

Structures of $\text{SO}_4^{2-}(\text{H}_2\text{O})_8$

8.7.9-1

atom	x	y	z
16	-0.238271	-1.097352	0.451994
8	-0.103631	-0.456341	-0.903850
8	1.078813	-1.654887	0.849176
8	-0.653413	-0.047353	1.433944
8	-1.269102	-2.153519	0.385093
8	0.781536	2.293095	1.676799
1	0.221455	1.486599	1.616809
1	0.740370	2.673144	0.780953
8	2.957637	-2.314999	-1.203518
1	2.272918	-2.268245	-0.508628
1	2.958123	-1.405614	-1.531671
8	2.911640	0.456432	1.342089
1	2.275002	1.162284	1.571561
1	2.346975	-0.342026	1.289127
8	-1.743524	1.600919	-1.451045
1	-2.283351	1.627340	-0.641461
1	-1.144412	0.831175	-1.280273
8	0.698999	3.083486	-1.127786
1	1.313712	2.350549	-1.325327
1	-0.185565	2.695263	-1.275199
8	-3.215977	0.904730	0.967114
1	-2.333610	0.589480	1.266317
1	-3.523322	0.160563	0.422343
8	2.307295	0.692747	-1.426760
1	1.443142	0.232282	-1.298365
1	2.682940	0.682502	-0.523291
8	-3.417344	-1.237623	-1.004166
1	-2.659906	-1.657708	-0.521630
1	-2.975576	-0.593458	-1.569910

8.7.9-2

atom	x	y	z
16	0.378888	-0.955866	-0.447319
8	1.795007	-1.143757	-0.873939
8	0.365702	-0.462182	0.967888
8	-0.236375	0.105052	-1.319048
8	-0.384385	-2.207349	-0.562299
8	-2.979088	-2.000246	0.445667
1	-2.791194	-1.354764	1.155008
1	-2.082459	-2.191951	0.093026
8	-0.000927	2.586665	-0.324755
1	-0.112669	1.669893	-0.688545
1	0.585056	2.448810	0.433650
8	3.846498	-1.206739	1.100632
1	3.554589	-0.372072	1.490100
1	3.151400	-1.360639	0.430826
8	2.763280	1.380199	-1.447521
1	1.922263	1.841538	-1.552354
1	2.484115	0.438478	-1.358890
8	-2.788519	2.253527	0.390444
1	-1.864620	2.509079	0.212567
1	-2.967256	1.563847	-0.284481
8	-2.067104	0.074008	2.181674
1	-1.177773	-0.117174	1.809111
1	-2.358363	0.860268	1.685695
8	2.267460	1.447736	1.425711
1	1.589853	0.733972	1.351989
1	2.625496	1.501757	0.522259
8	-3.007336	0.130497	-1.452374
1	-2.028840	0.093746	-1.533958
1	-3.185513	-0.630222	-0.865536

8.7.9-3

atom	x	y	z
16	-0.395001	-0.982718	-0.355194
8	0.220514	0.025508	-1.285190
8	-0.405142	-0.399651	1.025726
8	-1.804959	-1.213952	-0.784777
8	0.376729	-2.234423	-0.379192
8	-2.733364	1.239145	-1.593779
1	-1.877094	1.649298	-1.762011
1	-2.481239	0.302782	-1.407777
8	2.130317	-0.131412	2.114389
1	2.583163	-0.796294	1.561060
1	1.196550	-0.216943	1.817809
8	2.703267	2.224613	0.703787
1	1.813031	2.475792	0.392904
1	2.537923	1.442765	1.275381
8	2.977005	0.388390	-1.516476
1	2.015813	0.192734	-1.545017
1	3.030991	1.073244	-0.823954
8	-2.284758	1.566922	1.268641
1	-2.618840	1.546521	0.354298
1	-1.615976	0.840314	1.274851
8	0.062353	2.578487	-0.381352
1	0.151921	1.651033	-0.713897
1	-0.602252	2.491762	0.318379
8	3.094738	-1.954380	0.115560
1	3.238391	-1.203356	-0.491356
1	2.148786	-2.168587	-0.044199
8	-3.889364	-1.091722	1.149743
1	-3.597454	-0.227878	1.469149
1	-3.182370	-1.309873	0.510843

