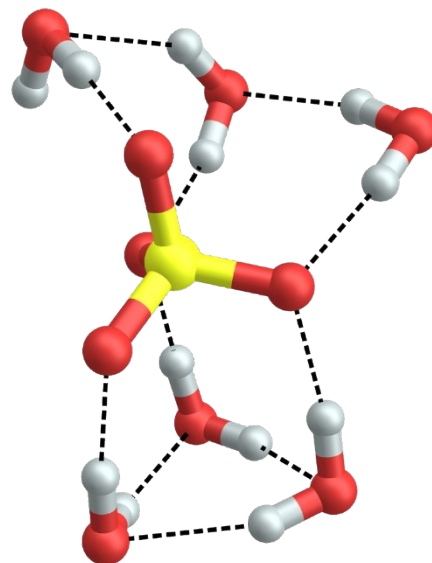


Structures of $\text{SO}_4^{2-}(\text{H}_2\text{O})_6$

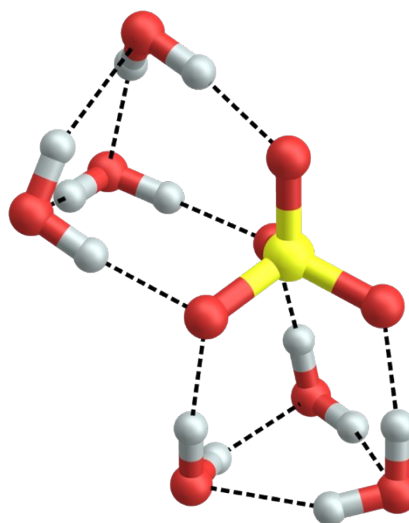
atom	x	y	z
8	1.367769	-1.033708	-1.266101
16	0.104667	-0.558772	-0.651051
8	0.317277	-0.409811	0.837632
8	-0.989715	-1.525892	-0.892922
8	-0.261150	0.775842	-1.213678
1	1.695784	0.627281	1.296879
8	2.596233	1.002626	1.445832
1	3.141651	0.293138	1.076316
1	-2.532802	-1.427594	-0.096178
8	-3.363440	-1.236422	0.405067
1	-3.015241	-0.775523	1.186772
1	2.189102	2.303047	-0.052341
8	1.771370	2.761017	-0.798888
1	1.061788	2.134155	-1.043500
1	-3.210724	0.643281	-0.429903
8	-2.830895	1.530311	-0.536477
1	-1.912905	1.334147	-0.840762
1	-1.072284	0.249632	1.746619
8	-1.902764	0.630068	2.118712
1	-2.202692	1.204566	1.395008
1	2.575757	-1.537246	-0.213314
8	3.178976	-1.780566	0.542137
1	2.538605	-1.816252	1.260715

6.6.5-1



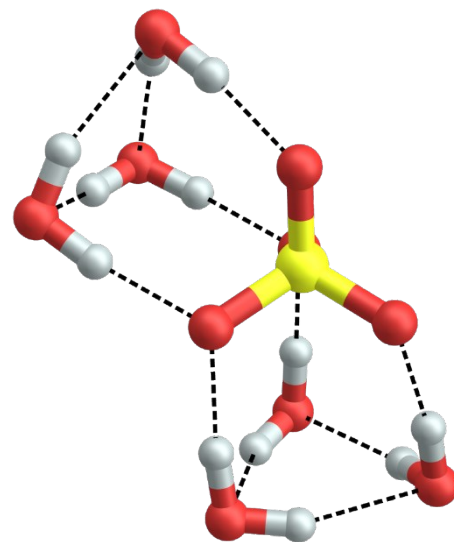
atom	x	y	z
8	1.216420	-1.767009	0.008507
16	0.000000	-0.924726	0.000001
8	-1.216420	-1.767008	-0.008502
8	0.005607	-0.040476	-1.216897
8	-0.005607	-0.040471	1.216895
1	3.004947	0.512711	1.200264
8	2.442865	1.158486	1.658370
1	1.548172	0.747973	1.589909
1	1.321748	1.152155	-1.301388
8	2.100174	1.754292	-1.223066
1	2.170062	1.871656	-0.261692
1	-1.321747	1.152161	1.301382
8	-2.100173	1.754298	1.223058
1	-2.170062	1.871657	0.261684
1	-3.004948	0.512704	-1.200262
8	-2.442867	1.158477	-1.658372
1	-1.548174	0.747965	-1.589911
1	2.802072	-1.107939	-0.274348
8	3.639380	-0.599093	-0.408266
1	3.320580	0.171633	-0.907402
1	-2.802071	-1.107937	0.274355
8	-3.639379	-0.599091	0.408274
1	-3.320577	0.171637	0.907405

6.6.6-1 (6-IV)



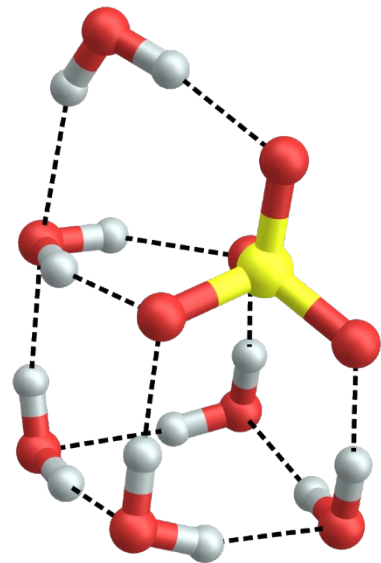
6.6.6-2

atom	x	y	z
8	-0.000001	-0.009967	1.207953
16	0.000000	-0.912640	0.004634
8	1.215806	-1.755668	0.020137
8	0.000001	-0.046917	-1.225544
8	-1.215806	-1.755668	0.020134
1	3.000126	0.553599	1.202727
8	2.431111	1.220631	1.620024
1	1.537164	0.806302	1.557258
1	2.817026	-1.123820	-0.218906
8	3.662759	-0.627426	-0.346968
1	3.362529	0.126209	-0.882614
1	-2.817025	-1.123819	-0.218911
8	-3.662757	-0.627423	-0.346975
1	-3.362525	0.126214	-0.882617
1	-1.365810	1.100576	-1.353629
8	-2.154363	1.689827	-1.286003
1	-2.206829	1.846888	-0.329004
1	-1.537168	0.806298	1.557259
8	-2.431115	1.220625	1.620026
1	-3.000128	0.553594	1.202724
1	1.365813	1.100574	-1.353632
8	2.154366	1.689826	-1.286008
1	2.206831	1.846889	-0.329010



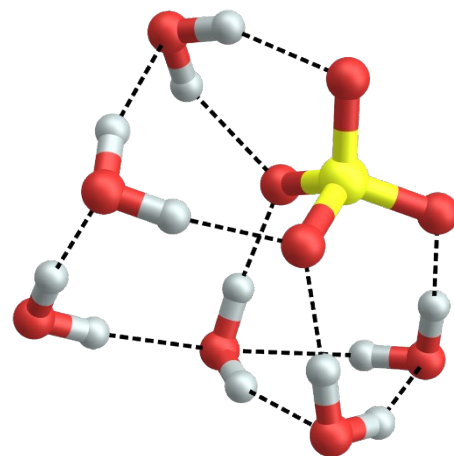
6.6.6-3

atom	x	y	z
8	-0.549372	-0.100042	-1.223571
16	-0.819727	-0.984952	-0.030731
8	-2.249968	-1.353228	-0.014008
8	-0.492331	-0.195510	1.208675
8	0.045086	-2.184672	-0.101890
1	1.007857	2.586961	-0.111544
8	1.975419	2.527264	-0.216037
1	2.087823	1.773751	-0.837946
1	2.146362	1.248877	1.299516
8	2.040638	0.505061	1.917496
1	1.121762	0.194562	1.722829
1	-0.863322	1.607181	-0.677965
8	-0.930868	2.273343	0.044755
1	-0.831278	1.637175	0.782843
1	1.787653	-1.956093	0.079176
8	2.731269	-1.683561	0.185808
1	2.665869	-0.982258	0.860783
1	2.472090	-0.427656	-1.254123
8	2.079556	0.245870	-1.841653
1	1.111439	0.087086	-1.709448
1	-3.054152	1.612461	0.065566
8	-3.799046	0.996694	0.069283
1	-3.339522	0.127434	0.041131



