5.422121715	2.349874681

H	9.325746562	-4.753486990	2.647063619
H	7.981142561	-4.883856276	1.952544016
O	4.668412518	-8.843883559	1.404771077
H	4.440971362	-7.993238326	1.868480496
H	4.607406865	-8.616505476	0.469151454
O	6.576685494	-3.848529904	1.089256113
H	6.421739744	-3.002946477	1.530868271
H	5.713111105	-4.292657553	1.133372467
H	-1.782059990	1.946768639	1.562675693
O	-2.614014653	3.589650672	1.286746677
O	-4.798433060	2.389841493	-0.109515742
O	-4.417536514	1.875578354	-3.140335612
H	-2.119834456	4.133093403	0.660397999
H	-3.354330310	3.234554876	0.747657956
H	-5.620287837	2.895088143	-0.048609025
H	-4.711979296	2.235617024	-1.066578180
H	-4.990275102	1.183292544	-3.485969886
H	-3.551991816	1.432357599	-3.031289396

### Cartesian coordinates of Model-I-SO<sub>4</sub><sup>2-</sup>:

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(Using OPBE potential, optimized in COSMO solvation model with  $\epsilon = 10$ .)

Fe	-0.011831201	0.334737042	0.495236000
Fe	-1.084583058	0.001156930	3.042470808
O	0.023399395	-0.851157471	2.018868450
O	-1.461481113	0.979734591	1.644674059
O	-1.222449482	-1.078146377	-0.546343393
H	-2.029549910	-1.232078723	0.024467361
H	-1.512445977	-0.555972456	-1.350817727
C	-1.246217343	2.820007696	-3.007448937
C	-1.128253766	1.541724618	-2.203981817
O	-1.676806663	0.488124834	-2.632821808
O	-0.444114920	1.630187148	-1.126640570
C	3.504327027	3.420511210	1.373270985
C	2.683240422	3.000263236	2.579640488
C	1.554281979	1.996829448	2.346589803
O	1.361961556	1.642597193	1.120513244
O	0.908660747	1.607251862	3.340396695
C	2.875459326	0.420378274	-2.346343869
C	2.710201289	-0.780968379	-1.482057665
N	1.727404933	-0.908397472	-0.515180854
C	3.458044711	-1.937554072	-1.505452815
C	1.891601018	-2.111762798	0.012859223
N	2.919722218	-2.762175740	-0.551886336
C	1.387057075	0.979548541	-9.711099040
C	0.477646548	0.502517441	-8.615593659
C	0.053146472	-0.833492802	-8.569976410
C	0.051874541	1.348361719	-7.587181312
C	-0.744483601	-1.314838867	-7.537016389
C	-0.748866947	0.884395353	-6.544877833
C	-1.141150269	-0.455178825	-6.507713312
O	-1.909037339	-0.972972047	-5.502126625
C	-5.389046668	1.177095930	4.154252836