8.7.9-4

atom	x	y	z
16	-0.236498	-1.325933	-0.084018
8	-1.561278	-1.951875	-0.259371
8	-0.134619	-0.125047	-1.008800
8	-0.087729	-0.817473	1.318148
8	0.850524	-2.269221	-0.401120
8	2.281120	0.521981	1.911362
1	1.426661	0.062921	1.748851
1	2.239651	1.317910	1.353376
8	2.430655	0.574777	-1.815378
1	2.933807	-0.070085	-1.280293
1	1.504480	0.285323	-1.659629
8	-0.730097	2.320879	-0.075744
1	-1.448927	2.379058	-0.724642
1	-0.415248	1.398830	-0.265405
8	-2.566859	1.083310	-1.957470
1	-1.747946	0.558652	-1.874300
1	-3.122695	0.678763	-1.261269
8	-3.710377	-0.316699	0.239674
1	-3.014380	-0.988287	0.046809
1	-3.298047	0.186322	0.967324
8	-2.004022	0.983855	2.147446
1	-1.365818	0.250886	1.989058
1	-1.656766	1.655902	1.536805
8	3.409215	-1.336196	0.059736
1	2.543811	-1.777082	-0.100628
1	3.190992	-0.717240	0.783321
8	2.138955	2.724757	-0.048503
1	2.318458	2.034091	-0.724613
1	1.172032	2.814568	-0.070329

8.7.9-5

atom	x	y	z
16	0.024287	-1.152873	-0.313150
8	0.277247	0.125106	-1.063981
8	-1.356843	-1.614611	-0.614678
8	1.017224	-2.166987	-0.714803
8	0.143465	-0.872917	1.153726
8	-3.165049	0.334059	-1.623059
1	-2.490294	-0.365059	-1.504348
1	-2.698786	1.117818	-1.280847
8	-3.662457	-1.079527	0.834829
1	-2.816291	-1.475640	0.537410
1	-3.841110	-0.497283	0.076358
8	3.629619	-1.350541	-0.724660
1	3.494119	-0.404000	-0.879460
1	2.711716	-1.710444	-0.780588
8	2.763147	-0.375110	1.912363
1	3.206590	-0.881635	1.212268
1	1.813034	-0.574833	1.751331
8	-1.843650	0.778194	2.124943
1	-1.068290	0.225234	1.875076
1	-2.587548	0.221908	1.834441
8	1.000800	3.940475	-0.268041
1	0.139884	3.487554	-0.247244
1	1.631051	3.199172	-0.272288
8	-1.349040	2.173454	-0.306865
1	-1.568170	1.867032	0.596211
1	-0.734398	1.466478	-0.622457
8	2.549870	1.444882	-0.355067
1	1.730789	0.988363	-0.668390
1	2.654442	1.089486	0.545265

atom	x	y	z
8	-0.098600	0.086002	1.138398
16	-0.877340	-0.419740	-0.038285
8	-2.283754	0.055846	0.081325
8	-0.833514	-1.900345	-0.067214
8	-0.274342	0.132149	-1.288312
1	1.438776	-0.197871	-1.704634
8	2.386511	-0.416024	-1.843636
1	2.840518	0.078097	-1.136572
1	2.089899	-2.117898	-1.067456
8	1.773232	-2.858217	-0.512729
1	0.826628	-2.636789	-0.383486
1	-0.478755	1.890722	-1.611135
8	-0.570058	2.869080	-1.568671
1	-1.286739	2.978501	-0.921543
1	2.214651	-1.928870	1.102154
8	2.238713	-1.250544	1.804383
1	1.365850	-0.815590	1.688795
1	0.712262	2.768694	-0.056223
8	1.066822	2.510642	0.812872
1	0.652776	1.625364	0.959084
1	3.144323	0.163841	1.010365
8	3.468838	0.929863	0.491119
1	2.747696	1.582151	0.574114
1	-3.554200	-1.493999	0.153783
8	-3.654969	-2.460972	0.144321
1	-2.713395	-2.686523	0.067849
8	-2.246803	2.686140	0.818288
1	-2.348669	1.728044	0.593838
1	-1.390790	2.709001	1.262475

