

Structures of $\text{SO}_4^{2-}(\text{H}_2\text{O})_7$

atom	x	y	z
8	-0.444186	-0.413285	1.286762
16	-0.477760	-1.234765	0.029778
8	-1.835708	-1.805631	-0.143248
8	0.542771	-2.298413	0.098720
8	-0.185595	-0.322963	-1.132559
1	0.921731	2.668403	-0.230020
8	1.872730	2.685913	-0.006991
1	1.958736	2.017356	0.707314
1	1.453099	0.127413	-1.698484
8	2.341737	0.512597	-1.871489
1	2.317621	1.327131	-1.336268
1	-2.881189	0.715308	-1.379513
8	-3.521324	0.133150	-0.954220
1	-2.955719	-0.641388	-0.688826
1	-3.081645	0.988808	0.813161
8	-2.512766	1.372970	1.501061
1	-1.781493	0.712166	1.552980
1	-0.615601	1.332867	-0.917764
8	-0.880970	2.270133	-0.744156
1	-1.396053	2.193070	0.078084
1	3.061806	-0.761819	-0.640330
8	3.157489	-1.392244	0.098813
1	2.264745	-1.807262	0.130747
1	2.576254	-0.064280	1.377797
8	2.049563	0.594187	1.869093
1	1.131932	0.257169	1.740389

7.6.7-1

7.6.7-2

atom	x	y	z
8	2.001572	-1.327254	-0.839046
16	0.628798	-1.022217	-0.365935
8	0.720785	-0.217622	0.905524
8	-0.127546	-2.263525	-0.107647
8	-0.082704	-0.202862	-1.399173
1	3.320793	-0.592024	-0.147814
8	4.060024	-0.151909	0.360433
1	3.723163	-0.195715	1.259972
1	0.065675	1.547506	-1.340385
8	0.099181	2.520290	-1.178340
1	0.814851	2.590033	-0.523893
1	-1.968221	1.215052	1.484257
8	-1.635559	0.565596	2.131429
1	-0.775034	0.284553	1.746391
1	-1.747724	-2.118453	0.646276
8	-2.623789	-1.876618	1.025629
1	-2.410506	-1.071235	1.536096
1	2.933957	1.674744	0.446495
8	2.143588	2.076772	0.834218
1	1.560336	1.281030	0.928118
1	-1.620919	2.469461	-0.389800
8	-2.514594	2.254242	-0.054177
1	-2.738696	1.426837	-0.529559
1	-1.864606	-0.287168	-1.462040
8	-2.840324	-0.253955	-1.332256
1	-2.958911	-0.854391	-0.571890

atom	x	y	z
8	-0.300197	0.024022	-1.222793
16	-0.199829	-0.799670	0.027172
8	-0.297631	0.115119	1.210904
8	1.122179	-1.485656	0.052163
8	-1.292614	-1.791625	0.066403
1	2.450769	-0.898826	1.275294
8	3.218999	-0.391171	1.607688
1	2.858963	0.518102	1.591227
1	3.737304	-0.581622	-0.328653
8	3.462389	-0.801484	-1.235754
1	2.562744	-1.146959	-1.047586
1	-1.945080	0.742618	1.553381
8	-2.881664	1.044582	1.596991
1	-3.360582	0.307112	1.184790
1	-2.714757	1.676519	-0.350615
8	-2.637294	1.520889	-1.306300
1	-1.786787	1.028063	-1.367589
1	-2.968158	-1.354338	-0.210943
8	-3.860913	-0.957409	-0.351308
1	-3.646153	-0.181458	-0.895931
1	0.961666	1.406693	1.284221
8	1.743806	1.999120	1.205959
1	1.870271	2.041738	0.239082
1	1.068104	1.129429	-1.553761
8	1.915239	1.623950	-1.646795
1	2.570573	0.904976	-1.624924

7.7.7-1

atom	x	y	z
8	-0.302692	-0.070918	1.221516
16	-0.200742	0.792836	0.000500
8	-0.296124	-0.083360	-1.213745
8	1.120819	1.480213	0.000027
8	-1.293612	1.785389	-0.011377
1	-3.662750	0.164475	0.879189
8	-3.869946	0.952836	0.349494
1	-2.974384	1.350080	0.229265
1	2.467079	0.970125	1.231357
8	3.241183	0.484032	1.582109
1	2.886481	-0.427202	1.609953
1	2.547725	1.091544	-1.102362
8	3.446726	0.741245	-1.284881
1	3.735572	0.571298	-0.371526
1	-1.805246	-1.059454	1.339601
8	-2.659381	-1.543418	1.261006
1	-2.728840	-1.679601	0.301799
1	-3.358096	-0.277399	-1.208649
8	-2.876638	-1.005512	-1.634475
1	-1.940276	-0.704976	-1.577666
1	1.059449	-1.209739	-1.493429
8	1.906961	-1.707687	-1.566884
1	2.560625	-0.987090	-1.587107
1	0.988057	-1.337714	1.358714
8	1.775969	-1.924275	1.302822
1	1.890349	-2.018083	0.337955

7.7.7-2

atom	x	y	z
8	-1.116591	-1.612430	0.647745
16	0.242221	-1.259042	0.150863
8	0.084015	-0.417466	-1.088122
8	1.052053	-2.445670	-0.156507
8	0.942319	-0.437709	1.198380
1	0.533029	1.165917	1.692666
8	0.222284	2.070444	1.937108
1	0.279906	2.557321	1.095810
1	-1.227936	0.667302	-1.161129
8	-1.951169	1.343127	-1.111967
1	-2.227725	1.275279	-0.177043
1	3.139456	-1.507675	-0.144274
8	3.499424	-0.732321	0.311186
1	2.691775	-0.490209	0.821931
1	1.430763	0.545689	-1.529086
8	2.206776	1.151926	-1.633392
1	2.839735	0.746864	-1.020129
1	-1.500522	1.284631	1.889213
8	-2.304786	0.775848	1.668065
1	-1.955516	-0.107714	1.427604
1	-2.543754	-1.677166	-0.584173
8	-3.293218	-1.459753	-1.174487
1	-3.104268	-0.536098	-1.387638
1	-0.497427	2.632127	-0.955418
8	0.312424	3.143839	-0.765788
1	1.038682	2.549724	-1.039912