C	-4.103614924	1.800893861	3.618569821
C	-2.977133763	1.856364937	4.636619024
O	-3.119239942	2.530592559	5.690214561
O	-1.877691546	1.226694587	4.413194730
C	-3.247335705	-4.529619653	2.472782738
C	-4.070671555	-3.249652630	2.613634110
C	-3.289138588	-2.028596167	2.132692260
O	-3.320434546	-1.762418670	0.901067074
O	-2.657703832	-1.392975612	3.038656641
C	-2.141616789	-1.410697250	6.443524824
C	-0.761059521	-1.606768940	5.927210789
N	-0.265982771	-1.099039010	4.735757445
C	0.246126684	-2.310380900	6.541830157
C	0.997344874	-1.492371087	4.654408190
N	1.340358648	-2.221140395	5.723394847
C	8.651145909	-8.820001412	-2.015707272
C	7.431090395	-7.962088719	-2.145805914
C	6.698489295	-7.463644959	-1.094568013
C	6.797748579	-7.461106471	-3.333384362
N	5.650966514	-6.705847118	-1.550442224
C	5.677039686	-6.682410116	-2.919156583
C	7.056484822	-7.578683299	-4.712334669
C	4.827926519	-6.041892882	-3.826246978
C	6.216280892	-6.941858060	-5.616293968
C	5.111833874	-6.181849603	-5.179485073
C	1.969990708	-5.218354234	2.469085881
C	3.257132090	-5.841081057	1.938805104
O	3.768860840	-6.775239957	2.627536525
O	3.741731888	-5.383360055	0.855297628
C	6.456954084	-3.631269009	6.936680780
C	5.211145913	-3.843821600	6.115188810
O	4.133780321	-3.290546667	6.402329309
N	5.338244426	-4.678569259	5.068696275
C	4.051760155	2.038995445	8.126486159
C	2.619873046	2.437818784	7.959904857
C	1.812423372	2.118823423	6.891859474
C	1.797584208	3.205461793	8.855990377
N	0.553542717	2.632165388	7.067989410
C	0.504783076	3.302554831	8.262096258
C	2.011304772	3.826777366	10.100516471
C	-0.553342001	3.986133302	8.870766688
C	0.964119301	4.508842185	10.708198263
C	-0.305610019	4.587350476	10.099431799
O	-4.362847207	1.336154689	8.339102503
H	-1.411114970	3.672436666	-2.340677582
H	-0.298344082	2.998727130	-3.531366315
H	-2.051920152	2.759170960	-3.743114217
H	4.015091082	2.566099515	0.914916298
H	2.879613709	3.882349846	0.600357929
H	4.268486585	4.149987649	1.671595322
H	2.216152620	3.875213370	3.053585167
H	3.327116514	2.564405996	3.355847508
H	3.778364311	0.323505959	-2.956951587
H	2.023044613	0.543556876	-3.024594035
H	2.952270829	1.335687688	-1.750782765
H	4.304133970	-2.233900499	-2.113892567
H	1.280617193	-2.537661507	0.794060193
H	3.233779550	-3.684464932	-0.254650197

H	2.198000000	0.260000000	-9.844000000
H	0.863471128	1.069176459	-10.672782846
H	1.826612433	1.954976045	-9.477405410
H	0.368024461	-1.524102054	-9.353376395
H	0.360014473	2.394458380	-7.583454286
H	-1.049580418	-2.360067105	-7.509909152
H	-1.060971459	1.565681004	-5.756634429
H	-1.942339916	-0.335549901	-4.768559404
H	-6.157141571	1.173338690	3.370712647
H	-5.226946755	0.138479600	4.466963404
H	-5.785600084	1.733637591	5.010309921
H	-4.301853085	2.838026162	3.314372989
H	-3.762459097	1.264523293	2.731451547
H	-2.326007146	-4.475843385	3.066265194
H	-3.823329944	-5.396711823	2.820086081
H	-2.965720969	-4.709155002	1.427464908
H	-4.357695217	-3.106150023	3.661474997
H	-4.985164348	-3.331234221	2.012704075
H	-2.286061991	-2.017393602	7.342684244
H	-2.317782244	-0.364320555	6.707552269
H	-2.891478359	-1.694593333	5.700737684
H	0.270185853	-2.857134466	7.475766664
H	1.671155518	-1.267011555	3.842159766
H	2.252227042	-2.635515204	5.888743482
H	9.468000000	-8.257999000	-1.544999000
H	8.463793245	-9.697112454	-1.383300979
H	9.003464930	-9.181881458	-2.985620707
H	6.844437026	-7.603707341	-0.030481249
H	4.954535407	-6.280683532	-0.952073151
H	7.904221008	-8.162410893	-5.071021579
H	3.973976674	-5.456295052	-3.484762344
H	6.411012369	-7.032163472	-6.684475651
H	4.467755385	-5.697303273	-5.912052799
H	1.606001000	-5.719001000	3.375999000
H	2.137980738	-4.159381746	2.693668223
H	1.192846589	-5.259505651	1.697139043
H	6.513000000	-4.433000000	7.686000000
H	7.369702724	-3.675704554	6.333865692
H	6.394917306	-2.672134935	7.454904857
H	6.203303208	-5.170245257	4.904551124
H	4.524030263	-4.991936294	4.560220149
H	4.382000000	1.434001000	7.275000000
H	4.717171084	2.909779944	8.198381701
H	4.205550082	1.445290402	9.037516548
H	2.044012447	1.559597885	5.994266059
H	-0.216878525	2.502877546	6.427153778
H	2.986984885	3.774807470	10.586919578
H	-1.530609763	4.049257349	8.396203120
H	1.123307428	4.992168937	11.671159880
H	-1.109165553	5.128900512	10.597314806
H	-3.960818069	1.675657704	7.523417238
H	-5.114827518	1.928971778	8.475402317
O	-4.840191530	4.736320748	6.105875929
H	-4.252403587	3.974694118	5.899214016
H	-4.429034363	5.466798596	5.623012351
O	8.654812181	-5.575606994	2.504976217
H	9.346071821	-4.899905299	2.536866456
H	7.905232067	-5.100816791	2.093843282