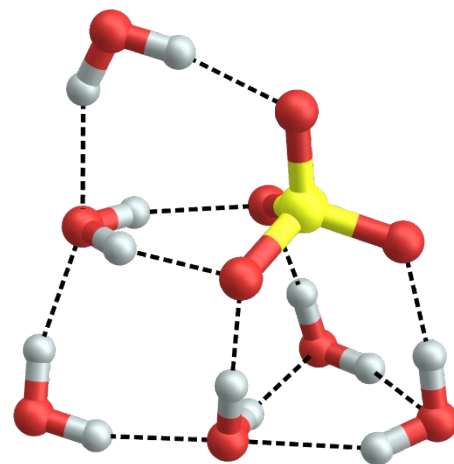
6.6.6-4

atom	x	y	z
8	0.729600	-2.411081	0.279399
16	-0.201084	-1.269976	0.133317
8	-1.606488	-1.734893	0.034762
8	0.156394	-0.490865	-1.103115
8	-0.063196	-0.350359	1.315168
1	-2.629494	0.787522	-1.295662
8	-3.276522	0.185372	-0.902857
1	-2.711244	-0.575947	-0.610589
1	2.133885	-0.728626	-1.363153
8	2.887734	-1.211707	-0.978344
1	2.361730	-1.846639	-0.446480
1	-0.385929	1.135042	-1.114781
8	-0.776392	2.046594	-1.071916
1	-1.142030	2.082021	-0.170998
1	0.968554	2.902704	-0.653637
8	1.843433	3.175795	-0.327016
1	2.126384	2.402686	0.199035
1	-1.378446	0.801876	1.541306
8	-2.107203	1.466748	1.486631
1	-2.730566	1.042249	0.875608
1	1.577633	0.443905	1.306796
8	2.488442	0.786607	1.157451
1	2.820457	0.175127	0.478187



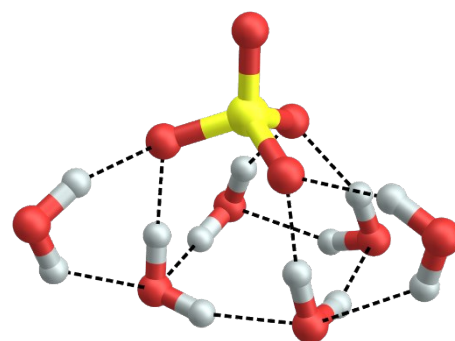
6.6.6-5

atom	x	y	z
8	-0.322977	-0.493379	1.233773
16	-0.443401	-1.159530	-0.110147
8	-0.292052	-0.083537	-1.158545
8	-1.766645	-1.797520	-0.239664
8	0.640883	-2.158638	-0.270922
1	1.320658	-0.138414	1.704307
8	2.273807	0.104754	1.819295
1	2.726677	-0.524772	1.236127
1	-3.426859	0.713004	0.190012
8	-3.963635	-0.085777	0.084926
1	-3.264688	-0.766356	-0.032544
1	-1.277301	1.241024	0.979686
8	-1.646451	1.830832	0.293715
1	-1.312333	1.331605	-0.484064
1	-0.396608	3.315404	-0.007520
8	0.370524	3.845346	-0.288299
1	1.018747	3.148526	-0.499444
1	3.004819	-0.425722	-0.943882
8	3.179058	-1.321553	-0.621352
1	2.262942	-1.695592	-0.543263
1	1.126146	0.901737	-0.957454
8	1.931318	1.438960	-0.737802
1	2.081568	1.216131	0.199391



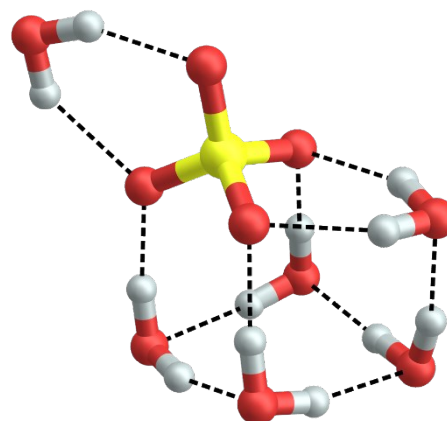
atom	x	y	z
8	-2.995869	-1.916503	1.307950
8	-0.505143	-1.313641	0.290159
16	0.241070	-0.898954	-0.946255
8	0.379604	-2.021210	-1.871144
8	-0.498097	0.242253	-1.585487
8	1.588194	-0.384245	-0.519787
8	1.456655	1.583779	1.324730
8	-1.248780	0.666453	1.972981
8	-2.244355	1.974187	-0.387049
8	3.410234	-0.841871	1.532035
8	0.419283	2.839284	-1.085705
1	-2.179323	-1.904199	0.763810
1	-2.889982	-1.091498	1.796126
1	-0.908432	-0.086898	1.424059
1	-1.689582	1.216587	1.299166
1	-1.850158	1.179109	-0.815648
1	-1.509863	2.597531	-0.516403
1	0.241269	1.932448	-1.423068
1	0.861881	2.645027	-0.240935
1	1.527113	0.877886	0.628224
1	0.591382	1.388656	1.726879
1	2.822180	-0.959967	0.756233
1	3.032579	-0.039295	1.912182

6.6.6-6 (6-VII)



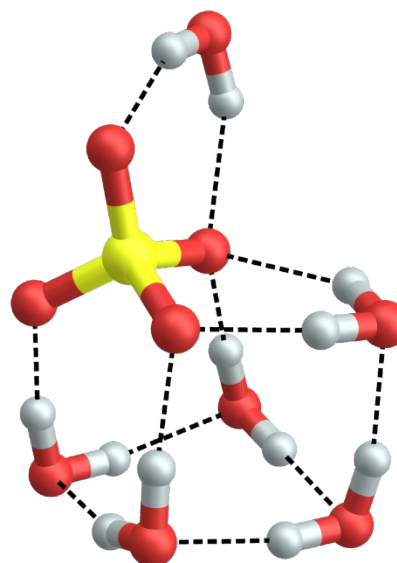
atom	x	y	z
8	0.206368	-0.858687	-1.184662
16	1.030688	-0.495817	0.019516
8	2.246457	-1.330738	0.067732
8	0.197163	-0.727495	1.245278
8	1.398664	0.949296	-0.061494
1	-2.985671	-1.121045	-0.140525
8	-3.507843	-0.303400	-0.267819
1	-2.952708	0.211212	-0.894016
1	-2.577400	0.531197	1.256991
8	-1.932928	0.879729	1.898246
1	-1.128100	0.335860	1.721351
1	-1.090610	-2.086384	-0.649602
8	-1.663952	-2.452857	0.058150
1	-1.172825	-2.060033	0.805152
1	0.165140	2.188580	0.085457
8	-0.631070	2.767210	0.167709
1	-1.152691	2.293056	0.842080
1	-1.375964	1.771934	-1.295107
8	-1.651381	1.047204	-1.888763
1	-0.951149	0.370358	-1.725061
1	3.466017	1.150496	-0.088121
8	4.269407	0.605721	-0.062243
1	3.817881	-0.260027	-0.007937

6.7.5-1 (=6.7.5-2) (6-VI)



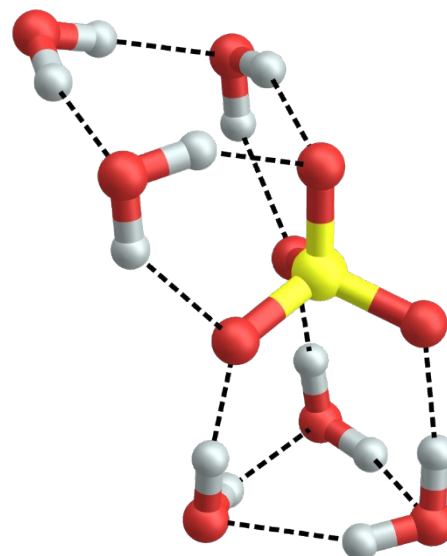
atom	x	y	z
8	0.142782	0.030808	-1.570810
16	1.038294	-0.513948	-0.490284
8	2.442775	-0.488709	-0.944032
8	0.611724	-1.890715	-0.150485
8	0.890126	0.374286	0.724280
1	-2.037508	2.144712	-0.184515
8	-2.888201	1.729006	0.063649
1	-2.871006	0.885561	-0.439051
1	-1.813548	-1.437810	1.573003
8	-1.822607	-2.241959	1.021068
1	-0.922329	-2.213629	0.613567
1	-0.171803	1.782690	-1.252341
8	-0.271245	2.568720	-0.666790
1	0.203887	2.198240	0.097054
1	-0.574942	0.324420	1.725005
8	-1.439512	0.352627	2.199603
1	-2.009885	0.856335	1.591914
1	-2.425475	-1.320889	-0.551210
8	-2.500204	-0.700719	-1.301854
1	-1.554363	-0.485230	-1.485612
1	2.806894	0.874040	1.450428
8	3.733236	0.803032	1.171801
1	3.566387	0.323708	0.334870