7.7.7-3

atom	x	y	z
8	-1.885687	0.820363	-0.126176
16	-1.158527	-0.483461	-0.094960
8	-0.063540	-0.447269	-1.119956
8	-2.077127	-1.599161	-0.362778
8	-0.528826	-0.644498	1.261160
1	0.874383	0.999802	-1.181778
8	1.432041	1.813070	-1.086506
1	0.817547	2.453393	-0.690765
1	1.760663	1.296267	0.909763
8	1.442817	1.136928	1.813266
1	0.667362	0.539981	1.660486
1	-3.895904	0.490604	-0.469952
8	-4.533407	-0.223658	-0.631602
1	-3.897049	-0.962201	-0.595643
1	-1.100555	2.288582	0.376567
8	-0.540381	3.054929	0.658262
1	0.047737	2.649769	1.312802
1	3.231302	1.003415	-1.376006
8	3.927933	0.336247	-1.471195
1	3.446527	-0.495500	-1.289456
1	2.146544	-0.981350	2.103934
8	1.798393	-1.873320	1.967683
1	0.873095	-1.662655	1.700293
1	1.400103	-1.480528	-1.056246
8	2.265790	-1.920300	-0.896461
1	2.260627	-2.030857	0.069780

7.7.7-4

atom	x	y	z
8	1.215334	1.434346	-0.005195
16	0.000000	0.578608	0.000003
8	-1.215332	1.434348	0.005205
8	0.003148	-0.292949	1.215841
8	-0.003148	-0.292943	-1.215840
1	2.827998	0.741028	0.262767
8	3.648935	0.211188	0.385583
1	3.321505	-0.546335	0.899650
1	-1.552004	-1.132060	1.589288
8	-2.437156	-1.557981	1.642075
1	-3.009332	-0.910866	1.197905
1	-3.321505	-0.546326	-0.899648
8	-3.648935	0.211193	-0.385576
1	-2.827998	0.741032	-0.262758
1	0.729835	3.391151	-0.001271
8	0.000003	4.033260	-0.000003
1	-0.729831	3.391152	0.001269
1	-1.325290	-1.512623	-1.316353
8	-2.100748	-2.113408	-1.236495
1	-2.163447	-2.241817	-0.275721
1	1.552004	-1.132051	-1.589293
8	2.437155	-1.557972	-1.642083
1	3.009332	-0.910861	-1.197907
1	1.325287	-1.512633	1.316347
8	2.100744	-2.113419	1.236485
1	2.163444	-2.241821	0.275710

7.8.6-1

7.8.6-2

atom	x	y	z
16	0.000000	0.568715	0.009062
8	0.000001	-0.299231	1.227521
8	-1.214820	1.425200	0.004441
8	1.214819	1.425201	0.004440
8	-0.000001	-0.306455	-1.204141
8	-3.671938	0.234447	0.324869
8	3.671938	0.234450	0.324863
8	2.419663	-1.601989	-1.618307
8	-0.000002	4.023909	-0.016722
8	2.156990	-2.062724	1.279507
8	-2.419665	-1.601987	-1.618310
8	-2.156986	-2.062729	1.279504
1	-3.364209	-0.510959	0.868209
1	-2.842944	0.754506	0.214500
1	2.842943	0.754508	0.214495
1	1.535766	-1.172497	-1.564622
1	0.729774	3.381748	-0.010901
1	-0.729776	3.381747	-0.010898
1	1.372063	-1.474875	1.357495
1	-3.000466	-0.939284	-1.209696
1	-1.535767	-1.172494	-1.564624
1	-1.372060	-1.474878	1.357492
1	-2.199286	-2.220736	0.321854
1	2.199290	-2.220733	0.321858
1	3.364211	-0.510954	0.868206
1	3.000465	-0.939286	-1.209697

7.8.6-3

atom	x	y	z
8	0.493901	-0.626850	-1.530708
16	-0.717898	-0.304984	-0.719691
8	-0.951111	1.165941	-0.727179
8	-0.476223	-0.747582	0.706226
8	-1.895516	-1.019654	-1.250731
1	3.216222	0.308111	-0.519710
8	2.889338	0.728607	-1.335804
1	2.024778	0.281369	-1.482096
1	1.431876	-2.103415	-0.673003
8	1.581260	-2.560533	0.176584
1	0.833692	-2.153934	0.658651
1	-3.627959	0.765613	0.811745
8	-3.506989	1.686876	0.533399
1	-2.648580	1.639994	0.070150
1	2.898462	-1.381879	0.867076
8	3.422426	-0.621190	1.186967
1	2.737479	-0.045276	1.593147
1	1.294786	1.681061	1.460913
8	1.266722	0.926697	2.080733
1	0.588575	0.344620	1.668634
1	-2.439975	-1.114813	1.465983
8	-3.324592	-1.245788	1.089273
1	-3.059435	-1.276979	0.143511
1	0.406590	2.278235	-0.365540
8	1.240241	2.744522	-0.128436
1	1.914209	2.208664	-0.587017

7.8.6-4

atom	x	y	z
8	0.910455	-1.633122	-0.049478
16	0.908028	-0.146997	-0.003706
8	2.298110	0.371918	0.024456
8	0.177277	0.321647	1.216085
8	0.204123	0.391641	-1.214573
1	-0.555086	1.993882	-0.707434
8	-0.891759	2.581213	0.004961
1	-0.617378	2.018047	0.756017
1	-2.109217	-1.602695	-1.254441
8	-2.168226	-0.832857	-1.852445
1	-1.285273	-0.412210	-1.725845
1	2.312979	2.256565	0.053880
8	2.161658	3.224452	0.065752
1	1.196766	3.277824	0.046911
1	-0.686498	-2.455813	0.110469
8	-1.620390	-2.752496	0.199430
1	-1.971840	-2.134935	0.868611
1	3.608530	-1.116314	-0.021634
8	3.755382	-2.078228	-0.053176
1	2.821071	-2.344390	-0.065329
1	-1.396443	-0.286250	1.732555
8	-2.327061	-0.561405	1.905300
1	-2.830548	-0.016730	1.274766
1	-3.064358	0.417307	-0.865245
8	-3.410558	1.097522	-0.245439
1	-2.663236	1.715383	-0.150964