O	4.934747284	-8.780462500	1.344509728
H	4.518276090	-7.992063302	1.799508221
H	4.651564153	-8.684811894	0.427496570
O	6.462314775	-4.178861516	1.201133570
H	6.278707222	-3.342069037	1.648050977
H	5.594255577	-4.624982604	1.178691291
C	2.684672848	-11.430271439	1.979531028
H	3.206970219	-10.518885926	1.690634625
H	2.111155627	-11.805042500	1.122095205
H	1.990574350	-11.175898543	2.784626764
N	3.605072176	-12.436113497	2.467404951
H	3.189295984	-13.192491163	2.997795222
C	4.887087191	-12.575216484	2.133257320
N	5.526811893	-11.629280412	1.425591404
H	6.527194063	-11.738415113	1.345101483
H	5.211768353	-10.660799637	1.492681782
N	5.529353452	-13.706342982	2.443662034
H	6.537899927	-13.693135929	2.456233561
H	5.070897823	-14.411807882	3.023629526
O	4.116506206	-15.597685432	4.034738492
S	3.561257306	-16.653106680	4.931778367
O	2.147415655	-16.275810972	5.299609418
O	3.554429064	-17.969967339	4.214917176
O	4.393551351	-16.749462398	6.173746115
H	4.069472939	-18.006207290	7.850384254
O	4.031026996	-18.555895352	8.653626855
H	4.479530638	-18.004121588	9.308790035
H	5.904900154	-15.230372143	6.267595502
O	6.638794040	-14.610216174	6.428378288
H	6.839745208	-14.757387105	7.363109348
H	3.892565314	-17.779016778	2.129420237
O	4.055100931	-17.826019725	1.169464445
H	3.639832092	-18.663405008	0.921830441
H	2.548821037	-19.631172789	4.819005313
O	2.127881834	-20.488957678	5.017264942
H	2.208162894	-20.962089986	4.177919764
H	0.990204809	-17.234036088	6.438346718
O	0.322166408	-17.652338585	7.023876841
H	-0.455880633	-17.093646550	6.891776969
H	1.544556286	-14.708277128	4.493568370
O	1.206799810	-13.900152216	4.046634646
H	0.412636356	-13.680711592	4.552653569

### Cartesian coordinates of Model-II-SO<sub>4</sub><sup>2-</sup>:

190

Fe	0.038467012	0.216608062	0.359085001
Fe	-1.159180386	-0.034661770	3.060550366
O	-0.184682468	-0.872642762	1.940164829
O	-1.604746556	1.047520278	1.501950849
O	-1.302064048	-1.029062086	-0.640435013
H	-2.057038837	-1.276544775	-0.036136033
H	-1.644636208	-0.450008142	-1.387369260
C	-1.031342856	2.950829330	-2.864170044

