

List of cartesian coordinates of all isomers proposed in this work

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**Cartesian coordinates of all the proposed isomers of
[Fe²⁺(H₂O)_{n=1-10}] at MP2/6-31++G(d,p) level of theory at
quintet spin-state**

Cartesian coordinates of the monomer : [Fe(H₂O)₁]²⁺

Cartesian coordinates of : 100-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.000000	-1.373576	0.000000
1	-0.787032	-1.960488	0.000000
1	0.787032	-1.960488	0.000000
26	0.000000	0.573446	0.000000

Cartesian coordinates of the dimer : [Fe(H₂O)₂]²⁺

Cartesian coordinates of : 200-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.960893	-0.000001	0.000000
1	2.546440	0.553835	-0.556694
26	0.000001	0.000001	0.000000
8	-1.960895	-0.000001	0.000000
1	-2.546441	-0.556703	-0.553830
1	2.546438	-0.553841	0.556694
1	-2.546442	0.556698	0.553832

Cartesian coordinates of : 200-4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.959993	0.000000	0.000000
1	2.545518	-0.783898	0.000003
26	0.000000	0.000000	-0.000001
8	-1.959992	0.000000	0.000001
1	-2.545517	-0.783898	0.000000
1	2.545520	0.783896	0.000003
1	-2.545519	0.783896	0.000000

Cartesian coordinates of the trimer : $[\text{Fe}(\text{H}_2\text{O})_3]^{2+}$

Cartesian coordinates of : 300-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.017704	-1.731828	0.000004
26	-0.012006	-0.000023	-0.000003
1	1.337077	-2.222115	-0.779915
1	1.337074	-2.222122	0.779919
8	-2.010103	-0.002862	0.000001
1	-2.591933	-0.786310	-0.000003
1	-2.594172	0.778918	0.000017
8	1.012736	1.734734	0.000003
1	1.330707	2.225925	-0.779919
1	1.330704	2.225942	0.779916

Cartesian coordinates of : 210-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.174709	1.428598	-0.000044
1	0.083279	2.398592	0.000245
26	-1.187979	0.000000	0.000001
8	0.174709	-1.428596	0.000041
1	0.083280	-2.398590	-0.000244
1	1.139829	1.180748	-0.000173
1	1.139828	-1.180746	0.000157
8	2.445379	-0.000002	0.000002
1	3.041424	0.000125	0.770862
1	3.041425	-0.000118	-0.770858

Cartesian coordinates of the tetramer : $[\text{Fe}(\text{H}_2\text{O})_4]^{2+}$

Cartesian coordinates of : 400-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
26	-0.000038	-0.000019	-0.000016
8	-1.262272	1.188785	-1.094328
1	-2.035038	1.671873	-0.753788
1	-1.164580	1.455896	-2.024233
8	1.262726	-1.188136	-1.094569
1	1.165342	-1.454802	-2.024631
1	2.035374	-1.671375	-0.753994
8	-1.262192	-1.189217	1.093999
1	-1.164593	-1.456396	2.023891

1	-2.034714	-1.672530	0.753235
8	1.261835	1.188615	1.094948
1	1.164041	1.455281	2.024966
1	2.034378	1.672178	0.754590

Cartesian coordinates of : 400-4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.110079	-0.000107	0.000045
1	-2.695892	-0.000127	0.776396
26	0.000004	0.000000	0.000003
8	2.110092	0.000090	0.000045
1	2.695955	0.000118	-0.776269
8	-0.000116	2.043379	-0.000047
1	0.781857	2.621371	-0.000083
1	-2.695943	-0.000160	-0.776269
1	2.695905	0.000113	0.776396
1	-0.782162	2.621273	-0.000074
8	0.000094	-2.043359	-0.000047
1	0.782127	-2.621271	-0.000067
1	-0.781891	-2.621336	-0.000079

Cartesian coordinates of : 310-5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.549808	1.311165	0.030079
1	-0.461926	2.490027	0.043821
1	-0.627636	-2.353625	0.045010
1	-1.632400	-1.103145	0.030715
1	3.324788	-0.064166	-0.686879
1	3.303854	-0.063095	0.879063
26	0.735421	0.024395	0.061558
1	-3.496111	0.168805	-0.765430
1	-3.516711	0.169912	0.774920
8	-2.911676	0.149043	0.012713
8	-0.581236	1.524987	0.042889
8	-0.680703	-1.382688	0.043638
8	2.733121	-0.043784	0.088309

Cartesian coordinates of the pentamer : $[\text{Fe}(\text{H}_2\text{O})_5]^{2+}$

Cartesian coordinates of : 500-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.133563	0.136385	-0.177948
1	2.711780	0.220663	-0.953385
26	0.000005	-0.000006	-0.104725
8	-2.133557	-0.136310	-0.177956
1	-2.723901	-0.087426	0.591057
8	-0.155545	1.972823	-0.728309
1	-0.980076	2.466048	-0.867504
1	2.723907	0.087516	0.591066
1	-2.711777	-0.220600	-0.953390
1	0.574395	2.584147	-0.917408
8	-0.000002	-0.000089	2.034936
1	-0.316006	-0.707505	2.619541
1	0.315977	0.707295	2.619591
8	0.155534	-1.972789	-0.728422
1	-0.574423	-2.584094	-0.917523
1	0.980053	-2.466041	-0.867596

Cartesian coordinates of : 410-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.752266	0.283396	1.202511
1	-0.720598	0.569466	2.381573
1	-0.720583	-0.569464	-2.381573
1	-1.752259	-0.283413	-1.202513
1	2.570343	1.797526	-0.660274
1	1.347262	2.623482	-0.163846
26	0.594924	-0.000002	0.000003
1	1.347341	-2.623465	0.163779
1	2.570357	-1.797491	0.660336
1	-3.707518	-0.748561	0.173046
1	-3.707523	0.748534	-0.173050
8	-0.798614	0.364390	1.436818
8	-3.112001	-0.000011	-0.000001
8	-0.798605	-0.364398	-1.436816
8	1.670719	-1.717046	0.301337
8	1.670679	1.717068	-0.301346

Cartesian coordinates of : 320-4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.941742	-1.075197	0.195180
1	-2.482867	-0.244020	0.270852
26	-0.000010	-0.846055	-0.142384
8	1.941698	-1.075206	0.195385
1	2.525979	-1.849976	0.158287
8	0.000008	1.144599	-0.361891

1	0.811121	1.688011	-0.294121
1	-2.526034	-1.849956	0.158004
1	2.482841	-0.244028	0.270954
1	-0.811090	1.688031	-0.294102
8	2.768194	1.469965	0.148931
1	3.389853	1.751894	-0.543626
1	3.084502	1.916011	0.952809
8	-2.768135	1.470017	0.149063
1	-3.389826	1.752053	-0.543422
1	-3.084379	1.915981	0.953011

Cartesian coordinates of the hexamer : $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$

Cartesian coordinates of : 600-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.121413	2.409604	-1.021067
1	0.065133	1.953623	-2.063932
1	-1.526103	2.175859	1.021257
1	-1.659353	1.032997	2.064004
1	-0.065134	-1.953610	2.063937
1	-1.121406	-2.409606	1.021072
1	1.724255	0.920334	2.064121
1	2.647389	0.233588	1.021329
26	0.000001	-0.000003	-0.000003
1	1.526100	-2.175869	-1.021264
1	1.659355	-1.033007	-2.064009
1	-2.647385	-0.233608	-1.021320
1	-1.724255	-0.920318	-2.064139
8	1.234530	-1.274315	-1.226691
8	1.720833	0.431844	1.226760
8	-0.486457	-1.706318	1.226595
8	-1.234520	1.274311	1.226692
8	-1.720828	-0.431847	-1.226767
8	0.486437	1.706338	-1.226579

Cartesian coordinates of : 510-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.996743	-1.756188	-1.056580
1	0.501632	-2.164319	-1.783947
26	0.488387	0.016096	-0.086791
8	1.000373	2.003608	-0.423150
1	0.476337	2.648833	-0.922856
8	2.301395	-0.164502	1.072223
1	2.389096	-0.218017	2.036842
1	1.665262	-2.401123	-0.777259

1	1.737403	2.487968	-0.019524
1	3.207416	-0.197228	0.725816
8	-1.223728	0.257771	-1.316014
1	-2.126397	0.196606	-0.932358
1	-1.315373	0.408594	-2.268448
8	-0.827875	-0.315121	1.480361
1	-1.800279	-0.272793	1.335164
1	-0.677991	-0.551698	2.406854
8	-3.355869	-0.054409	0.421730
1	-3.956059	-0.815353	0.358392
1	-3.927413	0.690774	0.669331

Cartesian coordinates of : 420-5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.373262	1.018709	1.096490
1	1.288065	1.675924	1.803927
26	-0.000002	0.000019	-0.000001
8	-1.373262	1.096537	-1.018665
1	-2.327141	0.918883	-0.853650
8	1.373231	-1.018702	-1.096503
1	1.288023	-1.675934	-1.803922
1	2.327141	0.853663	0.918868
1	-1.288066	1.803963	-1.675891
1	2.327112	-0.853675	-0.918875
8	-1.373228	-1.096526	1.018681
1	-2.327110	-0.918894	0.853661
1	-1.288018	-1.803965	1.675892
8	3.684483	-0.000026	-0.000001
1	4.279327	-0.563021	0.523007
1	4.279323	0.562938	-0.523048
8	-3.684481	-0.000028	0.000001
1	-4.279323	0.522975	0.563003
1	-4.279323	-0.523068	-0.562967

Cartesian coordinates of the heptamer : $[\text{Fe}(\text{H}_2\text{O})_7]^{2+}$

Cartesian coordinates of : 610-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.073260	-2.708969	-0.542418
1	-1.045442	-2.686778	0.534403
1	-2.364744	-0.776187	-1.913083
1	-2.364752	0.775738	-1.913254
1	0.073201	2.708882	-0.542927
1	-1.045537	2.686860	0.533858
1	1.096200	-0.000191	-2.380504

1	2.124732	-0.000122	-1.183292
26	-0.375727	0.000006	0.045891
1	2.148738	0.000145	1.173334
1	1.207875	0.000336	2.428993
1	-2.907128	0.000117	1.195929
1	-2.005865	0.000180	2.460076
8	1.212007	0.000187	1.461878
8	1.171816	-0.000134	-1.415604
8	-0.568996	2.131984	-0.102424
8	-2.037039	-0.000170	-1.434449
8	-1.983462	0.000132	1.491417
8	-0.568936	-2.132007	-0.101998
8	3.578756	-0.000009	-0.023335
1	4.172591	-0.767749	-0.023986
1	4.172605	0.767721	-0.024163

Cartesian coordinates of : 520-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.187148	0.849453	1.286725
1	-0.943020	1.317567	2.097676
26	-0.000002	-0.255910	0.000006
8	1.187141	0.849468	-1.286707
1	0.943009	1.317599	-2.097647
8	1.695734	-0.317311	1.291018
1	2.562617	0.034535	0.995847
1	-2.137821	1.019040	1.103271
1	2.137812	1.019057	-1.103249
1	1.754479	-0.490055	2.241812
8	0.000001	-2.337920	-0.000030
1	0.690604	-2.910797	0.366706
1	-0.690601	-2.910779	-0.366797
8	-1.695717	-0.317248	-1.291032
1	-1.754447	-0.489976	-2.241830
1	-2.562608	0.034583	-0.995863
8	3.713298	0.912476	-0.187025
1	4.441530	0.409833	-0.586425
1	4.120493	1.741185	0.112920
8	-3.713302	0.912452	0.187035
1	-4.441506	0.409759	0.586424
1	-4.120537	1.741156	-0.112867

Cartesian coordinates of : 610-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.187491	0.000813	-2.163839
1	3.112568	0.000563	-0.908386
1	1.035401	-2.777553	-0.529503

1	-0.075738	-2.797764	0.551016
1	-2.275316	-0.000346	0.755365
1	-1.409045	-0.000866	2.088789
1	-1.123525	-0.773346	-2.194455
1	-1.124020	0.774849	-2.193595
26	0.417581	-0.000009	0.025457
1	-0.075616	2.797374	0.553092
1	1.035239	2.777897	-0.527730
1	2.026015	-0.778048	2.226930
1	2.025729	0.776391	2.227738
8	0.471577	2.206599	0.014821
8	-0.669182	0.000694	-1.828851
8	-1.345775	-0.000520	1.123263
8	0.471571	-2.206625	0.013263
8	1.688443	-0.000646	1.757074
8	2.186799	0.000479	-1.194578
8	-3.744861	0.000048	0.030814
1	-4.332453	0.769072	0.063553
1	-4.332424	-0.769036	0.062679