6.7.5-3 (=6.7.5-4) (6-V)



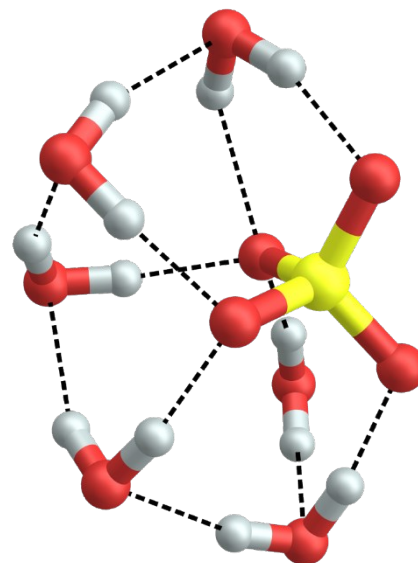
atom	x	y	z
8	-0.175639	-1.222425	0.151952
16	-0.095937	-0.000618	-0.710011
8	-0.169271	1.215549	0.160432
8	-1.213438	0.006556	-1.680809
8	1.213212	-0.001815	-1.434654
1	-1.539218	-1.312724	1.269220
8	-2.352360	-1.243663	1.826147
1	-2.439330	-0.282967	1.938604
1	-1.742708	1.574519	0.876362
8	-2.659917	1.640505	1.237310
1	-3.182992	1.197088	0.549568
1	-2.844446	-0.258857	-1.104932
8	-3.709670	-0.389762	-0.644408
1	-3.443963	-0.905472	0.134946
1	2.323330	1.339836	-0.728791
8	2.529211	1.996273	-0.031652
1	1.641745	2.009475	0.371004
1	3.674684	-0.760595	0.936072
8	4.192954	-0.001141	1.260846
1	3.675738	0.758090	0.933812
1	1.638665	-2.012441	0.373667
8	2.526454	-1.999203	-0.028115
1	2.321213	-1.343055	-0.725753

6.7.5-5 (=6.7.5-6)



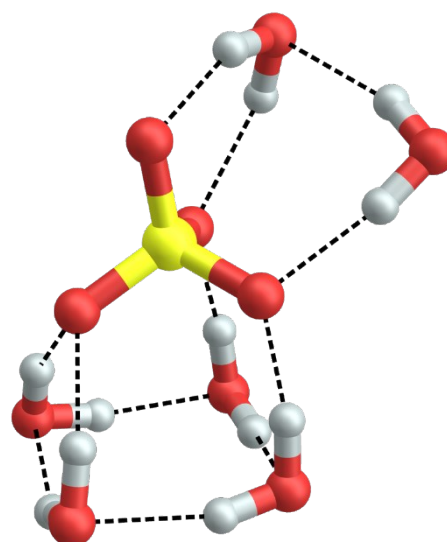
6.7.5-7

atom	x	y	z
8	-1.333643	-1.896949	-0.616569
16	-0.178394	-0.973048	-0.504833
8	1.084982	-1.648755	-0.858693
8	-0.103980	-0.454614	0.910360
8	-0.396664	0.201849	-1.418203
1	-2.968694	0.885884	0.020859
8	-2.635994	1.578794	-0.575290
1	-1.873288	1.121251	-1.002521
1	-2.180360	-0.454297	1.613396
8	-3.005115	-0.747591	1.197025
1	-2.601924	-1.289433	0.475820
1	0.972510	2.476206	-0.187545
8	1.408739	2.229498	-1.020882
1	0.818861	1.495568	-1.313453
1	-0.212954	1.320243	1.220651
8	-0.441090	2.276868	1.243499
1	-1.231124	2.290412	0.676131
1	2.921073	-0.308791	1.416827
8	2.444331	-0.524302	2.236089
1	1.531341	-0.603381	1.899482
1	2.791220	0.873897	-0.646943
8	3.269286	0.034047	-0.523282
1	2.560840	-0.629549	-0.687817



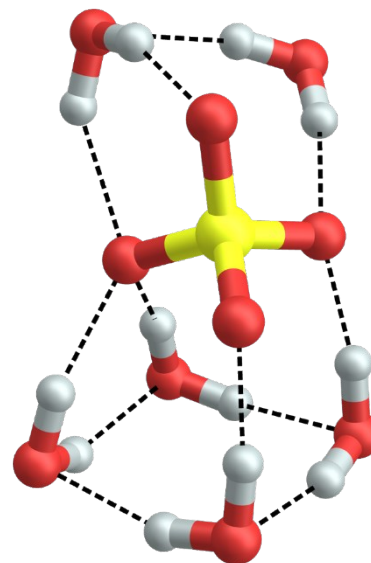
atom	x	y	z
8	0.554625	0.939950	-0.834556
16	0.506413	-0.522893	-0.517317
8	1.640593	-1.217848	-1.164124
8	-0.792105	-1.081982	-1.003458
8	0.591403	-0.701022	0.968315
1	-2.245046	-0.098293	-1.511500
8	-3.156135	0.257643	-1.405464
1	-3.418601	-0.229635	-0.605727
1	-2.082085	-1.548261	0.297323
8	-2.847463	-1.451961	0.902158
1	-2.504462	-0.784086	1.528779
1	-1.589708	1.289974	1.654121
8	-1.434586	0.580381	2.305749
1	-0.646720	0.124473	1.922096
1	2.601610	-0.792017	1.366140
8	3.447465	-0.908307	0.898758
1	3.067680	-1.128214	0.020268
1	-0.806110	1.918382	-0.271586
8	-1.662579	2.321659	0.011190
1	-2.305630	1.779049	-0.476988
1	2.265127	1.686626	-0.414150
8	3.172950	1.898232	-0.116852
1	3.447999	1.054329	0.274574

6.7.5-8



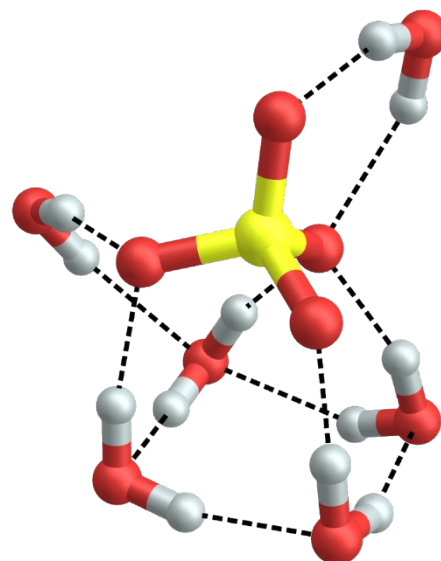
6.7.5-9

atom	x	y	z
8	0.562363	0.301527	-1.329471
16	0.482896	-0.850650	-0.376721
8	0.223698	-0.294684	1.004411
8	1.767233	-1.587893	-0.366352
8	-0.630405	-1.749379	-0.763604
1	-0.478549	1.476976	1.067633
8	-1.143017	2.196508	1.092483
1	-1.477395	2.175610	0.174716
1	3.214081	1.218543	-0.008920
8	3.008248	1.723610	-0.810632
1	2.168572	1.307948	-1.092552
1	-3.108174	-0.615082	0.385110
8	-3.167613	-0.828540	-0.562304
1	-2.273473	-1.222715	-0.722196
1	-0.989751	1.145719	-1.602653
8	-1.885914	1.558578	-1.589287
1	-2.455263	0.811795	-1.325333
1	2.217819	0.091023	1.790450
8	3.113604	-0.168741	1.525316
1	2.856587	-0.802773	0.814793
1	-2.198166	0.767227	1.951413
8	-2.316900	-0.179775	2.146326
1	-1.453003	-0.513556	1.819984