C	-1.048184903	1.626835095	-2.140887418
O	-1.772904876	0.683568482	-2.548010465
O	-0.272030623	1.564229454	-1.115490787
C	3.443608167	3.256658638	1.548460479
C	2.562110238	2.818863996	2.704420022
C	1.411078732	1.881616541	2.374780480
O	1.335315622	1.479408165	1.154476668
O	0.617835942	1.570064468	3.292752793
C	2.761836071	0.233236476	-2.344699270
C	2.610257741	-0.929011005	-1.428133976
N	1.624364318	-1.035741804	-0.459931905
C	3.365176671	-2.079277484	-1.392737847
C	1.796162504	-2.219951261	0.118179481
N	2.831221436	-2.875036228	-0.412406395
C	1.588227315	1.071959231	-9.447485022
C	0.692461250	0.561270549	-8.355662382
C	0.215099407	-0.756756825	-8.362097987
C	0.295283772	1.384724996	-7.297521957
C	-0.621572902	-1.239777611	-7.359369591
C	-0.543295523	0.921061960	-6.288647972
C	-1.003802956	-0.396939274	-6.311954271
O	-1.822590782	-0.905727708	-5.341954648
C	-5.511009060	0.815259811	4.318405591
C	-4.333751635	1.500779585	3.629638261
C	-3.153899330	1.739167903	4.549260374
O	-3.256648251	2.486179156	5.537016635
O	-2.000916896	1.171573227	4.304205348
C	-3.144749138	-4.642499932	2.590326707
C	-3.940884261	-3.348965279	2.757489049
C	-3.204452352	-2.144779340	2.185368638
O	-3.168013734	-1.998458660	0.944224638
O	-2.684839791	-1.351198679	3.057200201
C	-1.932324684	-1.391936778	6.519897702
C	-0.592010400	-1.562979924	5.899787853
N	-0.191071618	-1.064499052	4.666976631
C	0.472927212	-2.240014720	6.441976868
C	1.072733525	-1.438892826	4.495632861
N	1.502128501	-2.143947593	5.545684374
C	8.594130654	-8.831819820	-1.869730129
C	7.391984098	-7.943645118	-1.920327684
C	6.709323007	-7.472085408	-0.824433911
C	6.746015463	-7.361749096	-3.063013867
N	5.678096274	-6.656267602	-1.212157483
C	5.668901606	-6.563126028	-2.577385457
C	6.959002987	-7.422935059	-4.453537997
C	4.816453027	-5.852391763	-3.426706544
C	6.117991825	-6.711247260	-5.299452419
C	5.055447646	-5.935266388	-4.792900378
C	1.956097749	-5.176636200	2.488095040
C	3.318422000	-5.657594181	1.997235403
O	3.946141932	-6.480851227	2.720965191
O	3.756474249	-5.191096669	0.890000425
C	6.479815514	-3.617980621	6.952054259
C	5.345289774	-3.859542584	5.985118166
O	4.328506094	-3.139753570	5.967539553
N	5.503031445	-4.907867912	5.162022954
C	3.991307246	1.999596752	8.128513162
C	2.566702309	2.383949607	7.887662887

C	1.827760377	2.052848728	6.776637833
C	1.682946813	3.148740776	8.727428173
N	0.556837581	2.558611313	6.868579866
C	0.429325357	3.234396411	8.052999850
C	1.812592960	3.777469845	9.980680564
C	-0.669771936	3.910916944	8.590330525
C	0.722914503	4.453328647	10.515846410
C	-0.506481175	4.518629189	9.828917080
O	-4.517579891	1.559466057	8.532220110
H	-1.194521115	3.760105233	-2.143996688
H	-0.039226754	3.112417377	-3.303101541
H	-1.792266531	2.991502734	-3.646180906
H	3.950137051	2.405288919	1.080945026
H	2.865066518	3.766872275	0.770085806
H	4.212056063	3.951352053	1.909385017
H	2.115705560	3.685442752	3.210507550
H	3.159211013	2.312167620	3.475202283
H	3.683411640	0.132614183	-2.925059722
H	1.927189012	0.292060817	-3.053538862
H	2.795950108	1.180559869	-1.796959307
H	4.220782486	-2.382023005	-1.984021247
H	1.179537771	-2.623985906	0.904734058
H	3.168508435	-3.782367723	-0.039346934
H	2.198000000	0.259999000	-9.844000000
H	1.009552108	1.486395064	-10.284848984
H	2.254973898	1.862745906	-9.086755549
H	0.511586164	-1.432991626	-9.165269488
H	0.652643427	2.414229900	-7.248625950
H	-0.973318575	-2.270729969	-7.374180357
H	-0.838583622	1.585967728	-5.481321459
H	-1.896396859	-0.259485676	-4.621030151
H	-6.335055291	0.693483015	3.605001349
H	-5.235834816	-0.181071605	4.684029428
H	-5.881488348	1.403001539	5.165102918
H	-4.650283084	2.490886360	3.274510707
H	-4.019274833	0.926925702	2.756745401
H	-2.189063656	-4.598619653	3.127999856
H	-3.716329216	-5.488276243	2.991844197
H	-2.933350495	-4.847598322	1.534058961
H	-4.158940008	-3.173662988	3.816024228
H	-4.894757229	-3.433716601	2.220606308
H	-1.981976618	-1.982894795	7.438942124
H	-2.123375829	-0.346285199	6.779447083
H	-2.732947128	-1.722419874	5.853301877
H	0.575529065	-2.772754587	7.378565349
H	1.686800536	-1.212044610	3.638398044
H	2.431399934	-2.544147498	5.647932362
H	9.467999000	-8.258000000	-1.545000000
H	8.463993391	-9.649591571	-1.150582106
H	8.822757178	-9.275912710	-2.843020054
H	6.884365947	-7.668217647	0.226691972
H	5.028148860	-6.210201497	-0.575754780
H	7.773997765	-8.017454370	-4.866497926
H	3.990874721	-5.260077902	-3.032322061
H	6.278742389	-6.754486244	-6.376201352
H	4.408090069	-5.393497364	-5.481172749
H	1.606000000	-5.719000000	3.376000000
H	2.024405184	-4.114860471	2.747363906