7.8.6-5

atom	x	y	z
8	-0.958566	1.091696	-0.854244
16	-0.711984	-0.369281	-0.702958
8	-0.456977	-0.673298	0.753154
8	0.500039	-0.755865	-1.490555
8	-1.883846	-1.142979	-1.159289
1	0.944000	-2.132485	0.831096
8	1.651220	-2.520525	0.285996
1	1.399866	-2.088024	-0.558057
1	1.882964	0.379754	-1.545790
8	2.636593	0.998506	-1.410840
1	2.204735	1.735617	-0.935093
1	0.263860	2.253523	-0.235215
8	1.026048	2.744258	0.147701
1	1.205554	2.235155	0.960638
1	-2.413914	-1.002006	1.559452
8	-3.296234	-1.181663	1.197944
1	-3.031168	-1.294429	0.258146
1	-2.674282	1.604088	-0.102746
8	-3.532309	1.677975	0.357210
1	-3.634167	0.785848	0.724120
1	0.706733	0.289053	1.717142
8	1.425684	0.770173	2.186689
1	2.237005	0.372197	1.823303
1	3.391907	0.049670	-0.022669
8	3.621692	-0.507379	0.752663
1	3.041888	-1.286652	0.641582

7.8.6-6

atom	x	y	z
8	0.472258	0.942391	0.500973
16	0.735132	0.115741	-0.734484
8	1.923958	0.639650	-1.435557
8	-0.466105	0.196574	-1.619878
8	0.966265	-1.297736	-0.320849
1	-1.336748	-1.226794	1.818698
8	-1.344059	-0.332594	2.210996
1	-0.648956	0.130745	1.692865
1	2.111557	1.126575	1.548972
8	2.996593	1.072822	1.956501
1	3.441032	0.435742	1.375392
1	-2.805140	0.439180	1.433143
8	-3.482039	0.867263	0.863528
1	-2.954966	1.523600	0.366531
1	3.396346	-0.215933	-0.734081
8	3.830235	-0.877294	-0.151761
1	3.043238	-1.414048	0.037238
1	-1.980933	-0.713060	-1.389917
8	-2.844720	-1.123530	-1.157658
1	-3.209569	-0.499602	-0.503736
1	-0.381390	-2.286877	0.271562
8	-1.213247	-2.699100	0.601597
1	-1.881571	-2.326294	-0.003443
1	-1.410518	1.798262	-1.223759
8	-1.620994	2.495823	-0.570764
1	-0.889657	2.302499	0.045245

atom	x	y	z
8	0.071433	0.206872	-1.263726
16	1.006231	0.053107	-0.102437
8	2.186811	0.925500	-0.302719
8	1.402604	-1.373393	0.021195
8	0.295698	0.480030	1.149381
1	-1.187243	-0.222814	1.747986
8	-2.042249	-0.646929	1.993570
1	-2.648214	-0.319049	1.304404
1	-1.314825	-2.257709	1.272775
8	-0.842619	-2.924545	0.736942
1	-0.001791	-2.469445	0.513172
1	0.346071	2.239673	1.244829
8	0.525217	3.171740	0.971774
1	1.258830	3.000927	0.365388
1	-1.667707	-2.255375	-0.876146
8	-1.915109	-1.653369	-1.603125
1	-1.163295	-1.016932	-1.590709
1	-1.068219	2.830328	-0.311136
8	-1.566037	2.371497	-1.006081
1	-0.971280	1.605074	-1.191603
1	-3.044971	-0.395281	-0.818094
8	-3.496936	0.321630	-0.324980
1	-2.928109	1.099851	-0.481123
1	3.815606	-0.138215	-0.317736
8	4.258316	-1.005284	-0.258682
1	3.458416	-1.540748	-0.131402

7.8.6-7

atom	x	y	z
8	-1.286616	-0.663832	-1.192236
16	0.056222	-0.412425	-0.607598
8	-0.101544	-0.072953	0.853019
8	0.676335	0.774394	-1.285807
8	0.919351	-1.597054	-0.760870
1	-3.029353	0.605381	1.056732
8	-2.728061	0.070820	1.812922
1	-1.784721	-0.073414	1.584259
1	2.335989	1.225754	-0.747603
8	3.199940	1.400892	-0.309319
1	2.992501	1.209954	0.620694
1	-2.495318	-1.952795	-0.413864
8	-3.197463	-2.319137	0.155566
1	-3.212862	-1.656395	0.865001
1	-2.287171	2.115808	-0.483258
8	-2.998779	1.491796	-0.712098
1	-2.485921	0.706368	-1.004572
1	2.638946	-1.628918	-0.396976
8	3.580906	-1.486250	-0.142164
1	3.702931	-0.549511	-0.370734
1	1.456029	-0.048721	1.765750
8	2.371487	-0.027515	2.126738
1	2.824969	-0.700798	1.593334
1	-0.539818	2.176471	0.864355
8	-0.554551	2.793948	0.119926
1	-0.063801	2.248739	-0.536969