8.8.8-1

8.8.8-2

atom	x	y	z
16	0.882574	-0.411953	0.064622
8	2.291329	0.047088	-0.093987
8	0.831155	-1.890603	0.147378
8	0.306283	0.188330	1.305257
8	0.088130	0.059159	-1.114389
8	-1.126270	2.481364	-0.788318
1	-0.706529	2.776381	0.039209
1	-0.705523	1.602219	-0.940575
8	2.252612	2.636762	-0.933490
1	1.397220	2.633814	-1.378444
1	2.357895	1.688788	-0.667860
8	-2.371899	-0.996022	-1.880279
1	-1.452803	-0.697109	-1.712400
1	-2.894915	-0.351971	-1.366751
8	-3.482223	0.977102	-0.088122
1	-3.122948	0.440849	0.651685
1	-2.758860	1.597504	-0.301016
8	-2.274815	-0.660252	1.857189
1	-1.359933	-0.317868	1.747605
1	-2.229790	-1.512861	1.383880
8	3.647230	-2.476598	-0.077077
1	3.549070	-1.510228	-0.121501
1	2.705951	-2.695908	0.017892
8	-1.775653	-2.911970	0.144187
1	-2.097814	-2.390234	-0.616130
1	-0.827828	-2.660655	0.181887
8	0.633991	2.924782	1.481792
1	0.536959	1.948696	1.559389
1	1.329705	3.006681	0.808049

8.8.8-3

atom	x	y	z
16	-0.424001	-0.401445	-0.758722
8	0.832105	-0.775702	-1.466927
8	-1.560674	-1.169830	-1.294764
8	-0.256146	-0.711854	0.711106
8	-0.664906	1.064045	-0.904272
8	1.539878	2.694639	-0.414527
1	0.713067	2.212308	-0.633441
1	2.227778	2.122317	-0.803913
8	3.701522	-0.521202	1.251993
1	3.005271	0.083825	1.590337
1	3.189227	-1.314283	1.000862
8	1.518576	1.086278	1.947098
1	0.841816	0.469891	1.593827
1	1.554793	1.777279	1.257531
8	1.880472	-2.558967	0.400065
1	1.715523	-2.137604	-0.466694
1	1.122656	-2.170662	0.872395
8	-2.717563	-0.609628	2.041035
1	-3.299176	-0.815991	1.290780
1	-1.820665	-0.701729	1.651802
8	-4.119091	-0.520288	-0.553824
1	-3.245437	-0.813307	-0.901928
1	-3.945858	0.414424	-0.350013
8	3.230894	0.597912	-1.380521
1	3.542936	0.251989	-0.523931
1	2.372123	0.136171	-1.501319
8	-2.916328	1.911889	0.516087
1	-2.113633	1.717323	-0.016180
1	-2.826314	1.292842	1.259032

8.8.8-4

atom	x	y	z
16	0.420333	-0.487377	-0.709763
8	-0.833475	-0.948485	-1.375356
8	0.239180	-0.607620	0.783618
8	1.556196	-1.322764	-1.136406
8	0.665847	0.945388	-1.045277
8	-3.902994	-0.434860	0.847216
1	-3.328913	-1.225298	0.823672
1	-3.703238	0.011715	-0.003725
8	4.124120	-0.638870	-0.474572
1	3.967944	0.317841	-0.399950
1	3.245399	-0.958141	-0.784882
8	-1.940708	-2.496780	0.605848
1	-1.679299	-2.136037	-0.269615
1	-1.228350	-2.095264	1.128377
8	-1.351711	2.708111	-0.252600
1	-1.505532	2.304390	0.623237
1	-0.591735	2.184162	-0.586144
8	2.951330	1.930036	0.240870
1	2.846949	1.418535	1.060068
1	2.145785	1.681972	-0.263542
8	-1.680973	1.019384	2.023377
1	-2.494645	0.566607	1.735871
1	-0.963153	0.476632	1.631801
8	2.699767	-0.349349	2.096510
1	1.802015	-0.483585	1.721617
1	3.280024	-0.668400	1.385803
8	-2.992133	0.779669	-1.525651
1	-2.235566	0.155302	-1.586128
1	-2.558585	1.576722	-1.160886