H	1.212984607	-5.268322759	1.688247931
H	6.513000000	-4.432999000	7.686000000
H	7.447053871	-3.604734092	6.436547087
H	6.325764625	-2.670162339	7.470617564
H	6.330396164	-5.482325564	5.210323155
H	4.789150139	-5.176692309	4.497862156
H	4.382000000	1.434002000	7.274999000
H	4.635731623	2.877208202	8.272220966
H	4.101392235	1.374199533	9.024960225
H	2.123102472	1.482144891	5.907065772
H	-0.169531319	2.425010069	6.179933315
H	2.754810727	3.736986929	10.527628700
H	-1.617126769	3.961274792	8.055398103
H	0.816231005	4.940925667	11.485709991
H	-1.345497034	5.051800897	10.274400745
H	-4.160476486	1.837117542	7.676928348
H	-5.396168320	1.964555261	8.543698003
O	-4.531766607	5.331130038	5.375137487
H	-4.140081384	4.442491803	5.392418941
H	-4.054732255	5.762856954	4.652288928
O	8.834622796	-5.228802981	2.075883361
H	9.203802051	-4.633232875	2.742461609
H	8.034183928	-4.750847699	1.778118260
O	4.649553697	-8.796375879	1.434206968
H	4.433966311	-7.949499889	1.895195656
H	4.385940241	-8.627087267	0.521509027
O	6.527551328	-3.808502907	1.051278880
H	6.367417951	-2.968061514	1.500806712
H	5.678768089	-4.277753087	1.124917552
H	-1.466343153	1.973147783	1.758677775
C	2.7111035884	-11.471749517	2.010125768
H	3.212024054	-10.553800565	1.703107812
H	2.169019677	-11.898356026	1.156326562
H	1.992012849	-11.206471824	2.788773999
N	3.647364218	-12.425735707	2.568159372
H	3.238089903	-13.149811825	3.147935718
C	4.918202401	-12.599816292	2.201543387
N	5.523824333	-11.728054004	1.366715162
H	6.527978508	-11.820170127	1.302267472
H	5.209705900	-10.763419694	1.402469150
N	5.590170260	-13.659762935	2.640318369
H	6.565014458	-13.762779819	2.409587661
H	5.123276144	-14.410931888	3.155014042
O	4.094670057	-15.621645705	3.969659782
S	3.557409168	-16.650968651	4.906388624
O	2.149255152	-16.263394720	5.283256681
O	3.544384129	-17.983815870	4.220800071
O	4.404248918	-16.720166522	6.140500411
H	4.051683445	-17.979016953	7.828805133
O	4.002081372	-18.535977732	8.626139279
H	4.482635011	-18.009803613	9.279981726
H	5.904837431	-15.227942102	6.299243501
O	6.637849036	-14.611665605	6.480986481
H	6.832834991	-14.784343479	7.412381378
H	3.887138717	-17.764209745	2.121360761
O	4.039142400	-17.820522598	1.160756258
H	3.643111736	-18.672461305	0.931295858
H	2.555080748	-19.613729974	4.832577012

O	2.120506253	-20.464689055	5.035973069
H	2.213029454	-20.952271029	4.206121103
H	1.001806206	-17.220463802	6.417794690
O	0.335409167	-17.634819362	7.008093563
H	-0.443794400	-17.079185582	6.870461128
H	1.538871692	-14.689852368	4.489877518
O	1.210605505	-13.872267139	4.053021391
H	0.433643446	-13.637397125	4.578433197