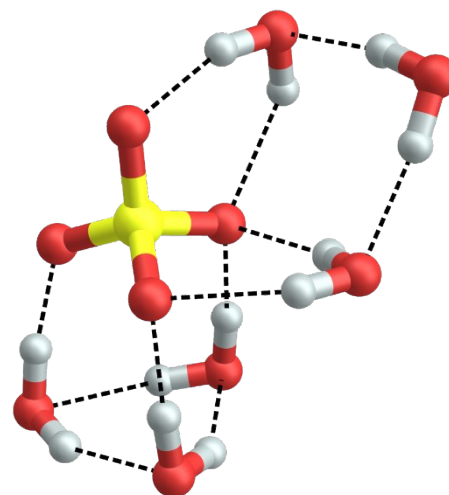
atom	x	y	z
8	-0.656662	-0.308272	0.724243
16	-0.838116	-0.204998	-0.777237
8	-0.147365	1.041033	-1.237742
8	-2.277411	-0.141397	-1.091443
8	-0.206068	-1.384434	-1.418535
1	1.647316	0.947401	-1.120988
8	2.587301	0.804780	-0.860796
1	2.652258	-0.168690	-0.835223
1	-3.343451	-0.470889	0.408258
8	-3.512634	-0.636686	1.358567
1	-2.591788	-0.590452	1.654944
1	1.398018	-1.859799	-1.018720
8	2.302332	-2.054336	-0.661498
1	2.131573	-2.077710	0.295429
1	0.606512	0.805901	1.406654
8	1.443828	1.226050	1.711057
1	1.995365	1.165120	0.904979
1	-0.221777	2.681298	-0.356071
8	-0.005895	3.434376	0.232519
1	0.516488	2.986088	0.912342
1	0.480742	-1.444492	1.538453
8	1.282422	-1.713012	2.046144
1	1.659820	-0.838617	2.225611

6.7.5-10



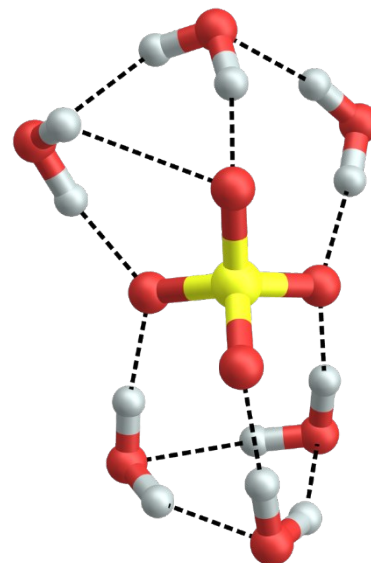
atom	x	y	z
8	0.285126	-0.114300	0.849766
16	-0.083920	-0.846317	-0.427068
8	-0.387397	0.181973	-1.471782
8	-1.276275	-1.687044	-0.175707
8	1.063158	-1.677235	-0.854066
1	3.908139	0.272481	0.373846
8	4.204565	1.138342	0.035585
1	3.360643	1.546222	-0.233233
1	-1.727956	1.280915	-1.124619
8	-2.463248	1.853123	-0.795151
1	-2.261588	1.908273	0.152678
1	2.442383	-1.550951	0.259179
8	2.939542	-1.252961	1.057542
1	2.210869	-0.765136	1.472704
1	-2.879046	-1.066162	0.060616
8	-3.722915	-0.573344	0.212635
1	-3.556176	0.246611	-0.282365
1	1.175345	1.469780	0.282125
8	1.507471	2.070947	-0.415252
1	1.023983	1.675460	-1.159903
1	-1.133101	0.607089	1.680500
8	-1.972016	1.000975	2.016635
1	-2.644874	0.392678	1.669906

6.7.5-11



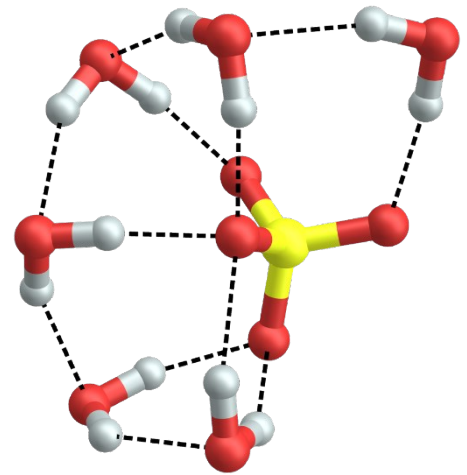
atom	x	y	z
8	0.020571	-0.939615	0.642348
16	0.080299	-0.201725	-0.669034
8	-0.124999	1.253882	-0.404798
8	-0.979749	-0.708531	-1.568823
8	1.418052	-0.423197	-1.281102
1	-3.405828	0.645790	-0.419943
8	-3.572914	-0.174327	-0.914290
1	-2.665867	-0.399328	-1.236924
1	3.468480	-0.409518	0.758672
8	3.651339	0.240878	0.067044
1	2.860549	0.104196	-0.515648
1	-1.584175	-1.113277	1.378865
8	-2.520320	-1.106095	1.691244
1	-3.015835	-1.047104	0.857967
1	1.308618	2.297598	0.253805
8	2.132241	2.727861	0.560077
1	2.770428	1.999663	0.503703
1	1.453938	-1.842701	1.014091
8	2.328108	-2.309081	0.988936
1	2.509273	-2.244210	0.044324
1	-2.483031	0.943640	1.497103
8	-2.463788	1.764636	0.978910
1	-1.609662	1.681559	0.492151

6.7.5-12



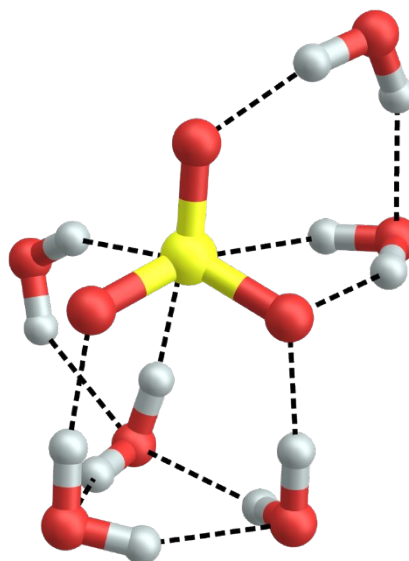
6.7.5-13

atom	x	y	z
8	-1.313751	-1.331961	-0.846577
16	0.069129	-0.838461	-0.534366
8	0.006526	-0.127935	0.807616
8	0.492314	0.128726	-1.571165
8	1.002397	-1.973428	-0.438564
1	2.770468	-1.560271	0.061695
8	3.629878	-1.227759	0.392596
1	3.395975	-0.331524	0.684306
1	2.145351	1.899466	0.572594
8	2.352901	1.288169	1.300679
1	1.566896	0.700031	1.270021
1	0.241756	2.836186	-0.410684
8	1.061171	2.708832	-0.917741
1	0.933437	1.784969	-1.242947
1	-2.218715	-1.645632	0.771499
8	-2.472248	-1.345443	1.669659
1	-1.673209	-0.822847	1.851392
1	-0.809913	1.450702	0.812029
8	-1.339277	2.274557	0.694821
1	-2.084661	1.938749	0.171070
1	-2.597276	-0.053932	-0.874488
8	-3.341043	0.493475	-0.526594
1	-3.407109	0.121619	0.365536