8.8.8-5

atom	x	y	z
16	0.423829	-0.375981	-0.755999
8	-0.834636	-0.742148	-1.465273
8	1.561925	-1.119218	-1.323387
8	0.652877	1.094382	-0.867591
8	0.267381	-0.723293	0.706171
8	4.036865	-1.021316	-0.153632
1	3.716863	-0.908523	0.757449
1	3.190382	-1.129722	-0.645697
8	-3.234615	0.624717	-1.372160
1	-3.554691	0.252775	-0.529687
1	-2.373367	0.168363	-1.496475
8	-1.557390	1.027218	1.966099
1	-0.871102	0.425239	1.608006
1	-1.588073	1.735546	1.293803
8	-1.870406	-2.575158	0.348188
1	-1.118983	-2.201418	0.840888
1	-1.697956	-2.123938	-0.502755
8	-3.723984	-0.575680	1.224045
1	-3.202566	-1.358403	0.959733
1	-3.034566	0.027273	1.579864
8	-1.554784	2.702202	-0.343835
1	-0.724567	2.228459	-0.570179
1	-2.238289	2.138733	-0.753364
8	3.218262	1.811600	-0.033846
1	3.673794	0.984380	-0.261679
1	2.307212	1.655511	-0.367518
8	2.568537	-0.042779	2.161135
1	1.732730	-0.339660	1.739918
1	2.761654	0.776862	1.676362

8.8.8-6

atom	x	y	z
16	0.418961	-0.486374	-0.705747
8	0.246762	-0.612236	0.787451
8	0.657917	0.948126	-1.038920
8	1.554627	-1.313761	-1.147978
8	-0.838301	-0.948238	-1.365531
8	-2.976294	0.803978	-1.521413
1	-2.541161	1.594724	-1.145620
1	-2.223877	0.174512	-1.581931
8	-1.951118	-2.501538	0.597172
1	-1.245954	-2.111917	1.136975
1	-1.675358	-2.128655	-0.269818
8	4.015751	-1.083657	0.029160
1	3.172118	-1.254094	-0.450126
1	3.689372	-0.816936	0.905214
8	3.243001	1.742231	-0.332139
1	3.684200	0.880869	-0.416006
1	2.330193	1.549480	-0.640172
8	-3.920832	-0.443261	0.819995
1	-3.345735	-1.232908	0.797650
1	-3.708368	0.013716	-0.022360
8	2.541641	0.288845	2.132952
1	2.751415	1.011565	1.518360
1	1.705506	-0.065633	1.759880
8	-1.705116	0.989446	2.029864
1	-2.516818	0.542972	1.727467
1	-0.983828	0.452698	1.637581
8	-1.332805	2.715721	-0.211919
1	-0.576216	2.188525	-0.549161
1	-1.500739	2.297824	0.654481

8.8.8-7

atom	x	y	z
16	0.000000	0.642650	0.000008
8	0.001402	-0.224599	-1.218583
8	1.217880	1.493991	0.000037
8	-1.217879	1.493993	0.000002
8	-0.001403	-0.224632	1.218576
8	-2.284646	-1.833909	1.291850
1	-2.410409	-1.903363	0.326082
1	-1.432645	-1.348998	1.354008
8	2.400536	-1.575758	1.570428
1	1.498675	-1.188394	1.507944
1	2.961173	-0.780077	1.584730
8	2.284646	-1.833873	-1.291899
1	2.410407	-1.903354	-0.326132
1	1.432644	-1.348961	-1.354044
8	-2.400538	-1.575714	-1.570470
1	-2.961174	-0.780033	-1.584750
1	-1.498677	-1.188353	-1.507975
8	-3.451398	0.732554	1.584921
1	-3.204689	-0.213775	1.607117
1	-2.625679	1.131543	1.245846
8	3.634556	1.031101	1.273787
1	2.702073	1.281399	1.103280
1	3.931004	0.892801	0.357194
8	3.451401	0.732595	-1.584902
1	2.625685	1.131581	-1.245814
1	3.204688	-0.213732	-1.607122
8	-3.634556	1.031136	-1.273758
1	-2.702073	1.281431	-1.103246
1	-3.931002	0.892812	-0.357168