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7.8.6-9

atom	x	y	z
8	0.149295	-1.211614	0.303635
16	0.148514	-0.001471	-0.572022
8	0.145479	1.227920	0.274647
8	-1.068853	-0.012781	-1.431205
8	1.371753	-0.010796	-1.426845
1	4.065616	0.753557	0.695598
8	4.608660	-0.005993	0.975151
1	4.062850	-0.765672	0.701417
1	2.553020	-1.359662	-0.824579
8	2.825264	-2.009887	-0.146190
1	1.984506	-2.023323	0.344478
1	-2.451516	1.226355	-1.000377
8	-3.264277	1.573746	-0.579575
1	-2.990598	1.609213	0.358310
1	-3.752432	-0.368641	-0.704657
8	-3.459549	-1.286296	-0.842832
1	-2.535516	-1.115483	-1.126139
1	-2.754205	-1.584608	0.967600
8	-2.167215	-1.562132	1.743700
1	-1.280587	-1.487005	1.318670
1	1.991479	2.022865	0.320337
8	2.834476	1.994763	-0.165735
1	2.559762	1.337923	-0.836688
1	-1.202057	1.358457	1.446901
8	-2.032581	1.311926	1.974542
1	-2.166170	0.348710	2.057130

atom	x	y	z
8	1.229940	1.013430	-1.167510
16	-0.056410	0.488400	-0.632516
8	-0.210254	-0.949359	-1.014748
8	-1.189850	1.273841	-1.153670
8	-0.020554	0.582956	0.872614
1	-3.399833	0.597827	0.777986
8	-3.687142	0.890521	-0.103129
1	-2.826489	1.117527	-0.527907
1	1.817981	-2.291225	0.785552
8	1.666912	-2.739946	-0.063724
1	0.955188	-2.185233	-0.456535
1	-2.437554	-1.232209	1.369700
8	-2.290207	-0.537855	2.032745
1	-1.458074	-0.119458	1.715471
1	2.863212	-0.452504	1.182766
8	2.253785	-0.677724	1.904016
1	1.426673	-0.221122	1.632543
1	1.689075	2.569927	-0.070319
8	1.647936	3.087966	0.754297
1	1.035117	2.524564	1.246873
1	2.725556	0.040360	-1.005957
8	3.471794	-0.569616	-0.808963
1	3.022822	-1.430199	-0.754155
1	-1.870910	-1.633053	-0.778514
8	-2.794315	-1.882344	-0.549886
1	-3.264557	-1.034556	-0.613577

7.8.6-10

atom	x	y	z
8	0.002743	-1.015224	0.952961
16	-0.695177	-0.366208	-0.199875
8	-1.965547	-1.069388	-0.489742
8	0.195540	-0.419895	-1.399766
8	-0.980390	1.063112	0.141674
1	-4.335230	0.057027	0.777439
8	-4.286256	-0.865657	1.062157
1	-3.421899	-1.117746	0.674784
1	3.056312	0.594809	-1.020932
8	2.480415	1.120606	-1.605093
1	1.633186	0.618774	-1.591429
1	1.738286	2.342381	-0.324531
8	1.213502	2.715188	0.409089
1	0.368374	2.216790	0.328794
1	1.235694	-0.019299	1.796839
8	1.975302	0.547815	2.114829
1	1.789057	1.396356	1.668398
1	1.436871	-1.918443	-1.163095
8	1.856634	-2.493696	-0.495578
1	1.271824	-2.247859	0.250038
1	3.269652	-0.175725	1.027795
8	3.820965	-0.593928	0.330755
1	3.257156	-1.331549	0.023816
1	-2.667178	1.527533	-0.359829
8	-3.568282	1.432160	-0.742636
1	-3.466285	0.547534	-1.119289

7.8.6-11

atom	x	y	z
8	-1.829257	0.924560	-0.027371
16	-0.884982	-0.221058	0.093990
8	-0.022761	-0.030567	1.300501
8	-0.007177	-0.274140	-1.117315
8	-1.638432	-1.497069	0.212569
1	-3.763507	0.271371	0.016238
8	-4.314041	-0.525603	0.089654
1	-3.587380	-1.169943	0.159454
1	0.500274	-2.195561	-1.369792
8	0.336238	-3.080921	-0.997955
1	-0.469935	-2.859263	-0.491949
1	1.563979	-2.525625	0.482895
8	1.998475	-1.998396	1.174930
1	1.346864	-1.279016	1.320482
1	0.236539	2.792517	-1.289784
8	-0.560833	3.189252	-0.911796
1	-1.095291	2.400194	-0.653204
1	3.404235	-1.075640	0.251752
8	4.034952	-0.533824	-0.259975
1	3.475917	0.187201	-0.596006
1	0.385361	2.970723	0.882428
8	0.989666	2.529809	1.501241
1	0.613675	1.621338	1.556470
1	1.933113	1.857228	-0.129953
8	2.047293	1.511972	-1.032806
1	1.342891	0.820829	-1.096288

7.8.6-12

7.8.6-13

atom	x	y	z
8	-2.132353	0.334592	0.261150
16	-0.686459	0.405064	-0.044471
8	-0.371093	-0.481752	-1.209464
8	0.104055	-0.065746	1.137811
8	-0.291250	1.803836	-0.372321
1	2.652624	1.762644	0.374177
8	2.449526	2.124093	-0.505775
1	1.463977	2.095053	-0.519662
1	-2.991113	2.137571	0.078475
8	-2.850559	3.078484	-0.124679
1	-1.895107	3.025766	-0.296377
1	-0.464710	-2.233186	-0.960735
8	-0.360069	-3.170433	-0.675268
1	0.449099	-3.112037	-0.147530
1	-2.108739	-2.827922	0.323651
8	-2.922077	-2.426368	0.667664
1	-2.734835	-1.471618	0.585940
1	2.843646	-0.150380	1.734343
8	2.547764	0.720102	2.037678
1	1.585744	0.650482	1.835346
1	2.331314	-1.536466	-0.232697
8	2.082642	-1.905918	0.636994
1	1.296832	-1.356092	0.862706
1	1.347753	-0.471820	-1.742565
8	2.328317	-0.440841	-1.818569
1	2.527632	0.446604	-1.465297

atom	x	y	z
16	-0.088523	-0.233445	-0.717124
8	1.245803	-0.524170	-1.309039
8	-0.208768	-0.992687	0.582371
8	-0.197977	1.226387	-0.422083
8	-1.165312	-0.652505	-1.634234
8	2.296882	-2.605566	0.120003
8	3.401418	1.361381	-1.311306
8	1.946102	-0.503712	2.232385
8	-2.583884	-0.440883	1.916189
8	-2.795208	1.963599	0.235623
8	1.965497	2.172089	1.088024
8	-3.756262	-0.653548	-0.756435
1	2.091029	-1.880577	-0.514908
1	1.430606	-2.685105	0.539039
1	2.689451	0.711515	-1.460179
1	3.093396	1.781929	-0.490302
1	1.079806	-0.584101	1.770453
1	2.494931	-1.065519	1.666566
1	-1.726334	-0.704122	1.511312
1	-2.662467	0.487501	1.639852
1	-1.855113	1.803865	-0.008723
1	-3.264063	1.277903	-0.267474
1	1.173478	1.955613	0.549791
1	2.102643	1.344478	1.581515
1	-2.856327	-0.701716	-1.157621
1	-3.561001	-0.809624	0.182687