Cartesian coordinates of : 430-4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.497140	-1.805748	-0.303012
1	-1.469605	-2.681431	-0.716894
26	0.000003	-0.436034	-0.000001
8	1.417789	1.017453	-0.169158
1	2.383004	0.857897	-0.183600
8	-1.417797	1.017445	0.169144
1	-1.209744	1.976360	0.167867
1	-2.439939	-1.522001	-0.222198
1	1.209729	1.976367	-0.167869
1	-2.383011	0.857884	0.183582
8	1.497149	-1.805740	0.303034
1	2.439947	-1.521992	0.222208
1	1.469618	-2.681418	0.716925
8	-3.812851	-0.415323	0.063883
1	-4.355553	-0.568069	0.854621
1	-4.452955	-0.300409	-0.657283
8	3.812849	-0.415317	-0.063902
1	4.355543	-0.568071	-0.854643
1	4.452960	-0.300395	0.657257
8	-0.000006	3.388410	0.000011
1	-0.103109	3.981375	-0.761785
1	0.103097	3.981361	0.761818

Cartesian coordinates of : 430-5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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1	-1.091713	-1.648562	-2.022183
1	-0.173127	-2.263047	-0.873018
1	1.224302	-1.542240	1.054183
1	2.067165	-0.186773	1.136477
26	-0.138148	0.341118	-0.333453
1	-1.670435	2.229524	0.761196
1	-2.653989	0.984926	0.516277
1	-4.464533	0.138837	1.478594
1	-4.805450	0.690681	0.072459
1	0.144334	-3.881549	0.875643
1	1.381819	-3.871575	-0.033614
1	1.314754	2.295430	-1.687917
1	2.183805	1.643015	-0.524092
1	3.630777	1.811165	1.403456
1	4.268673	0.860985	0.379474
8	-0.530706	-1.430220	-1.263653
8	0.676408	-3.299566	0.309394
8	-1.702227	1.327732	0.408156
8	-4.071453	0.401675	0.633852
8	1.189676	-0.572618	0.946852
8	1.308442	1.637319	-0.977307
8	3.409294	1.169442	0.709311

Cartesian coordinates of : 340-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.465700	-0.347218	0.328831
1	2.478837	1.280857	0.115682
1	-0.817032	-2.369182	-0.279091
1	0.817036	-2.369181	-0.279092
1	-2.465696	-0.347222	0.328825
1	-2.478839	1.280853	0.115678
26	0.000002	0.143166	-0.155853
1	2.949135	-2.758218	0.976891
1	3.278611	-2.587253	-0.510773
8	2.664787	-2.285219	0.178239
8	1.908888	0.445184	0.185676
8	0.000002	-1.843788	-0.412807
8	-1.908886	0.445182	0.185669
8	-3.233026	2.623858	0.012511
1	-3.762861	2.910875	-0.744633
1	-3.563704	3.113536	0.779034
8	-2.664780	-2.285224	0.178241
1	-3.278604	-2.587262	-0.510770
1	-2.949126	-2.758221	0.976895
8	3.233012	2.623869	0.012509
1	3.563688	3.113552	0.779030
1	3.762846	2.910886	-0.744636

Cartesian coordinates of the octamer : $[\text{Fe}(\text{H}_2\text{O})_8]^{2+}$

Cartesian coordinates of : 620-5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-2.596106	-0.455835	0.000004
1	-2.784620	1.115030	-0.000036
1	-0.776708	0.672590	-2.705204
1	0.776676	0.672629	-2.705200
1	2.596132	-0.455692	0.000008
1	2.784562	1.115182	-0.000024
1	0.800539	-2.147944	-0.000018
1	-0.800415	-2.147987	-0.000009
26	-0.000014	0.512448	-0.000001
1	-0.776710	0.672569	2.705201
1	0.776675	0.672615	2.705202
1	-0.000086	3.307946	-0.777002
1	-0.000109	3.307937	0.777045
1	-3.156452	-2.738720	0.766804
1	-3.156459	-2.738718	-0.766788
1	3.156600	-2.738551	0.766802
1	3.156617	-2.738543	-0.766790
8	-0.000086	2.730894	0.000018
8	-2.127226	0.405246	-0.000005
8	-0.000020	0.795654	-2.139448
8	0.000047	-1.591209	-0.000019
8	-2.740413	-2.314501	0.000007
8	-0.000021	0.795634	2.139448
8	2.740543	-2.314351	0.000004
8	2.127205	0.405363	-0.000001

Cartesian coordinates of : 620-6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.533858	2.704035	-0.571432
1	0.533849	2.704044	0.571400
1	1.568234	-0.051318	-2.399263
1	2.521384	-0.151703	-1.163325
1	0.533855	-2.704043	-0.571402
1	-0.533853	-2.704037	0.571428
1	-1.568234	0.051297	-2.399264
1	-2.521387	0.151677	-1.163327
26	0.000001	-0.000000	0.000000
1	-2.521387	-0.151679	1.163326
1	-1.568235	-0.051309	2.399265
1	2.521384	0.151706	1.163325
1	1.568234	0.051329	2.399264
8	-1.587235	-0.231616	1.448985

8	-1.587234	0.231611	-1.448986
8	0.000007	-2.133795	0.000016
8	1.587232	-0.231636	-1.448985
8	1.587232	0.231640	1.448985
8	0.000001	2.133795	-0.000016
8	-3.969538	0.000001	0.000000
1	-4.562396	0.763363	0.085388
1	-4.562397	-0.763359	-0.085387
8	3.969534	0.000000	0.000000
1	4.562393	-0.763359	0.085407
1	4.562393	0.763359	-0.085407

Cartesian coordinates of : 620-7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.795190	1.270483	-2.130236
1	-2.003335	1.196162	-1.131112
1	-2.488452	0.407937	1.037044
1	-1.997827	-0.632665	2.102511
1	0.757169	-2.261422	2.128174
1	1.844050	-2.173316	1.027977
1	1.802647	1.595653	0.814468
1	0.588210	1.695210	1.825502
26	-0.019811	-0.368762	0.051717
1	2.018025	-0.837809	-1.932461
1	2.571675	0.274507	-0.972091
1	-1.329522	-1.971509	-1.840075
1	-0.595998	-2.958689	-0.876796
1	-4.369037	1.161228	-0.377603
1	-3.708728	2.397263	0.251517
1	4.225329	1.585668	0.386481
1	3.562114	2.570180	-0.587874
8	-3.517806	1.496535	-0.054348
8	-0.671787	-2.027230	-1.131534
8	0.913045	1.245414	1.033579
8	-1.151163	0.780864	-1.375709
8	-1.715544	-0.117545	1.334037
8	0.924200	-1.943866	1.228764
8	3.397062	1.754224	-0.089792
8	1.876239	-0.404781	-1.078757

Cartesian coordinates of : 530-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.265131	-0.000000	1.508821
1	-0.908660	-0.000000	2.408000
26	-0.176948	-0.000000	-0.260832
8	0.294391	1.920344	-0.853308

1	-0.261856	2.552785	-1.329213
8	1.725976	0.000000	0.765702
1	2.298379	0.790422	0.763023
1	-2.243204	-0.000000	1.552234
1	1.116311	2.375824	-0.557591
1	2.298380	-0.790421	0.763023
8	0.294391	-1.920345	-0.853307
1	-0.261856	-2.552785	-1.329212
1	1.116312	-2.375824	-0.557591
8	-2.045941	-0.000000	-1.268152
1	-2.262182	-0.000001	-2.211315
1	-2.886028	-0.000000	-0.761678
8	2.677355	2.649556	0.266954
1	3.451288	2.837578	-0.287196
1	2.722886	3.300297	0.985208
8	-3.947871	-0.000000	0.765821
1	-4.518746	-0.768374	0.925022
1	-4.518746	0.768374	0.925022
8	2.677356	-2.649555	0.266954
1	3.451289	-2.837577	-0.287197
1	2.722888	-3.300295	0.985208

Cartesian coordinates of : 620-8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.995019	0.538949	0.838917
1	-1.775574	-1.019001	0.867944
1	0.536538	1.653359	2.325459
1	1.740883	2.207738	1.514719
1	-1.241502	1.904370	-1.016265
1	-0.227762	1.752721	-2.213379
1	-2.850148	2.972214	0.505950
1	-3.619267	2.050436	-0.446141
26	0.564808	0.091292	-0.035641
1	-2.967544	-2.872326	-0.432964
1	-2.057110	-3.549262	0.596347
1	2.102922	-1.050641	2.083269
1	1.780224	-2.215497	1.099938
8	-2.129081	-2.757145	0.041017
8	-2.762316	2.150915	-0.002637
8	-0.373656	1.532533	-1.283056
8	1.078196	1.501833	1.536827
8	1.726118	-1.256100	1.215296
8	-1.318142	-0.158452	0.927861
8	0.160026	-1.684556	-1.160503
1	-0.642242	-2.210700	-0.960658
1	0.481870	-1.947906	-2.034139
8	2.392789	0.456733	-1.159795
1	2.708383	1.274941	-1.570584
1	3.148864	-0.149066	-1.151824

Cartesian coordinates of : 611-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.235349	2.680339	-0.614893
1	2.341694	2.354338	0.424807
1	2.975819	0.036025	-1.935797
1	2.483691	-1.434764	-1.886872
1	-0.449104	-2.427990	-0.424767
1	0.654027	-2.763195	0.615766
1	-0.579389	0.383855	-2.365477
1	-1.531150	0.679817	-1.126031
26	0.866435	-0.013569	0.045823
1	-0.607504	0.625754	2.412285
1	-1.527910	0.751788	1.133993
1	3.292094	-0.754043	1.188319
1	2.439063	-0.470925	2.455538
8	-0.623909	0.516029	1.452328
8	-0.620670	0.409277	-1.399723
8	0.380319	-2.105198	-0.041058
8	2.445559	-0.587863	-1.418061
8	2.415279	-0.467890	1.487208
8	1.706978	1.950242	-0.186174
8	-2.838998	1.053627	-0.017861
1	-3.231001	1.939625	-0.037509
1	-3.606744	0.422030	-0.007607
8	-4.822162	-0.744656	-0.006021
1	-5.352717	-0.954750	0.774793
1	-5.402689	-0.903639	-0.763044

Cartesian coordinates of : 440-4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.594214	1.784588	-0.776048
1	0.575309	2.080238	0.458232
1	-1.388497	1.019838	1.665993
1	-2.478525	0.105901	0.937670
26	-0.080248	-0.342126	-0.249397
1	0.454786	-2.952281	-0.093864
1	1.743303	-2.235804	0.528715
1	3.256892	-2.698325	2.115443
1	3.924009	-2.696981	0.718545
1	0.083416	2.727878	2.828815
1	-0.881004	3.489143	1.910900
1	-1.491760	-1.093028	-2.548933
1	-2.492708	-0.770682	-1.359086
1	-4.426575	-1.249718	0.038347
1	-4.567918	0.168926	-0.532743
8	0.840571	1.426333	-0.220224
8	-0.394871	2.653210	1.988095

8	0.843601	-2.084874	0.090669
8	3.139110	-2.402161	1.201743
8	-1.525919	0.223273	1.116693
8	-1.545785	-0.840740	-1.616068
8	-3.906638	-0.483126	-0.251393
8	2.776983	2.261175	-1.738755
1	3.705590	2.337068	-1.479604
1	2.659505	2.853809	-2.494134

Cartesian coordinates of the nanomer : $[\text{Fe}(\text{H}_2\text{O})_9]^{2+}$

Cartesian coordinates of : 630-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.593204	-2.779524	0.653431
1	-0.854835	-2.586536	0.068713
1	-2.267082	-0.800234	-0.859365
1	-2.267597	0.799034	-0.859367
1	-0.856146	2.586218	0.067998
1	0.591980	2.780156	0.652148
1	2.110193	0.000145	-1.667541
1	0.719463	0.000019	-2.423882
26	0.123534	0.000120	0.306638
1	2.468529	0.001349	1.988653
1	2.995025	0.000473	0.506515
1	-0.788462	-0.781352	2.855051
1	-0.788760	0.782078	2.854760
1	-3.260092	-3.073801	-0.295818
1	-2.568083	-3.177461	-1.661069
1	4.439588	0.768339	-1.421266
1	4.439646	-0.767907	-1.421041
8	-2.522602	-2.712250	-0.811441
8	-0.489433	0.000330	2.368732
8	1.137030	0.000121	-1.552558
8	-0.111066	-2.131832	0.513351
8	-1.725395	-0.000425	-0.721933
8	-0.112035	2.132065	0.512632
8	3.894273	0.000229	-1.190876
8	2.192522	0.000557	1.062312
8	-2.524138	2.710923	-0.811821
1	-2.570020	3.175888	-1.661561
1	-3.261698	3.072249	-0.296140

Cartesian coordinates of : 630-4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.458680	0.046495	2.746192