atom	x	y	z
16	-0.426223	-1.018329	-0.432270
8	-0.054935	0.021995	-1.435996
8	-0.284313	-0.418089	0.949693
8	-1.849173	-1.412066	-0.629843
8	0.456126	-2.190382	-0.550905
8	2.363205	-0.511142	1.917258
1	2.783202	-0.974148	1.166352
1	1.413341	-0.547011	1.677818
8	-1.638451	2.298225	-1.426953
1	-1.044621	1.524275	-1.549018
1	-2.447622	1.879669	-1.084084
8	-2.799195	-0.961533	2.066273
1	-2.836878	-1.473624	1.243887
1	-1.880795	-0.639029	1.977520
8	2.576165	2.173496	1.025712
1	2.597713	1.276914	1.419849
1	1.620479	2.386698	1.020571
8	-3.707395	0.553359	-0.398784
1	-3.061307	-0.148756	-0.656302
1	-3.636045	0.504957	0.564475
8	2.582724	0.920324	-1.568349
1	2.643223	1.439213	-0.743853
1	1.647633	0.622426	-1.582225
8	3.176223	-1.676244	-0.562737
1	2.237776	-1.965197	-0.606842
1	3.139665	-0.796371	-0.987386
8	-0.244167	2.359636	1.080393
1	-0.695597	2.564379	0.241211
1	-0.275118	1.378227	1.088256

8.8.8-8

8.9.7-1

atom	x	y	z
8	0.307826	-0.345701	1.221621
16	0.200380	0.508947	0.002231
8	1.286180	1.520710	-0.001458
8	-1.125309	1.199224	0.000243
8	0.306633	-0.351779	-1.211907
1	-0.914856	-1.702970	-1.336117
8	-1.681887	-2.312841	-1.276040
1	-1.800724	-2.399778	-0.310723
1	-3.712056	0.140643	0.338250
8	-3.461868	0.320302	1.262269
1	-2.583043	0.724522	1.116159
1	1.966377	-0.998632	-1.578132
8	2.898098	-1.307186	-1.618722
1	3.381758	-0.579387	-1.194393
1	-2.532510	-1.361766	1.586660
8	-1.855554	-2.061642	1.578771
1	-1.025433	-1.539863	1.516589
1	2.734267	-1.982569	0.303545
8	2.663287	-1.849617	1.263450
1	1.812277	-1.366036	1.345205
1	-2.467108	0.575659	-1.264899
8	-3.220673	0.041331	-1.580448
1	-2.826045	-0.854093	-1.595068
1	0.577878	3.368448	-0.007266
8	-0.194720	3.959847	-0.010431
1	-0.882184	3.276444	-0.010466
8	3.879029	0.642353	0.362145
1	2.996024	1.059050	0.246437
1	3.660966	-0.142815	0.892590

8.9.7-2

atom	x	y	z
16	0.081642	-0.379238	-0.695826
8	0.401260	-1.816406	-0.891329
8	-1.184021	-0.038292	-1.407435
8	-0.104332	-0.120995	0.773825
8	1.182660	0.472093	-1.214939
8	0.708922	3.153504	-0.470685
1	-0.264470	3.097336	-0.450829
1	0.955390	2.276420	-0.829736
8	-3.328203	-1.387296	-0.235829
1	-2.778955	-2.037068	0.238227
1	-2.655381	-0.921023	-0.778424
8	3.102759	-2.455758	0.025905
1	3.384306	-1.546102	0.218757
1	2.189546	-2.330509	-0.289377
8	3.558286	0.443256	0.228445
1	3.114292	0.890592	0.970401
1	2.825358	0.410198	-0.420633
8	-2.613599	0.754710	1.594752
1	-3.084005	0.082842	1.069615
1	-1.678824	0.524422	1.403954
8	-2.102044	2.488732	-0.655547
1	-1.780436	1.669715	-1.089634
1	-2.397274	2.131143	0.200816
8	-1.214508	-2.866028	1.095814
1	-0.992842	-2.050527	1.566843
1	-0.635366	-2.746443	0.311266
8	1.604534	1.766945	1.921149
1	1.027388	1.024457	1.645602
1	1.371306	2.436642	1.253367