7.8.6-15

atom	x	y	z
8	-1.244360	-1.593559	-1.007161
16	-0.089361	-0.774000	-0.627009
8	-0.031869	0.479634	-1.439605
8	1.175533	-1.543633	-0.813892
8	-0.191927	-0.375787	0.832456
1	-0.794224	2.756754	0.265730
8	-1.503004	2.630470	-0.391142
1	-1.142151	1.874108	-0.900937
1	-3.066201	-1.463861	-0.589645
8	-3.957214	-1.269692	-0.239551
1	-3.753975	-0.543479	0.374438
1	-2.523348	1.491930	0.825817
8	-2.723562	0.756337	1.433080
1	-1.905876	0.224809	1.351477
1	2.698881	-0.885624	-0.472469
8	3.525813	-0.515743	-0.064875
1	3.314757	-0.619206	0.872722
1	1.400453	2.292928	0.605711
8	0.764058	2.253426	1.344368
1	0.435869	1.332545	1.279201
1	1.846834	-2.302771	1.181711
8	1.802707	-1.874115	2.047480
1	1.053768	-1.267103	1.862546
1	1.498611	1.436870	-1.295649
8	2.319251	1.911040	-1.029864
1	2.882972	1.189079	-0.698846

atom	x	y	z
8	0.253016	0.302292	-1.607097
16	1.016005	-0.473810	-0.580408
8	2.349651	-0.827999	-1.095693
8	0.246758	-1.699628	-0.221801
8	1.166729	0.383380	0.654438
1	-2.202972	-2.190927	1.049726
8	-1.566639	-2.210391	1.785315
1	-0.735498	-2.082365	1.278499
1	-1.496382	0.543887	-1.607530
8	-2.462801	0.719942	-1.531701
1	-2.515863	1.298338	-0.748874
1	3.718698	-0.365287	0.116503
8	4.066339	0.035410	0.938415
1	3.220312	0.352943	1.287136
1	-1.331888	-0.366095	2.300508
8	-0.956475	0.528674	2.384350
1	-0.164755	0.479209	1.797308
1	0.858267	2.244219	0.167653
8	0.431497	2.845873	-0.471894
1	0.292724	2.183442	-1.176373
1	-2.670418	-1.105571	-1.135091
8	-2.462576	-2.040725	-0.941825
1	-1.485574	-2.012288	-0.878475
1	-1.303574	2.742749	0.321742
8	-2.140094	2.472281	0.748720
1	-1.842399	1.785839	1.383989

7.8.6-16

atom	x	y	z
8	-0.154034	-2.341062	-0.683295
16	0.425343	-0.992540	-0.504131
8	-0.227972	-0.022100	-1.431397
8	1.892730	-1.024943	-0.762883
8	0.184630	-0.533268	0.912070
1	3.201233	1.128523	0.640293
8	3.277681	1.248724	-0.316074
1	2.796593	0.443339	-0.632779
1	1.750248	-0.493639	1.876867
8	2.714232	-0.597411	2.033700
1	2.939956	-1.036171	1.201714
1	-0.096632	2.500532	0.465952
8	-0.508677	2.160878	1.280749
1	-0.320262	1.201105	1.211234
1	-3.328143	1.385387	0.127848
8	-3.336708	2.143567	0.740817
1	-2.394084	2.229741	0.979349
1	-2.080637	-0.052315	-1.233209
8	-3.022514	-0.163280	-0.982993
1	-2.976126	-0.885205	-0.333171
1	-1.816113	-1.532686	1.468636
8	-2.295017	-2.221311	0.987236
1	-1.595093	-2.462315	0.334413
1	1.730787	2.279525	-0.929566
8	0.845826	2.538521	-1.240337
1	0.421365	1.668308	-1.412237

7.8.6-17

7.8.6-18

atom	x	y	z
8	-0.108270	1.047659	-0.368774
16	0.286552	-0.362626	-0.701209
8	0.307087	-1.152290	0.576833
8	1.642340	-0.379691	-1.304494
8	-0.696308	-0.947788	-1.636822
1	2.728170	2.218118	0.329472
8	2.015699	2.875925	0.312976
1	1.243938	2.333268	0.061806
1	-2.712576	1.816961	0.455657
8	-2.784982	1.900231	-0.512313
1	-1.868713	1.660699	-0.762430
1	-2.742055	-1.422745	0.789104
8	-2.228016	-1.553351	1.608651
1	-1.299547	-1.528739	1.282003
1	-1.990757	0.270175	2.061256
8	-1.738424	1.214782	2.055131
1	-0.984047	1.214979	1.436953
1	3.679435	-0.103660	0.753293
8	3.789478	0.534684	0.036057
1	3.020383	0.292835	-0.539819
1	1.861708	-1.821391	0.989515
8	2.794251	-2.152579	1.003254
1	3.007240	-2.078139	0.066711
1	-3.371151	0.065535	-0.844416
8	-3.336880	-0.899924	-0.968957
1	-2.404670	-1.017140	-1.272094