1	0.629034	-1.074937	2.666313
1	1.243767	2.067286	-0.193480
1	2.416524	0.983377	-0.185777
1	0.458680	0.046494	-2.746192
1	-0.629034	-1.074937	-2.666311
1	-1.243767	2.067286	0.193479
1	-2.416524	0.983377	0.185776
26	-0.000000	-0.385386	0.000000
1	-2.545922	-1.450089	-0.081001
1	-1.664008	-2.731752	0.106623
1	2.545922	-1.450089	0.081002
1	1.664008	-2.731752	-0.106621
8	-1.633057	-1.800152	-0.151265
8	-1.461946	1.124875	0.325525
8	-0.115487	-0.444524	-2.141926
8	1.461946	1.124875	-0.325526
8	1.633057	-1.800152	0.151267
8	0.115487	-0.444521	2.141926
8	-3.940198	-0.212220	0.001835
1	-4.553468	-0.255312	0.751942
1	-4.512785	-0.136123	-0.777153
8	3.940198	-0.212220	-0.001835
1	4.553467	-0.255312	-0.751943
1	4.512786	-0.136123	0.777152
8	0.000000	3.524714	-0.000000
1	0.091893	4.118372	0.761167
1	-0.091893	4.118373	-0.761167

Cartesian coordinates of : 540-4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-2.585277	0.798247	-0.078864
1	-2.585274	-0.798233	-0.078893
1	0.806262	2.432171	-0.630213
1	-0.806258	2.432172	-0.630212
1	0.806258	-2.432185	-0.630194
1	-0.806261	-2.432183	-0.630195
26	0.000000	-0.000001	0.332246
1	2.585278	0.798244	-0.078864
1	2.585273	-0.798236	-0.078893
1	-3.114737	2.820805	-1.507638
1	-3.106955	3.266378	-0.039148
1	3.114730	-2.820795	-1.507663
1	3.106982	-3.266351	-0.039167
8	-2.098424	0.000003	0.204621
8	-2.700247	2.633558	-0.651182
8	0.000001	1.907086	-0.462828
8	2.098424	0.000000	0.204621
8	-0.000001	-1.907102	-0.462799
8	2.700254	-2.633543	-0.651201
8	-2.700258	-2.633540	-0.651201
1	-3.106987	-3.266347	-0.039168

1	-3.114734	-2.820791	-1.507663
8	2.700250	2.633555	-0.651183
1	3.114741	2.820801	-1.507638
1	3.106959	3.266374	-0.039149
8	-0.000000	-0.000015	2.421321
1	-0.782626	-0.000025	2.991901
1	0.782626	-0.000026	2.991901

Cartesian coordinates of : 621-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.373034	2.657456	-1.642287
1	1.391420	3.096230	-0.541449
1	2.786806	0.094092	-1.773477
1	2.687101	-1.227438	-0.932093
1	-0.052030	-1.826731	1.511167
1	1.224194	-2.199523	0.649030
1	-0.694211	-0.398689	-2.294213
1	-1.769713	0.200819	-1.305510
26	0.608859	0.464056	0.074586
1	-1.184788	1.416127	2.082326
1	-1.995772	0.873103	0.841249
1	3.013841	1.063780	1.315331
1	2.005317	1.524502	2.397853
8	-1.101075	0.919069	1.257642
8	-0.806077	0.149253	-1.505805
8	0.600135	-1.482390	0.886051
8	2.406765	-0.291788	-0.971678
8	2.081589	1.281982	1.463724
8	0.933224	2.332725	-0.922301
8	-3.240129	0.568345	-0.360813
1	-3.786088	1.309102	-0.663707
1	-3.877667	-0.167760	-0.167121
8	-4.901294	-1.467282	0.192447
1	-5.476154	-1.496948	0.969217
1	-5.344309	-2.003212	-0.479253
8	2.649898	-3.003083	-0.215365
1	3.411914	-3.287232	0.313318
1	2.472487	-3.747777	-0.810842

Cartesian coordinates of : 630-5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.160362	2.494751	-0.032898
1	2.950508	1.735825	1.070090
1	3.263807	-0.368443	-1.549015
1	2.323689	-1.469515	-2.107595
1	-1.225046	-1.914556	-0.508374

1	0.082339	-2.751331	-0.354390
1	0.161420	1.093613	-2.399471
1	-0.747453	1.686780	-1.229630
26	0.931387	-0.095163	-0.002780
1	-1.383284	0.458069	1.428362
1	-0.246442	1.377659	1.986545
1	2.792321	-1.629794	1.545286
1	1.579070	-1.274034	2.457388
8	-0.404259	0.548380	1.512877
8	0.072154	1.152345	-1.438987
8	-0.249586	-1.845665	-0.426094
8	2.428576	-0.831835	-1.386335
8	1.980781	-1.103794	1.592280
8	2.279080	1.627286	0.381180
8	-2.034351	2.463597	-0.637385
1	-2.447403	3.260349	-0.996625
1	-2.722478	1.948010	-0.184526
8	-3.091625	0.368588	0.997289
1	-3.765057	0.497275	1.681992
1	-3.329231	-0.454750	0.530833
8	-3.071648	-2.049264	-0.556103
1	-3.447433	-2.843514	-0.144348
1	-3.488728	-2.009261	-1.431114

Cartesian coordinates of the decamer : $[\text{Fe}(\text{H}_2\text{O})_{10}]^{2+}$

Cartesian coordinates of : 640-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.639969	0.450861	-2.726045
1	0.640056	-0.450852	-2.726011
1	-2.178108	-1.701101	0.115987
1	-0.868294	-2.623711	0.116081
1	-0.450910	-0.640031	2.726014
1	0.450825	0.639976	2.726038
1	-2.623705	0.868272	-0.116062
1	-1.701092	2.178086	-0.116071
26	0.000001	0.000008	-0.000003
1	0.868320	2.623702	0.116122
1	2.178107	1.701051	0.116135
1	1.701071	-2.178114	-0.116052
1	2.623705	-0.868321	-0.116093
8	1.215561	1.725639	0.268318
8	-1.725650	1.215540	-0.268250
8	-0.000007	-0.000043	2.158667
8	-1.215567	-1.725646	0.268195
8	1.725649	-1.215578	-0.268293
8	0.000081	0.000079	-2.158670
8	-0.666009	3.840154	0.000036
1	-0.730905	4.432028	-0.764925
1	-0.804205	4.419320	0.764993

8	0.665984	-3.840184	0.000045
1	0.804152	-4.419360	0.764999
1	0.730912	-4.432046	-0.764922
8	-3.840192	-0.665980	-0.000037
1	-4.419375	-0.804080	-0.764999
1	-4.432052	-0.730954	0.764927
8	3.840161	0.666009	-0.000008
1	4.432054	0.730935	0.764935
1	4.419304	0.804191	-0.764985

Cartesian coordinates of : 640-4.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.249002	1.906656	2.149540
1	1.243148	1.946916	1.631808
1	2.728718	0.719738	0.128796
1	2.605149	-0.683596	-0.622898
1	0.794201	-1.984523	-1.658454
1	-0.567263	-1.516164	-2.282565
1	-1.243074	1.946990	-1.631776
1	0.249064	1.906624	-2.149544
26	0.000003	0.056735	0.000007
1	-2.605183	-0.683536	0.622856
1	-2.728708	0.719807	-0.128828
1	-0.794269	-1.984516	1.658425
1	0.567122	-1.516082	2.282630
1	3.679804	2.094680	2.068558
1	3.366886	3.068445	0.925103
1	-3.679722	2.094791	-2.068604
1	-3.366805	3.068544	-0.925139
8	3.077303	2.232628	1.321617
8	0.046798	-1.522280	1.468175
8	-0.380798	1.493891	-1.544420
8	0.380879	1.493791	1.544524
8	2.116054	0.094909	-0.299154
8	-0.046852	-1.522276	-1.468165
8	-3.077233	2.232722	-1.321650
8	-2.116063	0.094956	0.299117
8	2.640569	-2.383623	-1.562286
1	3.152408	-2.419701	-2.384908
1	2.878663	-3.194892	-1.088358
8	-2.640652	-2.383570	1.562241
1	-2.878765	-3.194837	1.088319
1	-3.152491	-2.419631	2.384863

Cartesian coordinates of : 631-3.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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1	0.692781	-1.974866	1.782326
1	1.753225	-0.900352	1.311165
1	1.970125	0.952449	-0.110542
1	1.010924	2.030146	-0.821943
1	-1.438662	2.450663	-0.887106
1	-2.780676	1.689882	-0.568442
1	-0.409371	0.847527	3.048377
1	-1.390105	1.877826	2.398544
26	-0.615932	0.110135	0.345344
1	-2.735367	-1.833928	0.225521
1	-2.866913	-1.144548	1.632134
1	-1.273178	-1.776756	-1.623798
1	0.047809	-1.044899	-2.100444
1	3.864641	-0.556590	0.190088
1	3.775906	0.365619	1.440974
1	5.486030	-1.058164	-1.494053
1	5.321904	-2.288037	-0.583108
8	3.230267	-0.052608	0.759068
8	-0.646691	-1.050218	-1.428646
8	-0.950558	1.025766	2.265971
8	0.793837	-1.070140	1.458357
8	1.055592	1.151244	-0.404637
8	-1.840487	1.739521	-0.348432
8	4.897073	-1.458894	-0.840758
8	-2.406120	-1.104113	0.783422
8	-0.035887	3.497771	-1.592936
1	0.066394	4.389493	-1.226386
1	0.014459	3.621105	-2.553158
8	-2.726312	-2.906579	-1.372946
1	-3.483362	-2.822686	-1.972964
1	-2.578022	-3.861407	-1.293840

Cartesian coordinates of : 541-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.076692	1.440103	-0.695813
1	-0.831959	2.359419	-0.909643
26	0.224367	0.013639	0.120338
8	1.781079	-1.369215	0.370760
1	2.713013	-1.093723	0.463165
8	-0.724819	-1.419851	-1.049646
1	-0.421537	-2.337102	-1.180253
1	-1.906180	1.183231	-1.140738
1	1.735788	-2.274079	0.005939
1	-1.644820	-1.300599	-1.353189
8	1.671727	1.502093	0.073901
1	2.623383	1.347834	0.225231
1	1.509205	2.419528	-0.219137
8	-3.204620	-0.205976	-1.291860
1	-3.893571	-0.244625	-1.971356
1	-3.658362	-0.253009	-0.432008
8	4.114721	0.215424	0.604955

1	4.557441	0.310409	1.462270
1	4.835744	0.187727	-0.042499
8	0.913723	-3.711223	-0.953255
1	0.699873	-4.516296	-0.457517
1	1.340396	-4.027910	-1.764194
8	0.432993	3.818883	-0.908453
1	0.254791	4.579870	-0.334967
1	0.679204	4.205090	-1.762909
8	-0.818298	-0.147509	1.900945
1	-0.496633	-0.455679	2.759041
1	-1.802365	-0.135227	1.917262
8	-3.591762	-0.136210	1.645614
1	-4.075649	-0.866092	2.063044
1	-4.035706	0.664477	1.966500

Cartesian coordinates of : 631-4.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.238619	-2.689209	0.232065
1	2.765178	-2.337459	-1.188114
1	4.011065	0.132304	0.679565
1	3.440897	1.494511	1.156649
1	-0.397403	2.209980	0.432726
1	0.929788	2.779731	-0.155824
1	1.137620	-0.499332	2.592624
1	-0.101126	-1.190225	1.860447
26	1.332971	-0.000762	-0.129247
1	-1.326311	-0.420248	-0.774824
1	-0.486724	-1.606667	-1.371640
1	2.854611	0.865612	-2.400363
1	1.403396	0.544349	-2.873939
8	-0.417435	-0.684360	-1.087028
8	0.809431	-0.788465	1.730914
8	0.516841	1.967356	0.167480
8	3.245445	0.721654	0.607133
8	2.014224	0.471484	-2.125652
8	2.357208	-1.960836	-0.395243
8	-1.577775	-1.791572	1.793977
1	-2.017350	-2.370159	2.430291
1	-2.256612	-1.264354	1.331822
8	-2.770440	-0.032057	-0.016343
1	-3.619615	-0.244545	-0.474227
1	-2.827615	0.895806	0.269792
8	-2.117742	2.669639	0.858306
1	-2.514544	3.398546	0.356530
1	-2.299909	2.883980	1.786281
8	-5.103254	-0.690036	-1.232555
1	-5.363917	-0.577615	-2.155831
1	-5.879329	-1.047644	-0.781520

Cartesian coordinates of : 433-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.435131	-1.437766	-1.406831
1	-1.148229	-1.118506	-1.401621
1	-0.800749	2.034165	0.569186
1	-1.862878	1.114516	-0.250140
1	1.704798	1.363646	0.762113
1	2.157414	0.084183	-0.114965
26	-0.145942	-0.461872	0.900295
1	2.564047	-0.716535	-2.420137
1	2.813410	-1.860789	-1.393396
1	-3.457394	-0.309745	-1.378245
1	-2.698683	0.481167	-2.483986
1	0.790894	3.455319	1.740537
1	1.000898	3.657277	0.217280
1	-1.069923	-1.532522	3.242052
1	0.290441	-2.239903	2.952807
8	-1.292092	1.180774	0.549073
8	0.751207	2.980423	0.896748
8	1.690786	0.383048	0.697346
8	2.247506	-1.067536	-1.574733
8	-0.385952	-1.430933	-0.865440
8	-2.575989	0.079387	-1.611297
8	-0.331677	-1.576806	2.614355
8	3.674366	-3.251783	-0.896519
1	3.572943	-4.112001	-1.326429
1	4.592383	-3.221050	-0.594248
8	-4.887844	-1.043950	-0.803239
1	-5.657958	-0.539870	-0.507029
1	-5.241946	-1.865779	-1.169522
8	1.436930	4.771589	-1.005410
1	2.336401	5.103414	-1.129479
1	0.855567	5.475745	-1.322703