8.9.7-3

atom	x	y	z
16	0.201442	0.502728	-0.005758
8	0.310356	-0.355514	-1.221325
8	-1.123287	1.194888	-0.008807
8	0.304151	-0.354831	1.212090
8	1.288183	1.513496	-0.000156
8	2.684714	-1.834339	-1.265586
1	2.747029	-1.977189	-0.306547
1	1.830490	-1.357041	-1.350169
8	-0.189225	3.954473	0.011178
1	0.582321	3.361674	0.008806
1	-0.877877	3.272339	0.003154
8	-3.246759	0.074248	-1.567580
1	-2.486299	0.600174	-1.253970
1	-2.857766	-0.823527	-1.593221
8	-1.718301	-2.285567	-1.298346
1	-1.823017	-2.386718	-0.332695
1	-0.945076	-1.684318	-1.359974
8	2.890531	-1.319302	1.624413
1	3.377763	-0.588308	1.209617
1	1.959367	-1.009461	1.579757
8	-3.444060	0.310641	1.284254
1	-2.565640	0.712802	1.130798
1	-3.709096	0.145986	0.361636
8	-1.844664	-2.081815	1.561202
1	-1.014389	-1.559716	1.498105
1	-2.520001	-1.380712	1.585037
8	3.888215	0.646668	-0.330697
1	3.677526	-0.134315	-0.870382
1	3.002761	1.060325	-0.222957

8.9.7-4

atom	x	y	z
16	0.000548	0.245843	-0.526765
8	-0.044667	-1.135804	-1.078977
8	0.012482	0.170386	0.974953
8	1.230465	0.939361	-0.990078
8	-1.194891	1.011952	-0.964114
8	3.666768	-0.051953	-0.135052
1	2.858231	0.387432	-0.480106
1	3.360195	-0.385531	0.725026
8	-3.674385	-0.188415	-0.703416
1	-2.843024	0.311782	-0.858266
1	-3.372090	-1.110214	-0.768048
8	0.095987	3.535586	-1.018726
1	-0.659300	2.921689	-1.058067
1	0.808346	2.873708	-1.078675
8	-2.220549	-2.682863	-0.267578
1	-1.425314	-2.229410	-0.621281
1	-2.281982	-2.309443	0.628312
8	-2.465811	-0.784529	1.926073
1	-1.578605	-0.431656	1.702912
1	-3.029892	-0.396327	1.237445
8	0.138692	2.975805	1.909343
1	0.101902	2.018298	1.739969
1	0.132621	3.341223	1.010864
8	2.351847	-2.556788	-0.864835
1	2.955398	-1.795064	-0.835289
1	1.481496	-2.131980	-1.021233
8	2.106586	-1.483090	1.876497
1	2.115544	-2.097085	1.124057
1	1.347521	-0.898106	1.667901

8.9.7-5

atom	x	y	z
16	0.101089	0.571234	0.000000
8	1.552038	0.237865	0.000000
8	-0.689717	-0.707391	0.000000
8	-0.241847	1.358295	1.212709
8	-0.241847	1.358295	-1.212709
8	0.064082	0.166157	3.686753
1	-0.085237	0.678935	2.861678
1	-0.163142	-0.735117	3.401641
8	0.064082	0.166157	-3.686753
1	-0.163142	-0.735117	-3.401641
1	-0.085237	0.678935	-2.861678
8	-2.354183	2.815191	0.000000
1	-1.796408	2.501614	-0.734407
1	-1.796408	2.501614	0.734407
8	2.536050	-0.742931	-2.417176
1	1.897740	-0.304755	-3.005287
1	2.295842	-0.381328	-1.536923
8	0.064082	-2.333343	-2.187744
1	-0.275606	-1.849904	-1.405670
1	1.002386	-2.082307	-2.201066
8	-3.527746	0.070743	0.000000
1	-2.634860	-0.317316	0.000000
1	-3.334739	1.021189	0.000000
8	2.536050	-0.742931	2.417176
1	1.897740	-0.304755	3.005287
1	2.295842	-0.381328	1.536923
8	0.064082	-2.333343	2.187744
1	1.002386	-2.082307	2.201066
1	-0.275606	-1.849904	1.405670