7.8.6-19

atom	x	y	z
8	0.072360	-0.895449	-0.698137
16	0.080085	0.324087	0.172179
8	0.909090	1.379185	-0.474533
8	0.613700	-0.013851	1.507769
8	-1.327589	0.824459	0.308280
1	2.585356	0.988254	-0.941639
8	3.484098	0.629576	-1.125534
1	3.296044	-0.310657	-1.284242
1	-3.803650	-0.431524	0.674424
8	-3.373837	-0.610663	1.524458
1	-2.532799	-0.123792	1.391207
1	1.645797	-1.779045	-0.806102
8	2.563378	-2.133188	-0.778907
1	2.856023	-1.879365	0.112343
1	3.572944	0.014999	0.831014
8	3.309572	-0.542387	1.581461
1	2.344789	-0.349581	1.655648
1	-3.068391	-1.000373	-1.356679
8	-3.405548	-0.088033	-1.380398
1	-2.651847	0.397759	-0.987425
1	-1.278206	-2.013141	-0.549042
8	-2.121468	-2.518731	-0.455595
1	-2.485870	-2.169509	0.371325
1	0.014658	3.115206	-0.400729
8	-0.777087	3.648112	-0.203244
1	-1.349560	2.923133	0.090071

7.8.6-20

atom	x	y	z
8	-1.681377	0.177997	-0.762050
16	-0.886767	-0.698458	0.165561
8	0.394567	-1.070035	-0.508152
8	-1.661714	-1.898080	0.512907
8	-0.564972	0.097219	1.398335
1	1.201719	1.795077	-1.262025
8	1.900094	1.129109	-1.127979
1	1.378984	0.302305	-0.980197
1	-3.380585	-1.929834	-0.412726
8	-3.999044	-1.500438	-1.032528
1	-3.444266	-0.729331	-1.235575
1	3.693290	0.251384	-1.383215
8	4.377720	-0.414264	-1.214980
1	3.941476	-0.979599	-0.548282
1	2.197364	1.140864	0.854096
8	2.059342	0.857150	1.773955
1	1.116847	0.574035	1.747536
1	-1.405509	1.631217	1.479869
8	-1.977744	2.417251	1.298042
1	-2.544251	2.040369	0.614687
1	-0.770454	2.896457	-0.418257
8	-0.560077	2.585054	-1.311185
1	-0.946164	1.674324	-1.269455
1	2.701441	-0.921926	1.320113
8	2.780125	-1.735669	0.787835
1	1.913028	-1.732367	0.330851

atom	x	y	z
8	1.501750	-1.860822	-0.801865
16	0.585050	-0.784649	-0.394428
8	-0.231161	-0.314362	-1.554995
8	-0.332221	-1.257263	0.686626
8	1.369980	0.387098	0.132569
1	0.358567	1.704879	0.646817
8	-0.258170	2.401063	0.987254
1	1.951844	0.760293	1.971709
8	1.992961	1.349018	2.748311
1	1.243854	1.931350	2.566425
1	-1.053606	1.883981	1.211795
1	-0.592874	2.677378	-0.940411
8	-0.718391	2.439462	-1.875733
1	-0.361253	1.525639	-1.893007
1	-1.600417	-0.160160	1.164362
8	-2.381524	0.433594	1.287706
1	-2.711822	0.524448	0.374008
1	-2.432127	1.387151	-1.718730
8	-2.849641	0.527989	-1.537336
1	-2.049146	-0.042333	-1.545790
1	3.254374	-1.252431	-0.938637
8	4.010698	-0.635275	-0.858917
1	3.536360	0.113794	-0.474337
1	-1.730240	-2.469184	0.935240
8	-2.622981	-2.739559	1.231112
1	-3.024693	-1.877965	1.393559

7.8.6-21

atom	x	y	z
8	-0.008490	-0.006363	-1.494146
16	0.883698	-0.007121	-0.291564
8	0.941508	-1.379270	0.278292
8	0.309725	0.938324	0.726028
8	2.244011	0.445662	-0.671660
1	-2.962639	1.360002	-0.652627
8	-3.627569	0.706567	-0.356972
1	-3.266438	-0.140195	-0.698149
1	-0.964800	1.534553	-1.531471
8	-1.411158	2.315726	-1.133136
1	-0.936666	2.310452	-0.286631
1	-0.496269	-2.118576	1.020961
8	-1.377381	-2.388979	1.366997
1	-1.704074	-1.556116	1.756912
1	-2.682993	0.473444	1.330666
8	-2.048451	0.311490	2.052477
1	-1.180177	0.529481	1.644973
1	3.522189	-1.053851	-0.564505
8	3.700449	-1.980503	-0.323870
1	2.811313	-2.195810	0.001387
1	-1.446534	-1.097336	-1.412531
8	-2.273152	-1.599035	-1.231158
1	-2.073703	-2.020188	-0.372570
1	1.739986	2.306945	1.335124
8	2.635390	2.613364	1.121532
1	2.822568	1.965285	0.418417

7.9.5-1

atom	x	y	z
8	-2.375258	-0.059251	-0.453662
16	-0.891788	-0.041157	-0.494872
8	-0.400847	-0.130797	-1.882455
8	-0.361328	-1.194597	0.313010
8	-0.398106	1.238111	0.134110
1	2.382496	1.147293	-1.254634
8	2.236817	1.830637	-0.571573
1	1.283220	1.716228	-0.361292
1	-1.991196	2.612675	0.261021
8	-2.956177	2.639828	0.172004
1	-3.085861	1.704964	-0.073516
1	1.309120	-0.344578	-2.266893
8	2.289120	-0.440698	-2.307300
1	2.460720	-1.039678	-1.556428
1	1.358464	-1.721631	0.169702
8	2.324365	-1.905180	0.157244
1	2.692115	-1.199665	0.720453
1	0.080089	0.899624	1.927364
8	0.380115	0.271183	2.615679
1	0.142689	-0.545016	2.140933
1	-3.035827	-1.750828	0.232117
8	-2.876894	-2.627228	0.629050
1	-1.911842	-2.560713	0.695126
1	2.888420	0.980599	0.930263
8	3.074856	0.425803	1.718291
1	2.202697	0.376747	2.158564