**Cartesian coordinates of all the proposed isomers of
[Fe²⁺(H₂O)_{n=1-10}] at MP2/6-31++G(d,p) level of theory at
singlet spin-state**

Cartesian coordinates of the monomer : [Fe(H₂O)₁]²⁺

Cartesian coordinates of : 100-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.340133	0.000000	0.000000
1	1.929388	0.789973	0.000001
1	1.929390	-0.789972	0.000001
26	-0.560763	0.000000	0.000000

Cartesian coordinates of the dimer : [Fe(H₂O)₂]²⁺

Cartesian coordinates of : 200-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.484878	0.639446	0.000000
1	1.971709	0.949262	-0.789771
1	1.971690	0.949285	0.789773
26	-0.006205	-0.558946	0.000000
8	-1.478394	0.674883	-0.000001
1	-1.396587	1.650840	-0.000006
1	-2.437342	0.468563	0.000002

Cartesian coordinates of : 200-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.505303	0.517375	0.000001
1	-1.978444	0.833087	0.804122
1	-1.978449	0.833132	-0.804099
26	0.000001	-0.446556	-0.000002
8	1.505300	0.517377	0.000001
1	1.978444	0.833092	0.804120
1	1.978439	0.833135	-0.804102

Cartesian coordinates of the trimer : $[\text{Fe}(\text{H}_2\text{O})_3]^{2+}$

Cartesian coordinates of : 300-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.648210	1.581411	0.391485
1	-0.501716	2.510688	0.134852
8	-1.045454	-1.352058	0.391491
1	-0.715988	-1.909479	1.119188
1	-1.923465	-1.689838	0.134821
8	1.693650	-0.229348	0.391493
1	2.011634	0.334696	1.119195
1	2.425186	-0.820845	0.134854
26	0.000005	-0.000001	-0.506072
1	-1.295668	1.574775	1.119196

Cartesian coordinates of : 210-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.118935	-1.393693	0.000012
1	1.093097	-1.158247	0.000008
26	-1.113138	0.000022	-0.000008
8	0.119012	1.393661	0.000014
1	1.093168	1.158153	0.000014
8	2.369005	-0.000020	-0.000009
1	2.965247	-0.000020	0.772256
1	-0.015443	-2.361742	0.000048
1	2.965217	-0.000015	-0.772297
1	-0.015317	2.361716	0.000037

Cartesian coordinates of : 300-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.391155	1.754439	0.000003
1	-0.514310	2.306849	0.800235
26	0.000001	-0.000002	-0.000002
8	-1.323814	-1.215970	0.000002
1	-1.740656	-1.598813	-0.800229
8	1.714970	-0.538466	-0.000001
1	2.254939	-0.708018	0.800238
1	-0.514350	2.306846	-0.800226
1	-1.740645	-1.598827	0.800232
1	2.254975	-0.708002	-0.800219

Cartesian coordinates of the tetramer : $[\text{Fe}(\text{H}_2\text{O})_4]^{2+}$

Cartesian coordinates of : 400-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.970210	-0.010293	-0.528306
26	-0.000062	-0.029368	-0.348661
1	-2.547697	0.646768	-0.105095
1	-2.504204	-0.465821	-1.201985
8	-0.000043	1.504537	0.888777
1	-0.000689	2.454002	0.680816
1	0.000200	1.414545	1.856224
8	0.000361	-1.439190	0.985739
1	-0.786535	-1.914501	1.300738
1	0.787589	-1.914074	1.300557
8	1.970087	-0.010005	-0.528456
1	2.547306	0.647710	-0.105890
1	2.504069	-0.465438	-1.202210

Cartesian coordinates of : 400-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.977801	0.002789	-0.482948
1	-2.654313	-0.049618	0.211984
26	0.000011	-0.000030	-0.290688
8	1.977822	-0.002650	-0.482935
1	2.454391	-0.056335	-1.329821
8	0.002127	1.595715	0.816858
1	0.779283	2.108947	1.091901
1	-2.454382	0.055786	-1.329870
1	2.654352	0.050154	0.211950
1	-0.784102	2.069799	1.133544
8	-0.002169	-1.595781	0.816811
1	0.784018	-2.069580	1.134027
1	-0.779362	-2.108947	1.091875

Cartesian coordinates of : 310-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.484148	1.085412	-0.265165
1	-0.470096	2.337147	-0.281714
1	-0.319626	-2.249508	0.631934
1	-1.375051	-1.183803	0.051503
1	1.754489	-0.898987	-1.661403

1	2.761554	0.230755	-1.237270
26	0.767157	0.145256	0.493522
1	-3.148723	-0.288480	-1.274711
1	-3.489168	-0.071946	0.212579
8	-2.738944	-0.140165	-0.404317
8	-0.571653	1.402157	-0.036349
8	-0.423978	-1.349937	0.277767
8	1.962661	-0.254211	-0.963016

Cartesian coordinates of : 310-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.502023	-1.285373	1.619039
1	2.797226	-0.608588	1.038137
1	-0.982099	-1.924293	-0.536442
1	-1.786911	-0.595531	0.003863
1	0.545459	2.008890	1.082726
1	-0.265423	2.391098	-0.208223
1	-3.435823	-0.126017	1.246374
1	-3.759376	0.113963	-0.252836
26	0.743224	-0.024747	-0.527711
8	-0.861467	-0.992494	-0.288026
8	0.317265	1.717150	0.183418
8	1.830112	-0.669866	0.940899
8	-3.028273	0.028867	0.379690

Cartesian coordinates of : 310-3.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.196749	-1.101124	0.220178
1	-2.560361	-1.263293	1.108298
26	-0.501757	-0.170665	-0.186100
8	1.262396	0.393762	-0.659424
1	2.153323	0.071408	-0.205789
8	-1.157807	1.544443	0.397004
1	-0.606912	2.339711	0.492102
1	-2.705068	-1.657585	-0.396436
1	1.485067	0.915944	-1.447070
1	-2.088529	1.799292	0.514390
8	3.297174	-0.433689	0.491006
1	3.878470	-1.114478	0.117850
1	3.849581	0.119140	1.065135

Cartesian coordinates of : 310-4.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.486013	-0.441923	0.000001
1	3.034065	-0.625628	0.783611
26	0.694848	0.355085	0.000002
8	-0.933412	1.398420	-0.000013
1	-1.045439	2.363616	0.000051
8	-0.319809	-1.275677	-0.000005
1	-1.317092	-1.264062	0.000005
1	3.034086	-0.625604	-0.783599
1	-1.818390	0.956926	-0.000002
1	0.007252	-2.191972	-0.000022
8	-2.866811	-0.501350	0.000003
1	-3.444203	-0.640609	-0.771333
1	-3.444177	-0.640641	0.771353

Cartesian coordinates of : 220-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.670369	-0.470059	-0.416343
1	-2.292873	0.406479	-0.225575
26	-0.000002	-0.863457	0.298710
8	1.670378	-0.470070	-0.416321
1	2.292873	0.406476	-0.225563
8	-3.018787	1.492641	0.088499
1	-3.169706	2.211682	-0.545599
1	-2.077391	-0.993127	-1.129008
1	2.077416	-0.993160	-1.128960
1	-3.814806	1.419274	0.639642
8	3.018781	1.492650	0.088487
1	3.169708	2.211678	-0.545625
1	3.814789	1.419303	0.639650

Cartesian coordinates of the pentamer : $[\text{Fe}(\text{H}_2\text{O})_5]^{2+}$

Cartesian coordinates of : 500-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.002370	-1.983984	-0.323159
1	-0.779215	-2.534377	-0.488218
26	0.000729	0.000002	-0.218995
8	-0.000617	1.983982	-0.323145
1	0.780840	2.534698	-0.487693
8	-2.008479	-0.001398	-0.297980
1	-2.589403	-0.001812	-1.075494
1	0.784749	-2.533456	-0.487488
1	-0.783129	2.533158	-0.487871

1	-2.578825	-0.002240	0.486751
8	-0.006858	-0.000029	1.756977
1	-0.001399	0.785906	2.325219
1	-0.000047	-0.785976	2.325188
8	2.010448	0.001435	-0.292621
1	2.580330	0.002202	0.492425
1	2.592231	0.001805	-1.069519

Cartesian coordinates of : 410-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.508668	1.163407	0.564298
1	0.234802	1.886106	1.195757
1	1.146956	-1.843745	-1.403925
1	1.940556	-0.803541	-0.498303
1	-0.652259	-2.073888	1.329925
1	-1.806142	-1.100296	1.751327
26	-0.557633	-0.090536	-0.341560
1	3.646489	0.098280	0.946278
1	3.685007	0.869843	-0.385573
8	3.083024	0.391983	0.210328
8	0.527815	1.268331	0.508223
8	1.048054	-1.164813	-0.717030
8	-1.171627	-1.303940	1.045238
8	-2.215518	1.003686	-0.265514
1	-3.119492	0.655366	-0.347654
1	-2.260117	1.940436	-0.521539

Cartesian coordinates of : 410-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.357365	0.729955	-0.207480
1	-1.483908	1.642173	-0.506685
26	0.350337	-0.097239	0.177528
8	1.914610	-1.097503	0.894035
1	2.696892	-0.643309	1.248421
8	0.759192	-0.586120	-1.661786
1	1.468762	-1.189315	-1.936909
1	-2.275037	0.320434	-0.003885
1	1.931335	-2.005376	1.240220
1	0.133415	-0.497155	-2.398832
8	1.417272	1.564438	0.212929
1	1.899067	1.884444	-0.567491
1	1.287679	2.324941	0.803456
8	-3.548883	-0.404953	0.347936
1	-4.166207	-0.755406	-0.311410
1	-4.079372	-0.199737	1.132323

Cartesian coordinates of : 320-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.861021	1.292428	0.127648
1	0.688760	2.319760	-0.262927
1	1.309239	-2.312045	-0.033790
1	2.131599	-0.984294	0.344380
1	-1.327830	-0.858212	1.482337
1	-2.462309	-0.102946	0.562342
26	-0.102204	-0.162592	-0.633459
1	3.535930	0.490131	1.635582
1	4.072332	0.440255	0.191895
8	3.252881	0.373689	0.712302
8	0.966602	1.389846	-0.287377
8	1.265263	-1.344653	0.034749
8	-1.483442	-0.459100	0.612133
8	-3.804161	0.410518	0.360054
1	-4.542318	-0.160339	0.096911
1	-4.186257	1.140258	0.870669

Cartesian coordinates of : 320-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.635988	-0.952368	-0.561269
1	2.170598	-0.116284	-0.623957
26	0.000012	-0.924785	0.425493
8	-1.635984	-0.952237	-0.561183
1	-2.021985	-1.648043	-1.117777
8	0.000136	0.967208	0.704803
1	-0.806639	1.484600	0.485888
1	2.021900	-1.648241	-1.117844
1	-2.170513	-0.116062	-0.623784
1	0.806925	1.484485	0.485578
8	-2.561011	1.528861	-0.247918
1	-3.296736	1.686750	0.368838
1	-2.731729	2.133154	-0.990437
8	2.560848	1.529004	-0.247914
1	3.296480	1.687000	0.368927
1	2.731566	2.133317	-0.990417

Cartesian coordinates of : 230.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.864464	0.887942	-0.255356

1	-2.008775	1.709514	-0.755407
26	-0.272694	0.479292	0.625633
8	1.356776	-0.170850	0.105932
1	1.586508	-1.172502	0.002588
8	1.792895	-2.640964	-0.057912
1	2.316823	-3.118666	0.603009
1	-2.700753	0.235321	-0.412691
1	2.116615	0.430770	-0.247250
1	1.873978	-3.139931	-0.884429
8	3.111047	1.449234	-0.687062
1	3.876142	1.696745	-0.145743
1	3.374278	1.584658	-1.609725
8	-3.746021	-0.657744	-0.532300
1	-4.568966	-0.545399	-0.030645
1	-3.977668	-1.083039	-1.372585

Cartesian coordinates of : 320-3.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.000022	2.250522	-0.000009
1	-0.401892	2.811433	0.689427
26	-0.000002	0.437985	-0.000002
8	-1.313285	-0.456210	-0.749165
1	-1.248647	-0.714004	-1.687601
8	1.313306	-0.456163	0.749173
1	1.248680	-0.713955	1.687611
1	0.401852	2.811435	-0.689441
1	-2.260982	-0.802066	-0.288219
1	2.261001	-0.802037	0.288219
8	3.372301	-1.183140	-0.299604
1	4.224207	-0.764965	-0.097685
1	3.540419	-2.111707	-0.524612
8	-3.372297	-1.183142	0.299608
1	-4.224201	-0.764980	0.097648
1	-3.540417	-2.111697	0.524662