8.9.7-6

atom	x	y	z
16	0.111556	-0.232792	-0.604659
8	-0.969186	-1.218867	-0.846943
8	0.354214	-0.100851	0.869845
8	1.363362	-0.656703	-1.275938
8	-0.306875	1.107835	-1.130800
8	1.263625	2.827993	0.292046
1	0.661115	2.340808	-0.319967
1	1.212582	2.260552	1.070493
8	3.092994	-2.632851	-0.104374
1	2.427227	-2.142137	-0.619499
1	3.226682	-2.025760	0.641276
8	3.024081	-0.306198	1.708790
1	2.062585	-0.316717	1.518047
1	3.366275	0.221019	0.964884
8	3.412919	1.197495	-0.747209
1	2.816009	1.907198	-0.450517
1	2.779688	0.520484	-1.067592
8	-1.971337	0.726375	2.175575
1	-2.363346	1.216917	1.428052
1	-1.096531	0.460032	1.817256
8	-3.684238	-0.771322	-1.227244
1	-2.721456	-0.853688	-1.388862
1	-3.729667	-1.164962	-0.337739
8	-2.860702	1.847075	-0.325515
1	-3.320970	1.052526	-0.649899
1	-1.941604	1.690805	-0.637369
8	-2.782017	-1.843774	1.275179
1	-2.626053	-1.003142	1.749284
1	-2.032151	-1.848909	0.649402

8.9.7-7

atom	x	y	z
16	-0.113407	-0.200652	-0.602102
8	-0.363838	-0.070449	0.873538
8	0.961532	-1.194136	-0.839685
8	-1.364816	-0.619131	-1.277953
8	0.314600	1.137163	-1.122153
8	1.999262	0.338065	2.286256
1	2.448365	-0.473033	1.988029
1	1.110971	0.241423	1.876430
8	3.621642	-0.360871	-1.372370
1	3.509096	0.505512	-0.932724
1	2.692139	-0.655855	-1.441859
8	-3.030799	-0.361127	1.703251
1	-3.381268	0.176222	0.970499
1	-2.069012	-0.348888	1.514746
8	-3.439859	1.189477	-0.721123
1	-2.850707	1.900348	-0.411957
1	-2.797167	0.526662	-1.052813
8	-1.295713	2.807159	0.344013
1	-1.229637	2.186932	1.080989
1	-0.685651	2.371129	-0.295656
8	2.980172	-2.003871	0.904735
1	2.104048	-1.931060	0.474398
1	3.520091	-1.523863	0.252442
8	2.738019	1.939520	0.020634
1	1.885974	1.767343	-0.435835
1	2.593858	1.508170	0.885021
8	-3.050455	-2.656159	-0.147843
1	-2.395990	-2.142421	-0.655003
1	-3.198596	-2.063304	0.606513

8.9.7-8

atom	x	y	z
16	0.123217	0.322975	-0.591750
8	0.255508	0.590994	0.882954
8	-1.146628	0.912871	-1.081287
8	1.279031	0.936967	-1.294498
8	0.111419	-1.150876	-0.819335
8	-3.425590	-0.743142	-1.464793
1	-2.607181	-0.221847	-1.582113
1	-3.123385	-1.423767	-0.830456
8	-2.092990	-2.336546	0.458413
1	-1.274944	-2.047729	0.000716
1	-2.150219	-1.699630	1.196549
8	1.595632	3.249034	0.366195
1	1.110373	2.678879	0.977660
1	1.628705	2.650916	-0.401857
8	2.742105	-0.296445	1.835958
1	3.266889	-0.061348	1.053536
1	1.848080	0.032572	1.599334
8	3.755572	-0.276902	-0.955429
1	3.433862	-1.181445	-0.801004
1	2.923799	0.205997	-1.154597
8	-3.458425	1.483445	0.358188
1	-2.558918	1.561150	-0.020709
1	-3.790243	0.735715	-0.169419
8	2.316053	-2.581920	0.086300
1	1.504215	-2.174815	-0.287933
1	2.455613	-2.043929	0.884229
8	-2.034935	-0.127856	2.292178
1	-2.645922	0.439872	1.789366
1	-1.166218	0.104816	1.895947