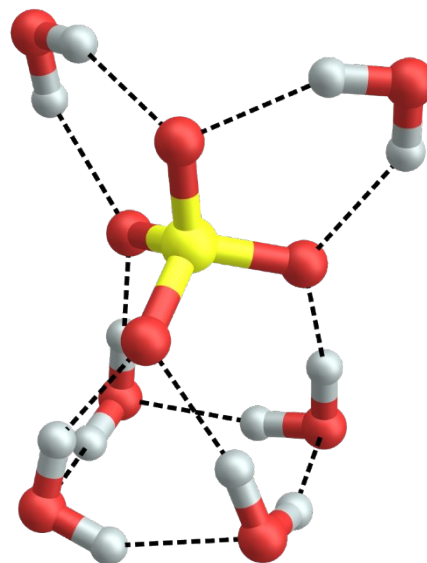
atom	x	y	z
8	0.677370	-0.071698	-1.778847
16	-0.461103	-0.114742	-0.833332
8	-1.731156	0.166922	-1.522473
8	-0.238503	0.912722	0.258948
8	-0.521911	-1.458372	-0.162794
1	2.271797	-0.584299	-1.357419
8	3.129210	-0.893222	-0.969704
1	2.824975	-1.566231	-0.338213
1	-1.464070	0.291864	1.751804
8	-1.948892	-0.485693	2.082050
1	-1.589196	-1.139176	1.451376
1	-3.560623	-0.146375	0.882653
8	-4.057821	0.030149	0.068320
1	-3.325082	0.096617	-0.579980
1	1.363703	0.793787	0.978585
8	2.304835	0.772881	1.281670
1	2.763340	0.396187	0.509836
1	0.878027	-2.007695	0.707497
8	1.706646	-2.202151	1.215655
1	1.908025	-1.340477	1.608497
1	0.431427	2.706535	0.142927
8	1.066076	3.410972	0.382215
1	1.788498	2.875059	0.735411

6.7.5-14



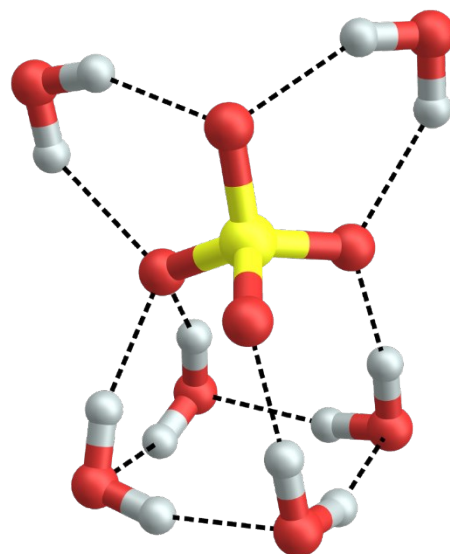
atom	x	y	z
8	-0.285024	-0.014860	-1.360675
16	0.697147	-0.003564	-0.234134
8	0.485781	1.230169	0.581262
8	2.084481	-0.019543	-0.768128
8	0.474598	-1.210915	0.618708
1	-3.058602	-0.355641	-1.276252
8	-2.743618	-1.273614	-1.344970
1	-1.777220	-1.102026	-1.400288
1	-1.074847	1.356186	1.415209
8	-2.002705	1.316772	1.749200
1	-2.160639	0.354710	1.790141
1	2.120014	2.427314	0.514698
8	3.024242	2.492923	0.163278
1	3.033241	1.631894	-0.293273
1	-2.550993	1.621301	-0.058723
8	-2.596089	1.584616	-1.034050
1	-1.710297	1.224595	-1.250869
1	-1.137416	-1.478364	1.262699
8	-2.099324	-1.558840	1.474263
1	-2.490414	-1.576768	0.583147
1	3.001243	-1.683420	-0.277188
8	2.978981	-2.536460	0.193818
1	2.080978	-2.444746	0.555197

6.8.4-1 (=6.8.4-2) (6-III)



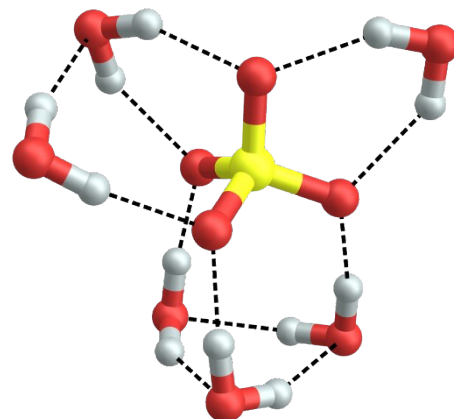
atom	x	y	z
8	-0.034269	-0.277575	-1.723980
16	-0.710272	-0.074979	-0.422114
8	-2.155692	0.212701	-0.623164
8	-0.068747	1.090348	0.288162
8	-0.558727	-1.294298	0.429786
1	1.641630	-0.805094	-1.693561
8	2.591839	-1.014095	-1.519474
1	2.547402	-1.422606	-0.634655
1	1.128747	0.835424	1.703469
8	2.028154	0.832098	2.096812
1	2.530141	1.180182	1.338970
1	-2.609345	1.991279	-0.048569
8	-2.368203	2.848664	0.351216
1	-1.437009	2.638615	0.526115
1	2.167725	-1.069307	1.611017
8	1.999344	-1.916969	1.163264
1	1.056358	-1.805553	0.889661
1	2.754828	0.810692	-0.984135
8	2.571359	1.686100	-0.590106
1	1.601924	1.637216	-0.457144
1	-3.263303	-1.243217	0.101263
8	-3.305573	-2.088444	0.584402
1	-2.350621	-2.176194	0.746051

6.8.4-3 (=6.8.4-4)



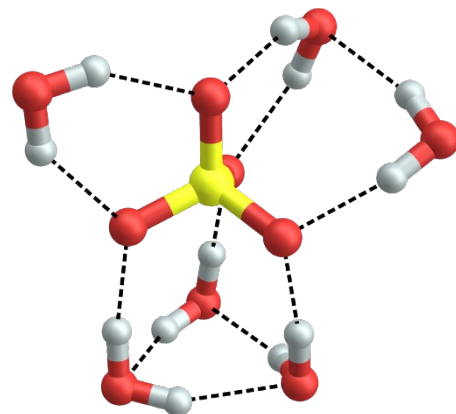
atom	x	y	z
8	0.157307	-0.354154	1.215535
16	0.369212	0.377614	-0.072398
8	0.065499	-0.541084	-1.209528
8	1.788393	0.822358	-0.152110
8	-0.534476	1.561554	-0.132935
1	-2.249315	1.352079	0.242876
8	-3.178054	1.084513	0.440425
1	-3.046007	0.306973	1.008762
1	0.540755	3.285291	-0.249349
8	1.446066	3.636039	-0.294328
1	1.906140	2.777462	-0.261480
1	-2.971612	-0.308646	-1.055244
8	-2.623848	-1.123876	-1.451900
1	-1.651428	-0.959003	-1.452498
1	2.393934	-2.401091	-0.346543
8	1.979283	-2.695496	-1.172554
1	1.288974	-2.014287	-1.296721
1	-1.400720	-1.149586	1.450683
8	-2.314015	-1.525219	1.459639
1	-2.466374	-1.706250	0.517680
1	1.905506	-1.280197	1.596811
8	2.841839	-1.295588	1.327815
1	2.818814	-0.496941	0.762920

6.8.4-5 (=6.8.4-7)



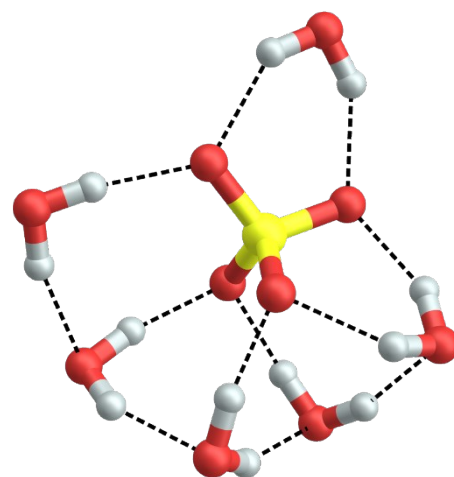
atom	x	y	z
8	-0.071806	-0.542853	-1.218522
16	-0.360427	0.372232	-0.074258
8	-1.772239	0.841035	-0.151563
8	0.561366	1.542551	-0.123325
8	-0.161283	-0.373298	1.207488
1	-1.858593	2.798107	-0.254211
8	-1.384576	3.649165	-0.284273
1	-0.485131	3.283424	-0.241023
1	3.156615	0.139908	-0.773453
8	3.244543	0.987139	-0.304378
1	2.305198	1.283603	-0.250920
1	2.869429	-0.187496	1.339050
8	2.460656	-0.934425	1.806087
1	1.497666	-0.759651	1.676122
1	1.517330	-1.353039	-1.188852
8	2.423934	-1.715450	-1.047166
1	2.472403	-1.769111	-0.078820
1	-1.360007	-1.976251	-1.313523
8	-2.071690	-2.634307	-1.188386
1	-2.467300	-2.335083	-0.354740
1	-2.824587	-0.442797	0.772876
8	-2.869408	-1.242314	1.335823
1	-1.932182	-1.255272	1.601349