Cartesian coordinates of : 500-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.947884	-0.589233	-0.037888
1	-2.411397	-1.001126	0.710906
26	0.000000	0.000001	0.023502
8	1.229529	1.621628	-0.038176
1	2.066811	1.566970	-0.529270
8	-1.162320	1.670460	-0.038129
1	-0.851655	2.449849	-0.529294
1	-2.593181	-0.052950	-0.529004
1	1.362400	2.227451	0.710501

1	-1.697345	1.984074	0.710595
8	-0.041540	-2.034628	-0.037783
1	0.207051	-2.602701	0.711008
1	-0.751039	-2.482646	-0.528796
8	1.922210	-0.668245	-0.037962
1	2.539382	-0.607332	0.710757
1	2.129002	-1.481483	-0.528965

Cartesian coordinates of the hexamer : $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$

Cartesian coordinates of : 600-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.026507	-2.454259	-0.517249
1	-1.938076	-1.390265	-1.207847
1	1.026771	-0.779153	-2.383971
1	1.938233	0.350962	-1.807728
1	1.938073	1.390262	1.207850
1	1.026506	2.454257	0.517249
1	1.938235	-1.740955	0.600118
1	1.026636	-1.674993	1.866852
26	0.000000	-0.000000	-0.000000
1	-1.026770	0.779149	2.383970
1	-1.938234	-0.350964	1.807727
1	-1.026646	1.674984	-1.866858
1	-1.938237	1.740954	-0.600117
8	-1.209171	0.250755	1.592618
8	1.209085	-1.253863	1.013581
8	1.208997	1.504747	0.579192
8	1.209170	-0.250755	-1.592620
8	-1.209082	1.253869	-1.013578
8	-1.208997	-1.504749	-0.579192

Cartesian coordinates of : 510-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.755956	1.473368	-0.459254
1	-1.572420	2.336399	-0.863025
26	-0.405936	0.026553	-0.174955
8	0.991003	-1.373639	-0.066379
1	0.869474	-2.300605	-0.319267
8	1.027745	1.378948	0.000407
1	1.975553	1.112269	-0.021341
1	-2.683271	1.266182	-0.657006
1	1.947343	-1.151969	-0.127856
1	0.966812	2.239799	0.439437
8	-0.913249	-0.191071	1.724524

1	-0.313144	-0.620048	2.354960
1	-1.405826	0.486013	2.215180
8	-1.832894	-1.327694	-0.612970
1	-2.280948	-1.840088	0.078175
1	-2.078581	-1.713218	-1.468209
8	3.381190	-0.018576	-0.169014
1	4.026713	-0.076218	0.554730
1	3.919933	0.040403	-0.975459

Cartesian coordinates of : 420-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.587301	1.160198	-0.666635
1	1.752356	1.868233	-1.308124
26	0.000002	-0.000010	-0.548416
8	-1.587323	-1.160182	-0.666641
1	-2.443529	-0.882092	-0.266094
8	1.003917	-1.241393	0.535251
1	0.625905	-1.977774	1.038321
1	2.443502	0.882103	-0.266078
1	-1.752357	-1.868284	-1.308062
1	1.930282	-1.071175	0.823249
8	-1.003907	1.241392	0.535234
1	-1.930264	1.071179	0.823255
1	-0.625867	1.977765	1.038294
8	3.504386	-0.177485	0.750973
1	3.880589	0.200327	1.563286
1	4.248397	-0.632634	0.322071
8	-3.504384	0.177501	0.750981
1	-4.248388	0.632675	0.322096
1	-3.880587	-0.200317	1.563292

Cartesian coordinates of : 420-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.363127	1.116890	-0.009692
1	1.336164	2.263292	-0.386124
1	1.336128	-2.263266	0.386191
1	2.363112	-1.116904	0.009698
1	-2.363132	1.116866	0.009688
1	-1.336180	2.263284	0.386095
26	0.000008	0.000014	0.000003
1	-1.336143	-2.263249	-0.386161
1	-2.363116	-1.116868	-0.009698
1	4.362580	-0.025877	-0.770061
1	4.362592	0.025818	0.770036
1	-4.362598	0.025804	-0.770041
1	-4.362589	-0.025881	0.770058

8	1.410740	1.372403	-0.012681
8	3.770178	-0.000025	-0.000008
8	1.410720	-1.372400	0.012696
8	-1.410724	-1.372367	-0.012705
8	-1.410746	1.372381	0.012685
8	-3.770187	-0.000029	0.000005

Cartesian coordinates of : 420-3.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.915136	0.865511	1.078989
1	0.600279	1.285224	1.892390
26	-0.110008	-0.239694	-0.136018
8	0.017184	-2.098641	0.416430
1	0.813852	-2.643369	0.320802
8	-1.839538	0.045092	0.713236
1	-2.073630	-0.099023	1.640813
1	1.866025	1.078255	0.935866
1	-0.627936	-2.592716	0.945197
1	-2.645737	0.444895	0.235269
8	1.500125	-0.422710	-1.271196
1	1.528513	-0.696941	-2.200919
1	2.319142	0.084526	-1.064210
8	-3.765887	1.037060	-0.621734
1	-4.522804	0.522428	-0.938335
1	-4.071663	1.953427	-0.554213
8	3.395930	1.103815	-0.022898
1	3.696227	1.961653	-0.367048
1	4.194347	0.692664	0.348246

Cartesian coordinates of : 420-4.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.382491	2.134409	0.667829
1	-1.148502	2.165328	1.142217
1	1.744059	-0.797625	-0.630376
1	1.743897	0.797956	-0.630367
1	0.382913	-2.134331	0.667869
1	-1.148039	-2.165477	1.142370
26	-0.693569	-0.000074	-0.310464
1	2.715471	2.616757	0.814075
1	2.157070	3.253311	-0.469994
8	2.025514	2.507578	0.139067
8	-0.478561	1.649084	0.671001
8	1.196936	0.000111	-0.791575
8	-0.478251	-1.649209	0.670964
8	-2.684809	-0.000229	-0.166012
1	-3.301776	-0.000481	-0.916208

1	-3.223399	-0.000218	0.640363
8	2.026029	-2.507165	0.139081
1	2.157710	-3.252876	-0.469980
1	2.716037	-2.616201	0.814059

Cartesian coordinates of : 330-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.074168	-1.309470	-0.645674
1	1.033966	-2.541823	-0.719036
1	0.706386	1.859731	0.219798
1	2.032321	0.943149	0.104509
1	-1.515185	1.161373	-0.306175
1	-2.393692	-0.248937	-0.298092
26	0.044145	-0.535962	0.688013
1	3.684163	0.087020	-1.630562
1	4.173521	-0.355974	-0.240837
8	3.365798	-0.168175	-0.748551
8	1.201745	-1.667807	-0.332723
8	1.141718	1.020691	0.506512
8	-1.515843	0.215867	-0.046364
8	-3.633358	-1.050005	-0.585493
1	-4.419827	-1.032431	-0.020230
1	-3.938502	-1.290574	-1.472430
8	-0.680083	2.871708	-0.302316
1	-1.003287	3.530304	0.335073
1	-0.621612	3.354402	-1.143192

Cartesian coordinates of : 240.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.745676	-0.000002	-0.080625
1	-2.278101	0.847360	0.150172
26	-0.000002	-0.000010	-0.644621
8	1.745679	0.000003	-0.080657
1	2.278109	-0.847353	0.150156
8	2.937440	-2.173170	0.407406
1	3.133930	-2.517542	1.291047
1	-2.278099	-0.847363	0.150186
1	2.278093	0.847368	0.150159
1	3.601317	-2.552117	-0.187906
8	2.937398	2.173200	0.407422
1	3.133879	2.517567	1.291067
1	3.601270	2.552165	-0.187884
8	-2.937412	-2.173196	0.407421
1	-3.133902	-2.517577	1.291060
1	-3.601284	-2.552145	-0.187894
8	-2.937424	2.173190	0.407393

1	-3.133914	2.517580	1.291027
1	-3.601298	2.552129	-0.187927

Cartesian coordinates of : 330-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.590384	-1.535106	-0.693972
1	1.338306	-2.105965	-0.190003
26	-0.132205	0.000003	-0.191614
8	0.590367	1.535118	-0.693976
1	0.306161	1.969611	-1.517975
8	-1.580577	-0.000016	0.823229
1	-1.511349	-0.000004	1.794483
1	0.306185	-1.969597	-1.517975
1	1.338288	2.105983	-0.190005
1	-2.599684	-0.000014	0.499507
8	-3.904765	-0.000010	0.036921
1	-4.476918	-0.781608	0.064161
1	-4.476953	0.781559	0.064232
8	2.311212	2.827835	0.489690
1	3.223223	2.909766	0.172793
1	2.111977	3.621560	1.008676
8	2.311236	-2.827828	0.489684
1	3.223253	-2.909743	0.172799
1	2.112003	-3.621564	1.008653

Cartesian coordinates of : 510-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.168543	1.889562	-0.154743
1	-0.557228	2.584603	-0.449362
26	-0.430190	0.001049	0.088148
8	-1.011171	-1.940032	-0.118036
1	-0.320928	-2.616498	-0.204117
8	-2.455370	-0.116064	-0.287403
1	-3.090432	-0.437771	0.374360
1	-1.798286	2.294518	0.464173
1	-1.723105	-2.153121	-0.742389
1	-2.912802	0.500772	-0.881259
8	1.094232	1.298171	0.347804
1	1.991771	1.059434	0.014034
1	1.208025	1.737903	1.206849
8	1.124119	-1.193504	0.504580
1	2.014279	-1.002167	0.120879
1	1.249178	-1.438439	1.437449
8	3.337684	-0.003916	-0.547886
1	4.197096	0.019238	-0.094032
1	3.559757	-0.049497	-1.492964

 Cartesian coordinates of the heptamer : [Fe(H₂O)₇]²⁺

Cartesian coordinates of : 610-1.log

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.129321	-2.454966	-1.030929
1	-1.331495	-2.505429	-0.034613
1	-2.252739	-0.067362	-1.942119
1	-2.124311	1.428722	-1.492247
1	0.426195	2.532847	-0.057593
1	-0.272552	2.324831	1.312530
1	0.930723	0.337831	-2.333234
1	1.989930	0.123487	-1.170292
26	-0.398534	0.001632	0.005283
1	1.949462	-0.331452	1.118158
1	0.974162	-1.286970	1.876790
1	-2.736789	0.062224	1.243971
1	-1.696141	-0.170343	2.378467
8	1.008361	-0.469217	1.359212
8	1.035712	0.131900	-1.394073
8	-0.204808	1.968753	0.413713
8	-1.862272	0.520926	-1.278899
8	-1.824522	-0.216322	1.419104
8	-0.753373	-1.907528	-0.532122
8	3.425123	-0.028402	0.005936
1	4.038772	-0.766524	-0.141011
1	4.002221	0.729786	0.191800

 Cartesian coordinates of : 520-1.log

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.429602	-1.397190	-0.033838
1	1.290975	-2.304020	-0.345286
26	-0.000428	-0.010937	0.017878
8	-1.415697	1.376237	-0.153003
1	-1.238452	2.253722	-0.524182
8	-1.420603	-1.400098	-0.110771
1	-2.344534	-1.146821	-0.332503
1	2.341109	-1.131905	-0.294019
1	-2.333858	1.124842	-0.397205
1	-1.452257	-2.232267	0.382400
8	0.054666	0.145453	1.990107
1	-0.688112	0.479786	2.514965
1	0.566022	-0.455139	2.553235
8	1.389872	1.396382	-0.203344
1	1.462335	2.118833	0.438651

1	2.305030	1.140545	-0.452159
8	-3.723203	-0.025966	-0.746079
1	-4.503060	0.016297	-0.168904
1	-4.085086	-0.077419	-1.645931
8	3.703522	-0.025857	-0.780349
1	4.489651	0.005847	-0.211003
1	4.056085	-0.059638	-1.684676

Cartesian coordinates of : 430-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.695662	-1.518497	-0.543364
1	-1.898959	-2.234989	-1.163355
26	-0.061912	-0.407370	-0.503798
8	1.539882	0.696583	-0.706235
1	2.399844	0.366300	-0.373360
8	-1.038496	1.021629	0.338657
1	-0.668803	1.924247	0.445667
1	-2.539377	-1.152971	-0.189775
1	1.476519	1.657752	-0.520996
1	-1.975579	0.962199	0.617629
8	0.872103	-1.651247	0.635418
1	1.829598	-1.554327	0.847872
1	0.472974	-2.358869	1.161930
8	-3.596970	0.029241	0.672570
1	-3.960106	-0.233862	1.533981
1	-4.352569	0.401939	0.189386
8	3.472185	-0.881014	0.598250
1	4.105080	-1.411375	0.086648
1	3.976525	-0.572888	1.368508
8	0.613001	3.205583	0.104289
1	0.420892	3.891064	-0.556263
1	0.995327	3.689177	0.854205