atom	x	y	z
16	0.169726	0.246427	-0.266438
8	-0.121228	-0.609911	0.927126
8	0.527123	-0.627709	-1.416288
8	-1.043525	1.049502	-0.595912
8	1.309096	1.163811	0.040490
8	-3.087164	-0.750578	-1.474034
1	-2.441690	-0.047379	-1.260164
1	-2.558933	-1.556899	-1.337712
8	3.285659	-0.136014	-1.558398
1	2.442837	-0.595620	-1.730107
1	2.927409	0.581858	-1.009060
8	2.321759	-0.203593	2.307655
1	1.495343	-0.670807	2.093377
1	2.229417	0.520944	1.663573
8	-2.312304	0.766318	2.008563
1	-2.183607	1.273706	1.192724
1	-1.572845	0.137168	1.897314
8	-1.098951	-2.775113	-0.837639
1	-1.037928	-2.440361	0.068856
1	-0.458844	-2.164364	-1.262536
8	0.152739	3.672899	-0.792291
1	0.836648	3.073355	-0.452228
1	-0.556235	3.018856	-0.897663
8	-4.675236	-0.510149	0.915850
1	-4.249780	-0.650999	0.049297
1	-3.950352	-0.114041	1.431198
8	4.535021	-1.318938	0.786816
1	3.825533	-1.048683	1.396779
1	4.193503	-1.023750	-0.076145

8.11.5-1

8.12.4-1

atom	x	y	z
16	-0.000001	0.293586	-0.000009
8	0.000012	-0.560943	-1.219198
8	-0.000016	-0.560973	1.219160
8	1.217000	1.166477	0.000016
8	-1.216998	1.166481	-0.000012
8	2.735354	-0.044617	2.012764
1	2.416153	0.610350	1.362626
1	1.931407	-0.584600	2.060776
1	-1.931411	-0.584553	2.060762
8	-2.735364	-0.044577	2.012756
1	-2.416175	0.610387	1.362612
1	-1.931454	-0.584590	-2.060779
8	-2.735395	-0.044603	-2.012728
1	-2.416168	0.610351	-1.362590
1	2.416182	0.610379	-1.362573
8	2.735405	-0.044567	-2.012721
1	1.931463	-0.584552	-2.060774
1	0.000016	-2.549230	-0.730824
8	0.000000	-3.186588	-0.000069
1	-0.000017	-2.549274	0.730724
1	-0.731309	3.147050	-0.000029
8	0.000003	3.784901	-0.000024
1	0.731315	3.147051	-0.000008
1	4.057781	-0.785952	0.759902
8	4.629112	-0.993769	0.000035
1	4.057801	-0.785933	-0.759843
1	-4.057796	-0.785948	-0.759843
8	-4.629111	-0.993770	0.000035
1	-4.057784	-0.785938	0.759902

8.12.4-2

atom	x	y	z
16	-0.654658	0.000005	-0.126717
8	-1.458730	-1.222115	-0.396169
8	-0.182767	0.000019	1.285455
8	0.542833	-0.000008	-1.045340
8	-1.458723	1.222123	-0.396196
8	2.584477	-0.000028	0.809333
1	2.105739	-0.000025	-0.044634
1	1.799731	-0.000013	1.386289
8	-1.730307	2.317356	2.228125
1	-1.104038	1.593018	2.371321
1	-1.888740	2.173812	1.279799
8	-3.684251	0.000002	-1.783068
1	-3.142259	-0.731947	-1.447462
1	-3.142248	0.731948	-1.447474
8	0.784247	-2.737441	-1.528670
1	0.869408	-1.765304	-1.591593
1	-0.051910	-2.773458	-1.042094
8	-1.730372	-2.317249	2.228189
1	-1.888784	-2.173738	1.279854
1	-1.104093	-1.592918	2.371370
8	0.784315	2.737411	-1.528684
1	-0.051842	2.773477	-1.042114
1	0.869436	1.765268	-1.591586
8	3.169148	-2.834103	0.146402
1	3.085632	-1.931614	0.494953
1	2.359988	-2.938043	-0.385071
8	3.169222	2.834026	0.146382
1	2.360064	2.937981	-0.385091
1	3.085684	1.931541	0.494939