6.8.4-6 (=6.8.4-8)



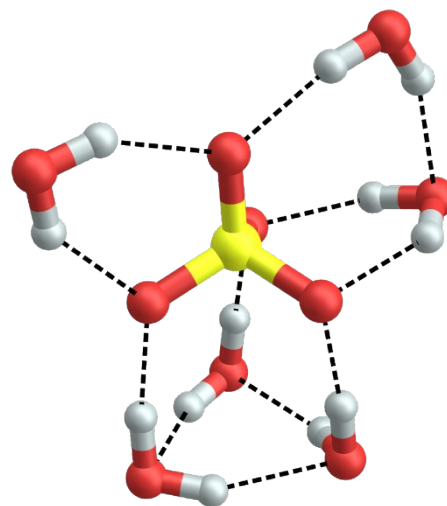
6.8.4-9

atom	x	y	z
8	-1.478646	-1.281913	0.339900
16	-0.660480	-0.073136	0.020905
8	-1.542176	1.097705	-0.195728
8	0.149189	-0.347462	-1.207477
8	0.272693	0.196719	1.162468
1	-0.449457	-2.768573	-0.196806
8	0.305528	-3.131220	-0.706456
1	0.493985	-2.326236	-1.222344
1	-3.502643	0.573750	0.010193
8	-4.085479	-0.180442	0.200840
1	-3.381612	-0.844772	0.319022
1	2.918122	-0.680620	-0.297292
8	2.872807	-0.064801	-1.048676
1	1.902125	-0.064166	-1.221089
1	1.522970	-1.110928	1.315684
8	2.169231	-1.842884	1.187017
1	1.663922	-2.451302	0.620910
1	2.593040	1.601831	0.036012
8	2.154583	2.160601	0.700223
1	1.433679	1.556369	0.988874
1	0.710220	3.269840	-0.132002
8	-0.147815	3.597004	-0.449573
1	-0.696009	2.788516	-0.415957



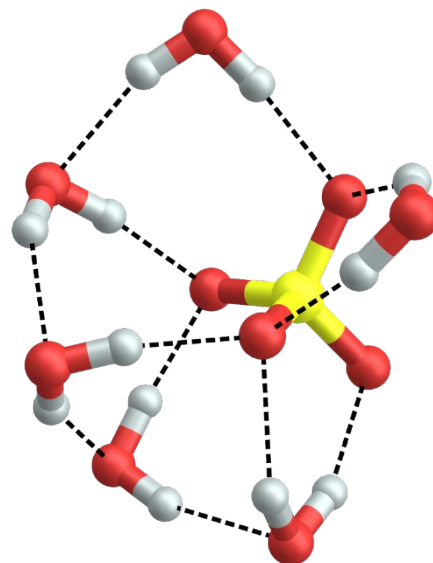
atom	x	y	z
8	-0.133506	-0.486597	1.200312
16	-0.393527	0.357250	-0.010701
8	0.487740	1.559646	0.022552
8	-1.815317	0.783081	-0.029466
8	-0.092228	-0.459853	-1.227090
1	-0.827465	-2.228672	0.722732
8	-1.131162	-2.843782	0.025770
1	-0.842437	-2.320768	-0.742200
1	-3.143934	-0.543446	-0.023256
8	-3.683000	-1.360625	-0.016266
1	-2.986582	-2.036533	0.006258
1	-0.607096	3.255415	0.027898
8	-1.511185	3.613193	0.019067
1	-1.976079	2.757673	-0.000679
1	1.549210	-1.108291	-1.359685
8	2.477209	-1.439658	-1.293854
1	2.567954	-1.590631	-0.338826
1	1.582513	-0.800723	1.556864
8	2.557732	-0.934405	1.625203
1	2.907677	-0.124343	1.219690
1	3.131599	0.414940	-0.856480
8	3.182841	1.215424	-0.307256
1	2.228098	1.437971	-0.192869

6.8.4-10



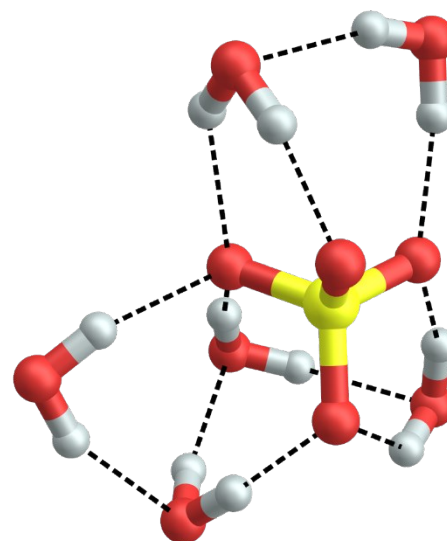
atom	x	y	z
8	-0.251992	-0.637636	0.833802
16	0.093853	-0.671979	-0.637468
8	-0.108437	0.702747	-1.199131
8	-0.815093	-1.620876	-1.319652
8	1.510402	-1.077800	-0.795982
1	2.005009	-2.275929	0.827295
8	1.701329	-2.541199	1.710686
1	0.911341	-1.973515	1.747145
1	-1.607556	1.949069	1.237388
8	-0.917309	1.809934	1.908046
1	-0.568954	0.932066	1.628909
1	0.757499	2.094548	-0.525511
8	1.125817	2.807875	0.044830
1	0.591083	2.679125	0.845653
1	-2.430884	-1.520657	-0.446899
8	-2.999958	-1.262851	0.313159
1	-2.281213	-1.053382	0.933280
1	-2.982903	0.674231	-0.214382
8	-2.653801	1.555746	-0.461571
1	-1.770683	1.336673	-0.837546
1	2.843223	0.251329	-0.507173
8	3.437088	1.007757	-0.333113
1	2.808012	1.708546	-0.097256

6.8.4-11



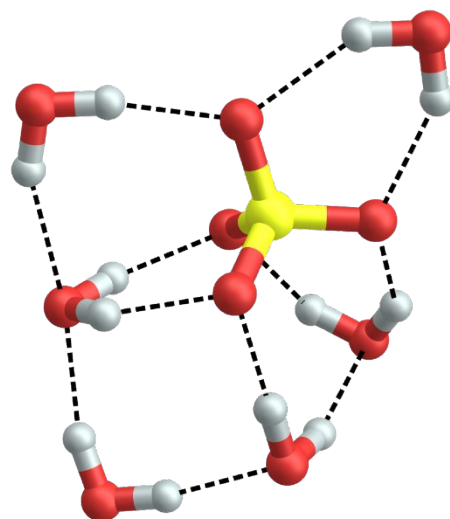
6.8.4-12

atom	x	y	z
8	-1.346792	0.668682	-1.529966
16	-0.387133	-0.074580	-0.688403
8	-0.978485	-1.384194	-0.264299
8	-0.083817	0.728599	0.550774
8	0.882228	-0.337472	-1.423113
1	2.468809	0.239503	-0.822246
8	3.286206	0.434440	-0.309627
1	3.047637	0.061382	0.557786
1	1.025801	2.287507	0.433849
8	1.810904	2.868302	0.414538
1	2.495438	2.231778	0.151616
1	1.735026	-1.581079	1.447245
8	1.876631	-0.750485	1.933789
1	1.152063	-0.183397	1.587530
1	-3.510107	-0.067331	0.872136
8	-3.551894	-1.036028	0.912930
1	-2.690286	-1.277822	0.515726
1	0.351887	-2.538409	0.005174
8	1.280926	-2.871407	-0.011445
1	1.634451	-2.237076	-0.653469
1	-2.501743	1.516454	-0.372246
8	-2.805674	1.814792	0.513629
1	-1.976701	1.659942	0.993663