7.9.5-2

7.9.5-3

atom	x	y	z
8	-1.724793	1.223630	-0.166794
16	-0.509072	0.373219	-0.069857
8	-0.528815	-0.373832	1.221874
8	0.714502	1.238125	-0.121828
8	-0.474406	-0.592765	-1.203568
1	2.439585	-1.321311	-1.414373
8	1.846875	-2.090285	-1.345270
1	0.961504	-1.659345	-1.341292
1	-3.277454	-1.665228	-0.355693
8	-2.971074	-2.074070	-1.180318
1	-2.107904	-1.636391	-1.307671
1	-2.490846	-0.739386	1.596362
8	-3.383944	-0.476978	1.311491
1	-3.120839	0.277783	0.748712
1	0.172323	3.270157	-0.302600
8	-0.624128	3.818662	-0.367705
1	-1.278444	3.096843	-0.320452
1	3.403838	0.435930	-0.306518
8	3.157188	0.495428	-1.246510
1	2.232936	0.805611	-1.149753
1	2.574734	-0.455194	1.708447
8	2.862876	0.474542	1.609030
1	2.065031	0.880802	1.217075
1	0.795961	-1.544241	1.494535
8	1.624263	-2.076112	1.523870
1	1.786366	-2.248268	0.576743

7.9.5-4

atom	x	y	z
8	-1.211982	1.393602	0.002240
16	-0.105777	0.399714	-0.002661
8	-0.196377	-0.452830	-1.222012
8	-0.191298	-0.458255	1.213201
8	1.210486	1.120564	-0.003939
1	-1.580313	-1.581388	-1.325135
8	-2.397407	-2.126382	-1.252739
1	-2.477251	-2.249348	-0.292421
1	2.360991	0.339387	-1.369233
8	2.509397	-0.391747	-1.997301
1	1.599939	-0.741693	-1.990542
1	-3.213990	-0.876730	1.198795
8	-2.688770	-1.571857	1.628468
1	-1.775691	-1.207003	1.575374
1	2.362363	0.346096	1.366484
8	2.509528	-0.383535	1.996468
1	1.600067	-0.733768	1.988260
1	0.926777	3.128509	-0.000179
8	0.266759	3.841272	0.002068
1	-0.525085	3.276882	0.002056
1	-2.880060	0.804160	-0.246797
8	-3.735511	0.331433	-0.365777
1	-3.469669	-0.439614	-0.894365
1	3.616109	-1.406145	0.761097
8	4.116697	-1.757843	0.002664
1	3.616059	-1.410149	-0.757552

7.9.5-5

atom	x	y	z
8	-0.603276	1.206447	-0.951992
16	0.243366	0.066561	-0.514410
8	-0.287505	-1.208662	-1.073253
8	0.237354	-0.006881	0.985865
8	1.646895	0.262659	-0.975557
1	0.084962	2.963837	-0.552979
8	0.576798	3.745931	-0.238773
1	1.294234	3.328834	0.264873
1	2.126812	-2.508121	0.816431
8	1.888129	-2.289062	1.730576
1	1.301326	-1.520308	1.604470
1	2.407744	-1.518742	-1.201377
8	2.240822	-2.480007	-1.230811
1	1.268077	-2.438104	-1.267432
1	2.443487	1.412436	0.252754
8	2.481262	1.921595	1.089753
1	1.771467	1.462775	1.563799
1	-1.875388	-1.802617	-0.512835
8	-2.763723	-1.986415	-0.130751
1	-2.685498	-1.596945	0.756250
1	-2.776428	0.483135	1.328324
8	-2.346549	-0.039869	2.024573
1	-1.401336	-0.017258	1.753713
1	-2.393442	1.058902	-0.799683
8	-3.335537	0.843597	-0.618732
1	-3.337230	-0.127472	-0.662928

7.9.5-6

atom	x	y	z
8	0.018908	0.032313	1.061497
16	0.656834	-0.449068	-0.208098
8	2.134015	-0.243404	-0.112109
8	0.124432	0.351152	-1.349198
8	0.360151	-1.888399	-0.407691
1	-0.695232	2.866198	0.314458
8	-1.313864	2.450041	0.940591
1	-0.908871	1.560637	1.053445
1	-3.346677	-1.609951	0.454996
8	-4.073648	-1.203926	-0.050727
1	-3.633161	-0.457281	-0.498868
1	-1.374655	-1.321329	1.632069
8	-1.747732	-2.187134	1.392998
1	-1.120039	-2.398182	0.674278
1	2.061570	-2.967510	-0.526120
8	3.032599	-2.929059	-0.496897
1	3.111721	-1.971059	-0.348410
1	0.612115	2.117778	-1.219232
8	0.838167	3.027546	-0.923480
1	1.490320	2.859399	-0.221558
1	-2.426581	1.576526	-0.477949
8	-2.601785	0.983249	-1.228269
1	-1.703895	0.625786	-1.394144
1	2.462662	1.181052	0.802730
8	2.402942	2.015373	1.334693
1	1.567891	1.860992	1.792604

atom	x	y	z
16	0.297828	0.014726	-0.485851
8	0.165474	-0.029450	1.010679
8	1.733048	0.101663	-0.851227
8	-0.302004	-1.230570	-1.047825
8	-0.419914	1.210016	-1.010397
8	3.258438	-2.242349	-0.238213
8	0.653376	-2.932468	0.972898
8	-2.489552	-0.392797	1.792441
8	-3.063972	1.538729	-0.323678
8	1.424404	2.366378	2.076021
8	1.863093	2.911239	-0.830822
8	-3.073425	-1.317099	-0.964406
1	2.849907	-1.397684	-0.510531
1	2.517985	-2.664241	0.225895
1	0.261156	-2.624056	0.131671
1	0.627651	-2.092167	1.456883
1	-1.533715	-0.247351	1.613118
1	-2.758350	-0.955369	1.048117
1	-2.124002	1.514432	-0.616533
1	-3.005868	1.128741	0.555647
1	0.985142	1.526975	1.843227
1	1.657634	2.715750	1.201860
1	2.189723	1.991849	-0.867621
1	0.917101	2.717006	-0.954238
1	-2.095970	-1.355533	-1.066684
1	-3.245368	-0.360291	-0.970957