Cartesian coordinates of : 430-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-2.022335	1.515550	-1.908257
1	-2.398805	1.195191	-0.394209
1	-1.373822	0.255241	1.476971
1	-0.281247	-0.910613	1.501041
26	0.032530	0.292975	-0.678110
1	2.421303	-0.669032	-0.962588
1	2.557754	0.528432	0.100341
1	3.808134	1.461860	1.721060
1	4.050215	2.195853	0.381090
1	-3.123601	1.996176	1.759331
1	-3.869952	0.693216	1.429631

1	-0.926949	-1.788938	-1.935196
1	-0.119660	-2.210735	-0.636042
1	0.986035	-3.126335	1.342450
1	-0.505629	-3.467348	1.419898
8	-1.750153	1.026214	-1.117495
8	-3.031907	1.158903	1.275419
8	1.915041	-0.098941	-0.364943
8	3.449675	1.583830	0.830451
8	-0.486026	-0.015428	1.162555
8	-0.212454	-1.523786	-1.336124
8	0.109922	-2.791526	1.092053

Cartesian coordinates of : 430-3.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.333170	0.767953	-0.072194
1	1.153134	1.891372	-0.084176
1	1.320211	-2.608234	0.505583
1	2.366850	-1.470713	0.109049
1	-2.333142	0.767906	0.072203
1	-1.153071	1.891328	0.084035
26	0.000008	-0.401916	-0.000003
1	-1.320183	-2.608243	-0.505612
1	-2.366832	-1.470718	-0.109048
1	4.328122	-0.505660	-0.826119
1	4.396816	-0.370050	0.707726
1	-4.396789	-0.370138	-0.707705
1	-4.328075	-0.505772	0.826137
8	1.366959	0.932601	-0.072187
8	3.772022	-0.417830	-0.034475
8	1.409527	-1.715360	0.141000
8	-1.409507	-1.715378	-0.141009
8	-1.366934	0.932555	0.072204
8	-3.771986	-0.417907	0.034489
8	-0.000093	3.306770	-0.000010
1	0.056817	3.898514	0.767998
1	-0.057161	3.898661	-0.767893

Cartesian coordinates of : 340-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.223076	-0.385293	0.376063
1	2.192805	1.259913	0.208935
1	-0.808129	-2.221425	-0.065702
1	0.808273	-2.221395	-0.065766
1	-2.223017	-0.385403	0.376121
1	-2.192870	1.259798	0.208921
26	-0.000001	0.098399	-0.699364

1	2.714896	-2.570450	1.451532
1	3.201195	-2.624164	-0.006057
8	2.530171	-2.217148	0.566312
8	1.711024	0.379420	0.034973
8	0.000049	-1.798555	-0.433905
8	-1.711018	0.379336	0.035008
8	-2.829887	2.635206	0.379505
1	-3.513232	2.984836	-0.210628
1	-2.938692	3.091952	1.225799
8	-2.530034	-2.217260	0.566401
1	-3.201029	-2.624290	-0.005990
1	-2.714765	-2.570581	1.451612
8	2.829701	2.635370	0.379605
1	2.938399	3.092129	1.225905
1	3.513059	2.985055	-0.210478

Cartesian coordinates of : 331.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-2.485070	0.812902	0.156315
1	-2.485012	-0.812991	0.156330
1	1.108333	-1.195076	0.587646
1	-0.253388	-2.081040	0.419013
1	1.108273	1.195074	0.587761
1	-0.253487	2.080999	0.419157
26	-0.401370	0.000027	-0.982424
1	-2.360916	2.768271	1.659704
1	-2.496967	3.280118	0.222953
1	-2.496947	-3.280155	0.222994
1	-2.360771	-2.768320	1.659740
1	3.118269	0.000006	0.740580
1	2.444557	-0.000058	2.158376
1	5.024755	-0.770821	-0.327867
1	5.024737	0.770919	-0.327836
8	0.357984	-1.448111	-0.012939
8	2.234442	-0.000018	1.211347
8	0.357913	1.448103	-0.012807
8	-2.122143	2.550355	0.743843
8	-2.182304	-0.000037	-0.308448
8	-2.122075	-2.550401	0.743860
8	4.451088	0.000040	-0.213836

Cartesian coordinates of the octamer : [Fe(H₂O)₈]²⁺

Cartesian coordinates of : 620-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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1	0.423863	-1.575300	-1.764999
1	1.759452	-1.392409	-0.937713
1	2.400847	-0.204075	0.980584
1	1.816694	0.977485	1.853584
1	-1.219837	1.515300	2.002187
1	-1.214780	2.590918	0.881900
1	-1.759500	-1.392318	0.937805
1	-0.423915	-1.575155	1.765108
26	-0.000003	0.361254	-0.000004
1	-1.816689	0.977434	-1.853621
1	-2.400858	-0.204075	-0.980565
1	1.219912	1.515066	-2.002249
1	1.214902	2.590788	-0.882060
1	4.179370	-1.239521	-0.449551
1	3.610728	-2.300073	0.502098
1	-4.179390	-1.239482	0.449572
1	-3.610745	-2.300073	-0.502034
8	3.370517	-1.490115	0.024542
8	0.754627	1.799993	-1.200535
8	-0.916072	-0.966838	1.196225
8	0.916018	-0.966951	-1.196150
8	1.583544	0.273391	1.232070
8	-0.754552	1.800118	1.200435
8	-3.370533	-1.490101	-0.024501
8	-1.583547	0.273363	-1.232079

Cartesian coordinates of : 620-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.513181	-0.238406	-0.056079
1	2.520364	1.331583	-0.255380
1	0.903903	0.483748	2.461712
1	-0.616013	0.181202	2.604348
1	-2.484305	-0.491318	0.057835
1	-2.626686	1.079586	0.245610
1	-0.689812	-2.053738	-0.031891
1	0.909582	-1.975069	-0.034319
26	-0.026529	0.518010	-0.003458
1	0.536502	0.330032	-2.598016
1	-0.968682	0.662778	-2.429918
1	-0.078394	3.046224	0.898434
1	-0.119339	3.117347	-0.667214
1	3.254395	-2.466869	-0.819088
1	3.334448	-2.408069	0.711253
1	-3.011940	-2.758456	-0.696944
1	-2.980118	-2.799299	0.835573
8	-0.199903	2.522912	0.092970
8	1.982784	0.582254	0.037025
8	0.047930	0.567808	2.015605
8	0.083347	-1.471855	-0.155824
8	2.844919	-2.048213	-0.045332
8	-0.101798	0.752658	-2.004823

8	-2.593604	-2.340911	0.072786
8	-2.027093	0.371655	-0.029406

Cartesian coordinates of : 620-3.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.684457	2.615366	0.728820
1	-0.544367	2.726091	-0.237734
1	-1.485896	0.681524	2.137409
1	-2.318067	-0.212953	1.160707
1	-0.214109	-2.482107	0.607811
1	0.180289	-2.381946	-0.897770
1	1.291901	-0.314337	2.306503
1	2.350374	-0.216053	1.148350
26	-0.000803	0.120879	0.009358
1	2.315606	-0.165188	-1.165531
1	1.482931	0.831407	-2.024896
1	-2.336626	0.058134	-1.133781
1	-1.306576	0.180528	-2.306281
8	1.400991	0.068243	-1.433085
8	1.439601	0.031569	1.414572
8	-0.187574	-1.883976	-0.152997
8	-1.405264	0.009513	1.445065
8	-1.442079	0.384980	-1.369460
8	0.140484	2.127384	0.093912
8	3.760982	-0.509730	-0.027791
1	4.486858	0.134454	-0.002029
1	4.203912	-1.371790	-0.077692
8	-3.728040	-0.474369	-0.021644
1	-4.101829	-1.365966	-0.104870
1	-4.500769	0.111062	0.029095

Cartesian coordinates of : 620-4.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.819717	0.677399	0.793001
1	-1.707309	-0.886217	0.899246
1	0.563317	1.755096	2.030869
1	1.643410	2.261501	1.026491
1	-0.932557	1.902263	-1.033250
1	-0.368626	1.057249	-2.217943
1	-2.485121	3.146263	0.501601
1	-3.308847	2.298601	-0.469156
26	0.550799	0.029972	-0.013831
1	-3.068071	-2.608233	-0.414920
1	-2.223410	-3.380050	0.601631
1	1.696460	-0.956087	2.164379
1	1.351988	-2.198719	1.295521

8	-2.223947	-2.573266	0.062585
8	-2.454985	2.321438	-0.008400
8	-0.163700	1.367798	-1.323046
8	1.099281	1.497007	1.266515
8	1.475504	-1.239343	1.264343
8	-1.195385	-0.056102	0.962215
8	-0.001516	-1.478675	-1.212325
1	-0.743806	-2.067962	-0.964654
1	0.608382	-1.962484	-1.787392
8	2.312428	0.111976	-0.992871
1	2.563664	0.804257	-1.622239
1	3.128020	-0.228802	-0.595699

Cartesian coordinates of : 611-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.864862	-2.559994	0.323274
1	1.569307	-2.322218	-1.039612
1	2.833985	-0.608398	1.706018
1	2.466594	0.886637	1.990134
1	-0.294299	2.355415	0.660820
1	0.958153	2.685553	-0.205838
1	-0.472511	-0.387487	2.300442
1	-1.415618	-0.725901	1.056774
26	0.879099	0.038339	-0.004282
1	-0.689353	0.580220	-2.074641
1	-1.399499	-0.472877	-1.152414
1	3.184801	0.631097	-1.129132
1	2.218144	0.414492	-2.329055
8	-0.517943	-0.122788	-1.432140
8	-0.491186	-0.525455	1.343957
8	0.547500	1.998773	0.341416
8	2.366281	0.163469	1.353386
8	2.248096	0.606266	-1.379784
8	1.369396	-1.907956	-0.186696
8	-2.703791	-1.009408	-0.093640
1	-3.057977	-1.905268	-0.201525
1	-3.500624	-0.414566	-0.038154
8	-4.754130	0.690691	0.064095
1	-5.319879	0.918595	-0.686738
1	-5.316461	0.779145	0.846226

Cartesian coordinates of : 530-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.353325	0.838685	-1.028984
1	-1.147013	1.141025	-1.926100
26	-0.100952	-0.378862	-0.066320

8	1.199075	-1.712858	0.650834
1	0.992396	-2.645207	0.811592
8	1.372835	0.632143	-0.929687
1	2.271866	0.248534	-0.968654
1	-2.322636	0.695052	-0.971830
1	2.128112	-1.669396	0.329401
1	1.451287	1.570531	-0.661788
8	-0.127378	0.778714	1.526149
1	0.227730	0.469132	2.372253
1	0.200255	1.692372	1.383319
8	-1.642247	-1.505938	0.495567
1	-1.695092	-2.011909	1.318805
1	-2.549685	-1.186589	0.293015
8	3.583726	-1.086273	-0.585117
1	4.380112	-0.865320	-0.076328
1	3.910627	-1.601612	-1.340130
8	-3.869310	-0.158586	-0.425655
1	-4.470985	0.326979	0.161211
1	-4.446881	-0.575605	-1.085347
8	1.024380	3.079596	0.438822
1	1.751143	3.566244	0.859462
1	0.441485	3.772340	0.090017

Cartesian coordinates of : 440-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.956962	-0.000128	-0.582383
1	-2.456488	-0.798358	-0.313938
26	-0.000003	0.000004	-0.455919
8	1.956956	0.000129	-0.582363
1	2.456591	-0.798026	-0.313901
8	-0.000125	1.758095	0.323587
1	0.816792	2.271509	0.503083
1	-2.456616	0.798006	-0.313895
1	2.456486	0.798344	-0.313880
1	-0.817104	2.271406	0.503103
8	0.000126	-1.758071	0.323616
1	0.817110	-2.271386	0.503095
1	-0.816787	-2.271503	0.503093
8	-2.623016	2.557505	0.362726
1	-3.135914	2.713921	1.171561
1	-2.939022	3.228385	-0.263799
8	2.623001	-2.557515	0.362704
1	2.939021	-3.228409	-0.263798
1	3.135871	-2.713920	1.171560
8	2.622651	2.557852	0.362693
1	2.938583	3.228763	-0.263835
1	3.135518	2.714338	1.171535
8	-2.622621	-2.557870	0.362691
1	-2.938542	-3.228823	-0.263799
1	-3.135491	-2.714315	1.171538

Cartesian coordinates of : 440-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.652534	-0.707479	-0.179466
1	2.197449	0.501210	0.809315
1	0.180307	1.507421	1.494438
1	-1.161299	1.673475	0.640747
26	0.003464	-0.367771	-0.241527
1	-2.179955	-1.229953	-1.361630
1	-2.344604	-1.522944	0.203380
1	-3.750727	-2.003263	1.920308
1	-3.127343	-3.310615	1.380206
1	2.013436	1.564346	3.087700
1	2.301114	2.673012	2.064347
1	0.610346	0.959940	-2.388624
1	-0.808812	1.391470	-1.832834
1	-2.943514	2.324897	-1.095822
1	-1.904731	3.451385	-1.090633
8	1.900962	-0.110805	0.107886
8	1.872359	1.807816	2.158796
8	-1.838373	-0.993128	-0.486977
8	-3.034131	-2.347461	1.368912
8	-0.518328	1.029369	0.996627
8	-0.164666	0.649649	-1.896632
8	-1.997436	2.493750	-0.961478
8	3.739367	-1.740601	-0.749389
1	4.087377	-2.501578	-0.263736
1	4.410343	-1.517991	-1.409944