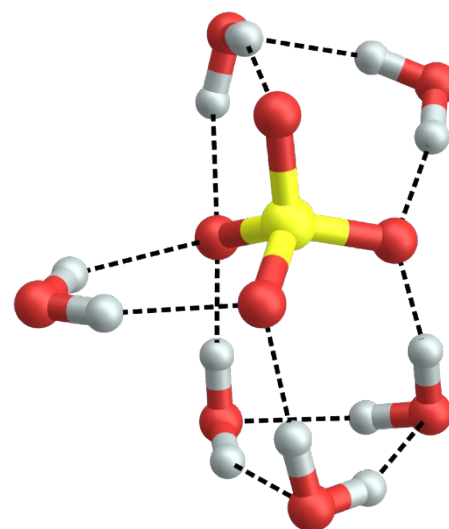
atom	x	y	z
8	0.173708	0.164900	-1.191936
16	-0.777109	-0.096379	-0.064474
8	-1.321908	-1.479723	-0.178722
8	-1.883103	0.894810	-0.104031
8	-0.022867	0.032084	1.225497
1	-1.315911	2.665716	0.122126
8	-0.862997	3.526330	0.243577
1	0.062640	3.249762	0.307816
1	-0.046570	-2.620397	0.710871
8	0.746521	-2.668718	1.280863
1	0.738366	-1.736079	1.571623
1	1.534906	-1.034570	-1.200923
8	2.261171	-1.677271	-1.028268
1	1.919870	-2.151907	-0.250560
1	1.254127	1.366481	0.928215
8	1.732582	1.946717	0.296542
1	1.364569	1.555026	-0.520394
1	-3.288266	-1.438890	-0.316426
8	-4.099580	-0.900395	-0.348417
1	-3.665598	-0.032937	-0.274940
1	3.448742	0.963623	0.080913
8	4.130971	0.311509	-0.154066
1	3.590872	-0.445713	-0.455052

6.8.4-13



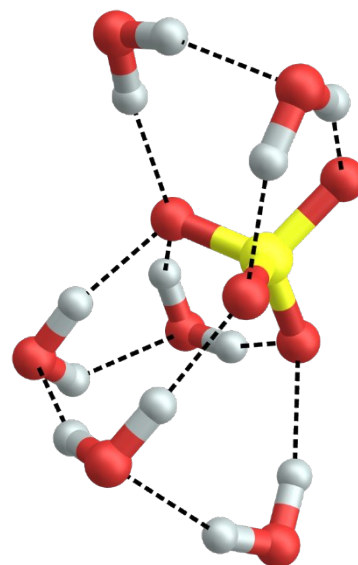
6.8.4-14

atom	x	y	z
8	-0.427239	-1.121759	-0.875198
16	-0.361666	0.348776	-0.625210
8	-0.290642	0.587328	0.862978
8	-1.566418	1.011246	-1.165184
8	0.870466	0.908686	-1.256130
1	0.801625	-2.219266	-0.230433
8	1.549955	-2.697332	0.199364
1	1.672528	-2.174156	1.009450
1	-3.229195	-1.207950	0.479631
8	-2.993812	-2.062214	0.084249
1	-2.116475	-1.863674	-0.297439
1	2.603756	-0.249515	1.266017
8	2.001316	-0.448968	2.000340
1	1.148819	-0.072794	1.675788
1	1.251446	2.585544	-0.306590
8	1.182672	3.146435	0.487913
1	0.626295	2.557934	1.019582
1	2.420611	0.062397	-0.983117
8	3.204629	-0.479545	-0.733781
1	2.809814	-1.358366	-0.602609
1	-2.860014	0.954338	0.152960
8	-3.163314	0.750526	1.064767
1	-2.283446	0.649889	1.465582



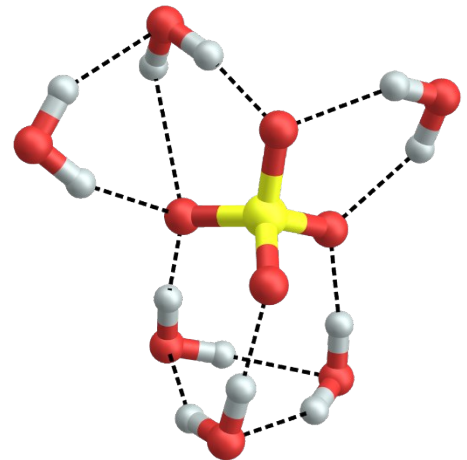
atom	x	y	z
8	-0.913243	-0.177130	-1.412458
16	0.389370	-0.131441	-0.685003
8	0.469290	-1.266239	0.281238
8	0.457097	1.163766	0.085695
8	1.520159	-0.198461	-1.634314
1	-0.814399	1.340107	1.314725
8	-1.683391	1.486749	1.760868
1	-2.231757	1.704548	0.993981
1	-0.880212	-1.456060	1.443544
8	-1.677514	-1.415416	2.020703
1	-1.830842	-0.455824	2.071512
1	2.947668	-0.938730	-0.709349
8	3.337530	-1.369346	0.082402
1	2.499417	-1.607932	0.514485
1	-2.337962	-1.327480	-0.945272
8	-3.056135	-1.833658	-0.518128
1	-2.764861	-1.815049	0.409493
1	3.363958	0.490530	0.945141
8	3.093782	1.378958	1.226704
1	2.184021	1.425055	0.871216
1	-1.793793	1.392118	-1.355900
8	-1.979673	2.330799	-1.122947
1	-1.114380	2.551589	-0.751627

6.8.4-15



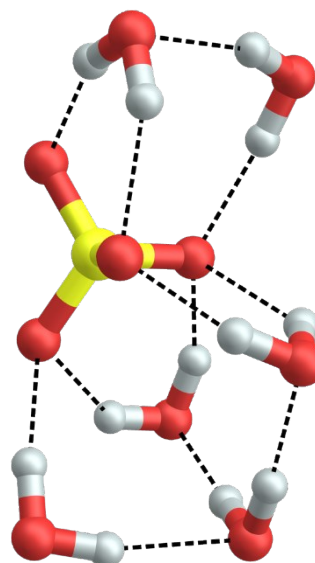
6.8.4-16

atom	x	y	z
8	0.384030	1.385578	-0.472671
16	-0.255795	0.328743	0.368953
8	-1.654434	0.740690	0.694130
8	0.520562	0.127545	1.611285
8	-0.301201	-0.950345	-0.416736
1	3.279557	0.606403	-0.033400
8	3.086296	1.117785	-0.836731
1	2.122739	1.307633	-0.731869
1	2.524507	-0.706050	-1.564061
8	2.161119	-1.604776	-1.501204
1	1.245930	-1.439142	-1.174770
1	-1.291339	-2.444273	0.215262
8	-2.056543	-3.042859	0.333874
1	-2.780447	-2.433224	0.130714
1	-1.917296	2.701365	0.256231
8	-1.517113	3.481464	-0.163837
1	-0.685366	3.054770	-0.436856
1	-2.653420	-0.965192	-1.429853
8	-3.370348	-0.662865	-0.860617
1	-2.853391	-0.093727	-0.235080
1	2.127579	-0.573335	1.480660
8	3.015809	-0.945972	1.259032
1	2.828244	-1.445064	0.447568



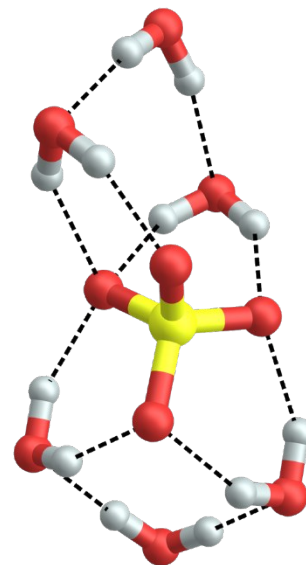
atom	x	y	z
8	1.702627	-1.470716	0.718237
16	0.513754	-0.743859	0.221981
8	0.421441	0.600697	0.911042
8	-0.728604	-1.510075	0.502449
8	0.646803	-0.501051	-1.248904
1	-2.951163	1.142453	0.471064
8	-3.252506	1.412231	-0.419371
1	-2.410978	1.596492	-0.884594
1	-0.286161	1.967875	-0.560695
8	-0.648051	1.887112	-1.457554
1	-0.281927	0.994290	-1.655950
1	-2.258706	-1.598337	-0.581555
8	-3.152843	-1.508023	-0.967374
1	-3.311592	-0.552383	-0.904521
1	2.686308	-0.263029	-1.536641
8	3.521522	-0.428231	-1.066060
1	3.135907	-0.923614	-0.310169
1	-2.008346	-0.454017	1.656701
8	-2.086331	0.448445	2.012769
1	-1.174322	0.738964	1.788644
1	3.341739	1.240964	0.125315
8	2.977166	1.882889	0.754943
1	2.089381	1.505858	0.919296