7.9.5-7

atom	x	y	z
8	0.980214	1.555614	-0.503692
16	-0.099291	0.569474	-0.237611
8	-1.348038	1.280260	0.145065
8	0.324985	-0.333049	0.893071
8	-0.334945	-0.268515	-1.446616
1	-2.073508	-2.410017	-0.177288
8	-2.299356	-2.189586	-1.095369
1	-1.611355	-1.521316	-1.319621
1	3.984292	-0.500400	0.336111
8	4.315250	-1.277900	-0.150293
1	3.489169	-1.672262	-0.483796
1	-3.486920	-0.798951	-0.283124
8	-3.703937	-0.109172	0.367133
1	-2.917633	0.480012	0.298269
1	1.302677	-1.796466	0.055939
8	1.648471	-2.233713	-0.744995
1	1.140297	-1.728572	-1.400952
1	2.443730	1.273802	0.555643
8	2.946241	0.836408	1.276604
1	2.232099	0.262844	1.595452
1	-1.140255	3.292311	-0.081908
8	-0.508466	3.993936	-0.310466
1	0.261584	3.420725	-0.467358
1	-2.552034	-1.249159	1.599496
8	-1.827216	-1.857599	1.819258
1	-1.029108	-1.337606	1.577334

7.9.5-8

7.9.5-9

atom	x	y	z
8	-0.106408	0.267977	-1.416715
16	0.874551	0.035953	-0.321979
8	1.034988	-1.431806	-0.112270
8	0.352119	0.655973	0.947233
8	2.181916	0.648463	-0.664968
1	-1.295571	1.266645	1.022267
8	-2.247148	1.525950	1.047812
1	-2.442199	1.706119	0.111104
1	0.082372	-1.977210	1.332322
8	-0.409452	-1.810861	2.167450
1	-0.227882	-0.857513	2.218928
1	-1.592326	-0.911243	-1.530229
8	-2.523973	-1.210968	-1.558385
1	-2.755510	-1.310980	-0.615459
1	2.688589	2.016991	0.597763
8	2.517087	2.552270	1.395011
1	1.664434	2.154696	1.628875
1	-2.874134	-0.208918	1.246966
8	-3.038004	-1.175432	1.273885
1	-2.183683	-1.529548	1.593647
1	-2.801307	0.747292	-1.861064
8	-2.439060	1.650835	-1.835055
1	-1.486343	1.437264	-1.740760
1	3.566835	-0.763106	-0.936065
8	3.773701	-1.713462	-0.906864
1	2.897766	-2.017258	-0.613711

atom	x	y	z
8	0.215135	-0.746549	0.929569
16	-0.554107	0.059739	-0.074296
8	-2.016571	-0.132247	0.153362
8	-0.196539	-0.398901	-1.444548
8	-0.204864	1.496914	0.088008
1	-1.792917	-1.076548	-2.445861
8	-2.750726	-1.240865	-2.413185
1	-2.900223	-0.925598	-1.506996
1	-1.817059	2.614226	0.493497
8	-2.778082	2.613726	0.641592
1	-2.920126	1.659122	0.534929
1	2.703662	1.130005	1.155821
8	2.610248	0.499058	1.896789
1	1.692416	0.187025	1.772411
1	1.508007	-0.343406	-1.955587
8	2.488177	-0.358692	-2.051813
1	2.742578	-0.959842	-1.329161
1	-2.349650	-1.359919	1.688729
8	-1.980154	-1.920898	2.391977
1	-1.042297	-1.762000	2.199594
1	1.475686	1.977112	-0.313214
8	2.441985	2.054788	-0.482970
1	2.599988	1.315174	-1.100161
1	2.999623	-1.185480	0.933750
8	2.700407	-1.923067	0.372471
1	1.733891	-1.771819	0.410956

7.10.4-1

atom	x	y	z
16	0.333264	0.031438	-0.086832
8	1.799525	-0.081447	-0.331021
8	-0.111689	1.432662	-0.295071
8	-0.394430	-0.884940	-1.010610
8	0.036681	-0.377081	1.328577
1	2.192398	-1.482300	-1.823445
8	1.756303	-2.086538	-2.443966
1	0.838008	-1.883617	-2.195967
1	2.546763	1.663640	-0.986262
8	2.380155	2.592249	-1.218999
1	1.432720	2.610010	-1.011484
1	2.735732	-0.863343	1.217863
8	2.716293	-1.224269	2.121241
1	1.770070	-1.102543	2.289524
1	-1.874618	1.849924	-0.896170
8	-2.811493	1.940932	-1.151660
1	-3.128905	1.027844	-1.071037
1	-2.157482	-0.901485	-1.095930
8	-3.123821	-0.980555	-0.920993
1	-3.111808	-1.280301	-0.000769
1	-1.223238	-1.575210	1.498106
8	-1.875664	-2.314842	1.434430
1	-1.578486	-2.744733	0.626213
1	-0.434580	1.143870	2.410313
8	-0.701846	2.064874	2.582639
1	-0.698898	2.386879	1.671824

7.11.2-1

atom	x	y	z
8	-2.681134	0.580449	-2.568299
8	-1.858833	-0.448947	-0.000025
16	-0.431080	-0.024264	-0.000010
8	-0.143073	0.787468	-1.218746
8	0.447915	-1.239747	-0.000202
8	-0.143001	0.787140	1.218927
8	0.177528	3.388405	0.000316
8	-2.681086	0.580115	2.568403
8	-1.530606	-3.322046	-0.000248
8	2.280313	-0.495457	-1.994988
8	2.280297	-0.496040	1.994863
1	-2.789096	0.118477	-1.721282
1	-1.751863	0.838638	-2.455232
1	0.092401	2.755097	0.730825
1	0.092321	2.755103	-0.730197
1	-1.751783	0.838212	2.455383
1	-2.789106	0.118323	1.721296
1	-0.637583	-2.940027	-0.000299
1	-2.025741	-2.487247	-0.000123
1	1.802328	-1.064186	-1.362500
1	1.644711	0.239980	-2.004875
1	1.802363	-1.064640	1.362227
1	1.644664	0.239373	2.004885
8	4.359215	-0.081752	0.000006
1	3.751684	-0.137895	0.759069
1	3.751690	-0.137673	-0.759078

7.12.2-1