### Cartesian coordinates of Model-I-Asp237H-SO<sub>4</sub><sup>2-</sup>:

190

Fe	0.025035480	0.347185992	0.542207289
Fe	-1.074834413	-0.027023965	3.067683094
O	0.070408873	-0.857825740	2.057029930
O	-1.437249390	0.959891264	1.675939805
O	-1.124918734	-1.089597023	-0.509374002
H	-1.933094342	-1.279781829	0.053634710
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C	1.582450681	2.011856942	2.394761229
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N	1.795605351	-0.813218380	-0.589831867
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C	1.939082518	-2.072735635	-0.212439278
N	2.910672930	-2.683311675	-0.913145523
C	1.358034254	0.949981260	-9.716167497
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C	-0.755738388	0.895398562	-6.532865531
C	-1.140904127	-0.445046436	-6.469337936
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C	0.522812178	3.328185506	8.284582181
C	2.036916334	3.807472657	10.130552681
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C	-0.272073469	4.593564052	10.142478517
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H	3.339229306	2.631419267	3.399554513
H	3.784856525	0.639597270	-2.958665996
H	2.033123123	0.891395030	-2.965373945
H	2.998095154	1.523974959	-1.631875785
H	4.222693038	-2.025156219	-2.487870090
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H	-4.128094767	-5.335875252	2.867696218
H	-3.191123564	-4.760913456	1.474901570
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H	-1.502112009	4.100375216	8.429375698
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O	8.815361806	-5.919809638	2.532674322
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H	2.902112910	-10.876986305	2.669703523
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H	4.857714034	-11.319333198	1.335306801
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O	4.348153429	-16.026467428	4.345944173
S	4.095255955	-17.305069532	5.077272794
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O	5.144538907	-17.495426188	6.132482259
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H	2.030848924	-15.369820593	5.104962082
O	1.347182845	-19.193728253	7.522251696
H	0.522056793	-18.698740042	7.619872276
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H	0.832273175	-14.479982834	5.403103814
H	3.711944623	-20.426392499	4.646310482
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O	3.525156969	-21.371640562	4.795809068
H	3.290132924	-21.680344872	3.913749649
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### Cartesian coordinates of Model-II-Asp237H-SO<sub>4</sub><sup>2-</sup>:

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O	-0.290549869	1.560586087	-1.122777100
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C	2.580920952	2.773050677	2.735923314
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O	0.638445365	1.515395926	3.305946073
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C	2.617210843	-0.810365862	-1.517516178

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C	1.822059740	-2.212900087	-0.058306252
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C	-1.978220678	-1.342374558	6.524753976
C	-0.642006558	-1.556884577	5.909144117
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C	6.759352073	-7.479490695	-0.932503046
C	6.762620580	-7.437600550	-3.172066926
N	5.711417765	-6.686560441	-1.329468035
C	5.679762677	-6.643153663	-2.696212731
C	6.995571219	-7.492120306	-4.560060484
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H	1.937134580	0.541080809	-3.034484638
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H	7.016220871	-7.574453106	0.116185295
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H	2.933359319	-10.831357443	2.591065164
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H	3.193480632	-13.471133665	3.517543714
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H	6.242688380	-12.310025681	1.172306788
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H	6.439363805	-14.176600146	2.420774935
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O	4.302485181	-16.014337292	4.345566679
S	4.030757636	-17.275859432	5.102011685
O	2.672860949	-17.154702252	5.736364056
O	4.049734852	-18.442654908	4.160550362
O	5.076821186	-17.462070733	6.161653334
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H	1.986787976	-15.275718782	5.092343341
O	1.421499549	-19.043631600	7.651939438
H	0.523269047	-18.687040332	7.617192232
O	1.571801552	-14.432053819	4.828859858
H	0.785927211	-14.390689074	5.391347217
H	3.878824766	-20.532082248	4.626303818
H	4.202355003	-17.927751883	2.126867297
O	3.848792681	-21.502190920	4.703246936
H	3.272399573	-21.753725027	3.968361925
O	4.273067355	-17.805358702	1.162486938
H	4.056418507	-18.682153903	0.817116816
H	5.315662999	-19.123268525	7.377376076
H	6.574570954	-15.975359027	6.393831961
O	7.321971561	-15.371425478	6.555153320
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O	5.557143462	-19.844572384	7.987110387
H	5.711792678	-19.374538439	8.818045240