Cartesian coordinates of : 440-3.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.337114	-1.150757	-0.000030
1	1.170677	-2.291212	-0.000022
1	1.170839	2.291113	0.000003
1	2.337199	1.150572	-0.000018
1	-2.337197	-1.150592	-0.000001
1	-1.170822	-2.291117	0.000004
26	0.000001	-0.000003	0.000002
1	-1.170653	2.291206	0.000012
1	-2.337105	1.150759	0.000024
1	4.370074	-0.000162	0.769901
1	4.370100	-0.000174	-0.769892
1	-4.370120	0.000185	0.769830
1	-4.370036	0.000195	-0.769963
8	1.373445	-1.331972	-0.000048
8	3.778899	-0.000143	-0.000005
8	1.373544	1.331859	-0.000002

8	-1.373434	1.331967	0.000040
8	-1.373540	-1.331865	0.000022
8	-3.778891	0.000160	-0.000034
8	-0.000172	-3.718032	0.000022
1	-0.000208	-4.309534	-0.769704
1	-0.000185	-4.309481	0.769789
8	0.000143	3.718032	0.000006
1	0.000176	4.309517	0.769746
1	0.000166	4.309500	-0.769746

Cartesian coordinates of : 332.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.040735	0.725517	0.409064
1	1.288954	2.155277	0.172184
1	-2.040735	0.725546	0.409239
1	-1.288908	2.155287	0.172362
1	-0.818123	-1.317576	0.741117
1	0.818142	-1.317555	0.741074
26	-0.000062	0.315587	-0.938783
1	2.756109	-0.769993	2.102374
1	3.207276	-1.265340	0.685258
1	-0.000007	4.305765	-0.058461
1	0.000118	3.915355	1.422193
1	-3.207247	-1.265370	0.685303
1	-2.756096	-0.770110	2.102455
1	-5.148911	-1.674247	-0.536851
1	-4.394934	-3.000882	-0.318558
8	-1.472099	1.266939	-0.201604
8	-2.486363	-0.772981	1.171056
8	-0.000007	-1.207431	0.196218
8	2.486376	-0.772939	1.170975
8	1.472080	1.266909	-0.201766
8	0.000044	3.532792	0.529860
8	-4.285393	-2.039891	-0.298970
8	4.285506	-2.039879	-0.298910
1	5.149023	-1.674224	-0.536777
1	4.395062	-3.000869	-0.318478

Cartesian coordinates of : 350.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.000013	1.500326	-1.440475
1	-0.000039	2.511346	-1.197663
26	0.000002	0.109122	-0.325995
8	-1.518602	-0.579219	0.225318
1	-2.005263	-1.329397	-0.263144
8	1.518615	-0.579180	0.225337

1	2.013299	-0.277084	1.062854
1	-0.000003	1.370445	-2.403817
1	-2.013305	-0.277140	1.062833
1	2.005313	-1.329333	-0.263119
8	2.726191	-2.448862	-1.023535
1	3.473090	-2.317472	-1.624173
1	2.749765	-3.377213	-0.752964
8	-2.755382	0.188334	2.323232
1	-3.550396	0.739419	2.320215
1	-2.746405	-0.276862	3.171261
8	-0.000075	3.924793	-0.850463
1	-0.778680	4.496481	-0.911889
1	0.778499	4.496525	-0.911896
8	2.755329	0.188430	2.323263
1	2.746399	-0.276786	3.171281
1	3.550276	0.739612	2.320271
8	-2.726069	-2.448969	-1.023552
1	-3.472956	-2.317624	-1.624215
1	-2.749614	-3.377313	-0.752955

Cartesian coordinates of the nanomer : $[\text{Fe}(\text{H}_2\text{O})_9]^{2+}$

Cartesian coordinates of : 630-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.778941	-2.594664	0.324223
1	-0.727944	-2.486296	-0.145230
1	-2.243668	-0.733030	-0.654283
1	-2.183326	0.866166	-0.675382
1	-0.645703	2.480946	0.047603
1	0.862796	2.523777	0.474191
1	1.925491	0.007844	-1.654179
1	0.494960	-0.110433	-2.312937
26	0.127065	-0.009441	0.303334
1	2.177885	-0.021724	2.010463
1	2.798000	-0.051418	0.546455
1	-0.937648	-0.888243	2.585215
1	-0.957305	0.676048	2.632896
1	-3.114794	-3.111201	-0.218300
1	-2.651612	-2.992668	-1.675502
1	4.287195	0.733949	-1.318124
1	4.307730	-0.799015	-1.273031
8	-2.484321	-2.642022	-0.786804
8	-0.552648	-0.088759	2.199096
8	0.969396	0.153140	-1.513208
8	0.002992	-2.018342	0.307229
8	-1.659048	0.046073	-0.603600
8	0.057149	1.990750	0.523423
8	3.743921	-0.033635	-1.079979
8	1.977301	-0.134565	1.071301
8	-2.319766	2.768064	-0.718270

1	-2.381154	3.178948	-1.594725
1	-2.973340	3.240861	-0.179524

Cartesian coordinates of : 630-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.263499	0.316133	2.625531
1	0.948658	-0.671510	2.561269
1	1.200749	2.007605	-0.088031
1	2.332770	0.882154	-0.200702
1	0.221856	0.155750	-2.489206
1	-0.494202	-1.221147	-2.381765
1	-1.171517	2.013176	0.135388
1	-2.296648	0.893970	0.005208
26	-0.007904	-0.340149	0.073442
1	-2.328193	-1.483970	0.026399
1	-1.440600	-2.300337	1.021478
1	2.359476	-1.494730	-0.169156
1	1.295711	-2.655788	-0.255950
8	-1.408103	-1.772679	0.209538
8	-1.393656	1.081368	0.326883
8	-0.342825	-0.384848	-1.917210
8	1.378115	1.066265	-0.280991
8	1.436060	-1.746132	0.041905
8	0.169687	-0.357097	2.081363
8	-3.741272	-0.329092	-0.333481
1	-4.482092	-0.305945	0.292654
1	-4.160985	-0.372035	-1.206720
8	3.819206	-0.351301	-0.307950
1	4.334311	-0.328786	-1.129675
1	4.486247	-0.403033	0.394515
8	0.033421	3.497269	0.038768
1	0.049150	4.090561	0.805842
1	0.009241	4.091793	-0.727181

Cartesian coordinates of : 621-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.927500	-2.288123	-0.900172
1	-2.743636	-1.864317	0.364792
1	-2.988853	0.765680	-1.616028
1	-1.992132	1.966940	-1.506080
1	1.004424	1.892438	-0.145187
1	0.004864	2.344153	0.972362
1	0.056841	-0.354804	-2.402092
1	0.932911	-1.188460	-1.354586
26	-0.916557	0.070777	0.012310
1	1.208639	-0.603979	1.363543

1	0.229309	-1.807623	1.306073
1	-2.825290	1.162252	1.640717
1	-1.812123	0.313613	2.479901
8	0.248555	-0.838475	1.347507
8	0.316614	-0.416509	-1.472664
8	0.078389	1.802655	0.173874
8	-2.106891	1.024665	-1.313795
8	-2.119736	0.502485	1.580175
8	-1.971904	-1.646087	-0.177823
8	1.926766	-2.364659	-0.713246
1	2.265355	-3.151695	-1.163461
1	2.671144	-1.973682	-0.225411
8	2.919827	-0.357012	1.077642
1	3.563301	-0.462427	1.794373
1	3.148163	0.473801	0.621041
8	2.799218	2.056495	-0.493042
1	3.235167	2.873010	-0.201142
1	3.073190	1.954570	-1.417743

Cartesian coordinates of : 540-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.485751	-0.816789	-0.231230
1	2.488554	0.793375	-0.202048
1	-0.803751	-2.502524	-0.144088
1	0.802770	-2.502851	-0.144007
1	-0.804022	2.465321	-0.346137
1	0.805114	2.464948	-0.346242
26	0.000000	-0.004147	0.044202
1	-2.486087	-0.815747	-0.231212
1	-2.488203	0.794424	-0.201941
1	2.961023	-3.028609	-1.322248
1	3.181014	-3.170655	0.190887
1	-3.065931	3.001609	-1.218874
1	-3.158831	3.123887	0.310081
8	1.981433	-0.015613	0.012246
8	2.659951	-2.684104	-0.467008
8	-0.000398	-1.989200	0.070696
8	-1.981418	-0.014799	0.012282
8	0.000412	1.915389	-0.407278
8	-2.695342	2.646673	-0.395714
8	2.696366	2.645657	-0.395766
1	3.159963	3.122638	0.310116
1	3.067173	3.000520	-1.218859
8	-2.661061	-2.683013	-0.467065
1	-2.962326	-3.027389	-1.322288
1	-3.182258	-3.169378	0.190860
8	0.000064	0.235978	2.006819
1	0.778897	-0.040553	2.512137
1	-0.778916	-0.040152	2.512130

Cartesian coordinates of : 540-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.971717	1.600378	-0.322155
1	-2.491089	0.185526	-0.821401
1	-1.716287	-1.912580	-0.000769
1	-0.280263	-2.514455	0.396568
1	-0.539952	1.632396	1.619095
1	-0.162205	0.273411	2.314341
26	0.040813	0.010116	-0.251491
1	1.866073	1.751146	-0.898204
1	0.616813	2.044333	-1.818360
1	2.637388	-0.313685	-0.046024
1	1.950443	-1.739599	0.258283
1	-3.679288	-1.855682	-1.580188
1	-4.175201	-1.576323	-0.154629
1	-2.518000	3.164185	1.605608
1	-1.380721	3.795119	0.792901
1	4.270966	1.258094	-1.097094
1	3.989092	1.794937	0.315910
8	0.016435	0.828818	1.541884
8	-1.712689	0.777015	-0.781609
8	-0.807290	-1.697224	0.288292
8	-3.401837	-1.476217	-0.731471
8	0.889831	1.670512	-0.967730
8	-1.758969	2.938411	1.045165
8	1.813927	-0.836348	-0.086855
8	3.585009	1.297171	-0.411982
8	1.313060	-3.477679	0.656942
1	1.558111	-4.171583	0.024836
1	1.464869	-3.874310	1.528980

Cartesian coordinates of : 441-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.876096	1.485807	-0.388323
1	-1.749611	1.309476	0.034421
26	0.421822	0.019504	-0.398188
8	1.680691	-1.464587	-0.659036
1	1.435621	-2.353876	-0.329189
8	1.835191	1.182837	0.193470
1	2.772167	0.904955	0.272235
1	-0.579366	2.386304	-0.151964
1	2.635035	-1.316411	-0.502064
1	1.703392	2.135080	0.391843
8	-0.793955	-1.099910	0.573219
1	-0.642964	-2.048224	0.759185
1	-1.694156	-0.782633	0.839536
8	0.740155	3.681797	0.391369

1	0.622160	4.162229	1.225886
1	0.961378	4.366592	-0.259727
8	0.342027	-3.626143	0.510211
1	-0.025819	-4.316427	-0.064169
1	0.666101	-4.101279	1.291436
8	4.151379	-0.280013	-0.013563
1	4.785135	-0.089823	-0.723637
1	4.698418	-0.554039	0.739396
8	-3.000590	0.338799	0.872074
1	-3.803637	0.123230	0.324801
1	-3.341302	0.638959	1.727987
8	-5.095145	-0.262522	-0.665217
1	-5.565856	0.369995	-1.224507
1	-5.713324	-0.989726	-0.512206

Cartesian coordinates of : 441-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.684364	-2.323848	-0.302275
1	-1.786113	-1.118949	-0.494310
1	2.734634	-1.177157	0.285703
1	1.605414	-2.338251	0.087292
1	-0.684386	2.323844	-0.302173
1	-1.786130	1.118941	-0.494219
26	0.475098	-0.000001	-0.092756
1	2.734618	1.177160	0.285779
1	1.605399	2.338250	0.087361
1	0.376720	-4.383364	0.634222
1	0.633052	-4.365127	-0.883599
1	0.376722	4.383460	0.634066
1	0.633020	4.365029	-0.883759
8	-0.843179	-1.359504	-0.318422
8	0.497505	-3.783485	-0.118813
8	1.788332	-1.375607	0.129388
8	1.788304	1.375608	0.129528
8	-0.843209	1.359500	-0.318267
8	0.497483	3.783485	-0.118896
8	-3.098943	0.000001	-0.754117
1	-3.522154	0.000018	-1.626123
1	-3.844848	-0.000011	-0.095058
8	4.148626	0.000018	0.522915
1	4.603486	0.000009	1.380221
1	4.859700	0.000036	-0.137569
8	-5.063704	-0.000016	1.050256
1	-5.588486	0.771025	1.303785
1	-5.588536	-0.771040	1.303730

Cartesian coordinates of : 360.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.705197	-1.615514	0.000005
1	0.931588	-2.133927	-0.840438
26	0.000004	-0.000006	-0.000004
8	-1.751670	0.197034	0.000021
1	-2.313784	0.260384	0.840475
8	1.046479	1.418465	-0.000034
1	1.382217	1.873730	-0.840486
1	0.931430	-2.133981	0.840455
1	-2.313836	0.260155	-0.840415
1	1.382399	1.873624	0.840403
8	1.896671	2.570166	2.133237
1	2.784928	2.469237	2.501836
1	1.537124	3.388011	2.503245
8	-3.174286	0.356614	-2.133232
1	-3.704221	-0.363367	-2.501809
1	-3.529553	1.176326	-2.503244
8	1.278211	-2.927319	-2.133270
1	0.745942	-3.644851	-2.503257
1	2.166680	-3.026244	-2.501903
8	1.895972	2.570633	-2.133326
1	1.537391	3.389528	-2.501950
1	2.783501	2.468456	-2.503330
8	-3.174147	0.357491	2.133302
1	-3.702644	-0.362808	2.503318
1	-3.530874	1.177212	2.501890
8	1.277564	-2.927557	2.133308
1	2.165633	-3.025093	2.503270
1	0.746047	-3.646332	2.501961

Cartesian coordinates of the decamer : $[\text{Fe}(\text{H}_2\text{O})_{10}]^{2+}$

Cartesian coordinates of : 640-1.log

Atomic number (AN) and Cartesian coordinates			
AN	X	Y	Z
1	-0.284579	-1.926712	-1.896206
1	1.233496	-1.956960	-1.445141
1	2.568999	-0.677824	0.053958
1	2.331416	0.700604	0.812776
1	0.434729	1.945820	1.506273
1	-0.715785	1.126638	2.172894
1	-1.233558	-1.956990	1.445060
1	0.284543	-1.926925	1.896052
26	0.000004	-0.090168	0.000006
1	-2.331422	0.700654	-0.812743
1	-2.569000	-0.677810	-0.053993
1	-0.434740	1.945879	-1.506178
1	0.715892	1.126806	-2.172734
1	3.671740	-2.013032	-1.834343
1	3.429626	-2.943661	-0.639775
1	-3.671809	-2.012909	1.834289

1	-3.429733	-2.943614	0.639773
8	3.075540	-2.157419	-1.083216
8	0.350631	1.391134	-1.315689
8	-0.411220	-1.428264	1.446879
8	0.411216	-1.428143	-1.446980
8	1.923583	-0.150847	0.561774
8	-0.350612	1.391020	1.315829
8	-3.075610	-2.157368	1.083175
8	-1.923578	-0.150798	-0.561766
8	2.239117	2.475002	1.502890
1	2.687289	2.664871	2.341811
1	2.474758	3.214753	0.922414
8	-2.239070	2.475064	-1.502900
1	-2.474747	3.214836	-0.922465
1	-2.687203	2.664894	-2.341850

Cartesian coordinates of : 640-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.552877	0.002699	-2.472283
1	-0.993585	-0.096161	-2.434411
1	-0.645759	2.564427	-0.187665
1	-2.013039	1.738753	0.005590
1	-0.211410	0.887409	2.492645
1	0.316252	-0.572243	2.539494
1	1.699048	1.951925	-0.327337
1	2.529918	0.611610	-0.105177
26	0.001843	-0.008053	0.043068
1	1.995304	-1.723215	0.144462
1	0.637714	-2.534154	-0.107895
1	-2.554046	-0.624943	0.319016
1	-1.716623	-1.967204	0.094242
8	1.024904	-1.712151	0.247821
8	1.684036	0.980723	-0.426566
8	0.327530	0.241461	2.013323
8	-1.039759	1.706250	0.058103
8	-1.676090	-1.040888	0.401800
8	-0.191014	-0.331985	-1.948119
8	3.703392	-0.855661	0.221983
1	4.379003	-1.032285	-0.450701
1	4.173983	-0.926112	1.066720
8	-3.735342	0.908755	0.200121
1	-4.221194	1.109939	1.015048
1	-4.403268	0.973395	-0.499684
8	0.881134	3.693539	-0.393045
1	1.020028	4.200488	-1.207866
1	1.051439	4.328043	0.320169
8	-0.919560	-3.628257	-0.406459
1	-1.047003	-4.367267	0.208443
1	-1.071401	-4.009998	-1.284274

Cartesian coordinates of : 631-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.524959	-2.025917	1.562537
1	1.643877	-0.923976	1.295935
1	1.797198	1.108028	0.254654
1	0.817786	2.046269	-0.608253
1	-1.503605	2.084498	-1.015376
1	-2.774356	1.223598	-0.674862
1	-0.475999	0.746033	2.937935
1	-1.363127	1.810980	2.227167
26	-0.625659	0.081780	0.410226
1	-2.460146	-1.853740	0.095928
1	-2.716927	-1.146665	1.496308
1	-0.891283	-1.537566	-1.650798
1	0.564018	-0.957675	-1.708756
1	3.740933	-0.401854	0.240169
1	3.650854	0.319263	1.621795
1	5.275837	-0.629861	-1.560125
1	5.132068	-1.987195	-0.853005
8	3.107133	-0.003220	0.887791
8	-0.332431	-0.776446	-1.394396
8	-1.084248	0.883740	2.196656
8	0.676600	-1.087375	1.389976
8	0.866420	1.368175	0.089436
8	-1.881414	1.443503	-0.376964
8	4.685285	-1.140283	-0.989134
8	-2.091193	-1.246011	0.765440
8	-0.227947	3.184514	-1.780326
1	-0.270364	4.124867	-1.546347
1	-0.096390	3.174418	-2.740641
8	-2.353728	-2.745968	-1.571942
1	-3.052037	-2.643172	-2.237132
1	-2.191971	-3.701654	-1.535301

Cartesian coordinates of : 631-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-2.032642	-2.402395	-0.963883
1	-2.658498	-2.322216	0.464000
1	-3.758320	0.502062	-0.797928
1	-3.013932	1.857876	-0.546742
1	0.267369	2.080359	-0.005256
1	-0.421239	2.094226	1.401229
1	-1.071873	0.220718	-2.468213
1	0.191341	-0.592280	-1.929608
26	-1.299083	-0.054289	0.158499
1	1.216712	-0.576191	0.644473
1	0.421715	-1.914398	0.637531

1	-2.790310	0.272078	2.386503
1	-1.458397	-0.461101	2.775451
8	0.325084	-0.974502	0.852285
8	-0.537969	0.043172	-1.682367
8	-0.512363	1.755632	0.499765
8	-2.996667	0.908025	-0.359599
8	-2.029657	-0.212123	2.033798
8	-2.248861	-1.797305	-0.239882
8	1.456448	-1.635132	-1.923190
1	1.816983	-2.139014	-2.665853
1	2.203989	-1.206617	-1.464079
8	2.661884	-0.031768	0.013466
1	3.512690	-0.229600	0.476110
1	2.679800	0.910469	-0.226537
8	1.822374	2.657258	-0.750814
1	2.240599	3.446740	-0.372938
1	1.816284	2.819745	-1.706411
8	5.005545	-0.641515	1.221778
1	5.228683	-0.642408	2.161604
1	5.818672	-0.880479	0.757659

Cartesian coordinates of : 541-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.904468	1.355248	-1.010918
1	-0.756250	2.310957	-0.880801
26	0.291177	0.007667	-0.213299
8	1.620057	-1.364607	0.344484
1	2.568440	-1.134265	0.407281
8	-0.890627	-1.406647	-0.919035
1	-0.691735	-2.359425	-0.869693
1	-1.854843	1.157714	-1.126058
1	1.518718	-2.291184	0.048765
1	-1.839235	-1.238740	-1.084889
8	1.632335	1.417829	0.147666
1	2.581010	1.244346	0.290326
1	1.463828	2.363430	-0.027652
8	-3.272240	-0.054499	-1.001629
1	-4.008823	-0.058005	-1.630872
1	-3.659962	-0.059174	-0.107699
8	4.036622	0.039330	0.563274
1	4.496647	0.068478	1.416485
1	4.744997	0.015000	-0.098502
8	0.580311	-3.776819	-0.634884
1	0.413426	-4.516833	-0.031125
1	0.882884	-4.192978	-1.457033
8	0.377568	3.807391	-0.550112
1	0.159508	4.471560	0.121499
1	0.625363	4.319413	-1.335588
8	-0.513847	0.121338	1.586311
1	-0.038622	-0.294861	2.319051
1	-1.472225	-0.028695	1.729211

8	-3.326766	-0.106258	1.874856
1	-3.716770	-0.883028	2.305177
1	-3.698519	0.648512	2.357773

Cartesian coordinates of : 442-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.256911	1.499689	0.377572
1	2.176689	1.340386	0.062284
26	-0.000008	-0.000001	0.251159
8	-1.256924	-1.499696	0.377558
1	-0.963819	-2.383163	0.078799
8	-1.352816	1.104543	-0.540859
1	-2.268704	0.770543	-0.710523
1	0.963810	2.383160	0.078821
1	-2.176699	-1.340397	0.062262
1	-1.237793	2.054295	-0.745383
8	1.352845	-1.104574	-0.540744
1	1.237808	-2.054313	-0.745319
1	2.268722	-0.770563	-0.710447
8	-0.274710	3.645680	-0.642675
1	-0.058289	4.116084	-1.462696
1	-0.582702	4.335975	-0.034613
8	0.274686	-3.645686	-0.642684
1	0.582667	-4.335989	-0.034626
1	0.058290	-4.116078	-1.462719
8	-3.549387	-0.389361	-0.611622
1	-4.286545	-0.203474	0.029114
1	-3.980974	-0.686706	-1.426273
8	3.549372	0.389377	-0.611607
1	4.286552	0.203497	0.029108
1	3.980932	0.686708	-1.426278
8	5.468620	-0.132327	1.174517
1	5.854185	0.520298	1.774209
1	6.114633	-0.848656	1.113845
8	-5.468578	0.132354	1.174560
1	-5.854125	-0.520255	1.774281
1	-6.114589	0.848685	1.113900

Cartesian coordinates of : 433-1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.807163	-1.466449	1.104454
1	0.807210	-1.466462	1.104369
1	1.212282	1.619469	-0.437899
1	1.982423	0.373457	0.243618
1	-1.212233	1.619544	-0.437720
1	-1.982374	0.373567	0.243876

26	-0.000084	-0.450343	-1.062794
1	-2.623446	-0.541924	2.417079
1	-3.182919	-1.428381	1.258949
1	3.183008	-1.428439	1.258720
1	2.623605	-0.541880	2.416802
1	0.000009	3.598422	-1.125413
1	0.000103	3.544335	0.427219
1	0.783303	0.436404	-3.460087
1	-0.783760	0.436465	-3.459971
8	1.480389	0.677144	-0.549221
8	0.000046	2.973894	-0.384672
8	-1.480411	0.677234	-0.549014
8	-2.433235	-0.827374	1.511379
8	-0.000006	-1.541596	0.542518
8	2.433344	-0.827399	1.511134
8	-0.000191	0.333135	-2.899159
8	-4.367792	-2.473551	0.666913
1	-4.447277	-3.399238	0.934633
1	-5.261582	-2.193449	0.427189
8	4.367875	-2.473664	0.666809
1	5.261659	-2.193593	0.427024
1	4.447357	-3.399329	0.934605
8	0.000179	4.464558	1.857953
1	-0.769499	4.953678	2.179077
1	0.769897	4.953657	2.179010

Cartesian coordinates of : 442-2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.136716	2.325246	-0.284986
1	2.224820	1.126064	-0.568825
1	-2.224834	1.126063	0.568773
1	-1.136737	2.325249	0.284932
1	1.136738	-2.325250	-0.284924
1	2.224836	-1.126064	-0.568763
26	-0.000001	-0.000001	0.000001
1	-2.224825	-1.126069	0.568820
1	-1.136718	-2.325250	0.284992
1	0.185213	4.378008	0.746952
1	-0.185189	4.378074	-0.746827
1	0.185175	-4.378074	0.746838
1	-0.185227	-4.378008	-0.746942
8	1.297294	1.361698	-0.325476
8	0.000007	3.787487	0.000038
8	-1.297325	1.361700	0.325359
8	-1.297294	-1.361701	0.325488
8	1.297322	-1.361701	-0.325366
8	-0.000019	-3.787487	-0.000028
8	3.522630	-0.000007	-0.928236
1	3.879097	-0.000016	-1.829338
1	4.314942	0.000003	-0.327977
8	-3.522633	0.000006	0.928241

1	-3.879108	0.000014	1.829339
1	-4.314938	0.000007	0.327974
8	5.624480	0.000006	0.726584
1	6.165343	-0.770965	0.943423
1	6.165347	0.770968	0.943446
8	-5.624459	0.000001	-0.726608
1	-6.165359	-0.770958	-0.943400
1	-6.165293	0.770976	-0.943506