6.8.4-17



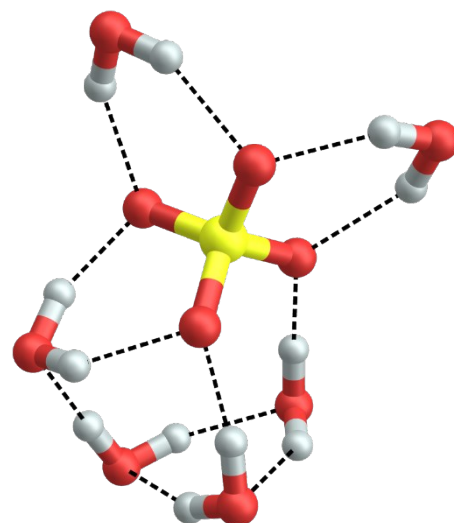
atom	x	y	z
8	0.439849	-0.214467	0.853406
16	0.046202	-0.643403	-0.540447
8	-0.097911	0.574782	-1.391770
8	-1.269677	-1.353881	-0.469704
8	1.082848	-1.541189	-1.091268
1	1.221505	1.571819	0.717261
8	1.511869	2.286902	0.119997
1	1.054720	1.957487	-0.677928
1	2.591946	-1.535117	-0.045655
8	3.067401	-1.308979	0.783649
1	2.308080	-0.902200	1.236241
1	-1.167791	-0.298422	2.049538
8	-2.056589	-0.693529	2.096093
1	-2.025534	-1.135852	1.222100
1	-3.399259	0.586949	1.505497
8	-4.050976	1.124460	1.018897
1	-3.716206	1.079872	0.104255
1	3.962725	0.369433	0.414349
8	4.229761	1.298667	0.284952
1	3.371895	1.740566	0.143722
1	-2.002464	0.981149	-1.654799
8	-2.897078	0.596683	-1.593387
1	-2.614835	-0.276839	-1.254347

6.8.4-18



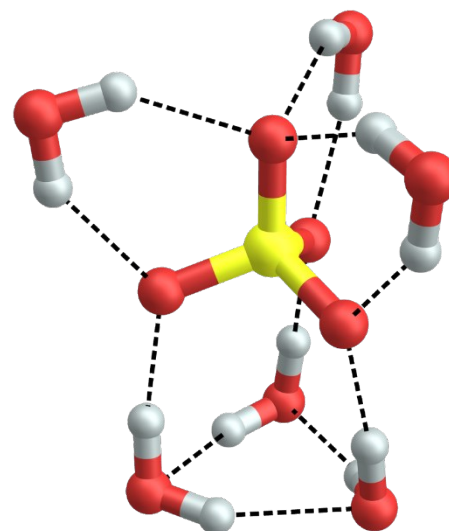
6.8.4-19

atom	x	y	z
8	-0.448633	1.205501	-0.663271
16	-0.768418	-0.016032	0.132669
8	-2.130130	0.116133	0.715800
8	0.240251	-0.176442	1.225650
8	-0.715777	-1.219318	-0.754268
1	0.763139	-2.194451	-0.409299
8	1.549140	-2.419398	0.139458
1	1.343729	-1.808665	0.869858
1	1.182038	1.563006	-1.087767
8	2.141788	1.795813	-1.168642
1	2.403515	1.854337	-0.236743
1	3.057155	0.081058	-1.141405
8	3.563952	-0.686674	-0.814411
1	2.880011	-1.347197	-0.575321
1	1.802109	0.612907	1.505701
8	2.739825	0.911011	1.574507
1	3.203583	0.303231	0.977211
1	-2.450596	-2.213786	-0.697846
8	-3.352838	-2.226927	-0.333199
1	-3.278636	-1.402330	0.180000
1	-1.935759	2.603464	-0.488276
8	-2.811333	2.742435	-0.090801
1	-2.885569	1.867857	0.334590



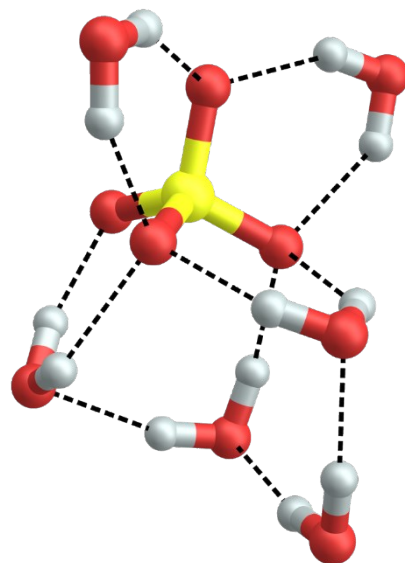
atom	x	y	z
8	1.205859	0.723560	-0.154359
16	0.000000	0.000000	0.342619
8	-1.229551	0.682525	-0.154359
8	0.000000	0.000000	1.837909
8	0.023692	-1.406084	-0.154359
1	-1.586342	0.569551	-1.886858
8	-1.641500	0.454209	-2.865180
1	-1.181743	-0.391410	-2.996474
1	-0.005879	-1.902620	2.546405
8	0.000000	-2.843413	2.303318
1	0.011476	-2.717153	1.338308
1	0.299925	-1.658588	-1.886858
8	0.427394	-1.648685	-2.865180
1	0.929843	-0.827715	-2.996474
1	1.286417	1.089037	-1.886858
8	1.214106	1.194476	-2.865180
1	0.251900	1.219125	-2.996474
1	-2.358861	1.348638	1.338308
8	-2.462468	1.421707	2.303318
1	-1.644778	0.956401	2.546405
1	2.347385	1.368515	1.338308
8	2.462468	1.421707	2.303318
1	1.650657	0.946219	2.546405

6.9.3-1 (6-I)



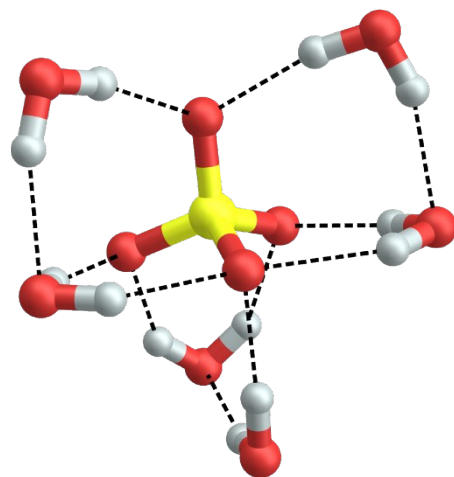
atom	x	y	z
8	-2.220323	0.197729	-0.186878
16	-0.804382	-0.192612	-0.412079
8	0.036528	1.046845	-0.554661
8	-0.675845	-1.023383	-1.631155
8	-0.297796	-0.970447	0.772659
1	-1.195505	2.663882	-0.945567
8	-2.129410	2.929039	-0.936188
1	-2.496660	2.067632	-0.664172
1	0.822632	1.495491	1.286147
8	1.084316	1.045954	2.107588
1	0.659199	0.185420	1.914027
1	0.738588	-2.080085	-1.433154
8	1.519726	-2.476772	-0.978236
1	1.269976	-2.248281	-0.069889
1	2.957999	0.902567	1.672142
8	3.821295	0.846181	1.222156
1	3.550321	0.617630	0.312282
1	2.442322	-0.746142	-1.270243
8	2.631312	0.207725	-1.313084
1	1.748844	0.594681	-1.123464
1	-1.899299	-1.624944	1.862167
8	-2.860635	-1.535278	1.972087
1	-3.001646	-0.886810	1.258682

6.9.3-2



6.9.3-3

atom	x	y	z
8	1.216420	-1.767009	0.008507
16	0.000000	-0.924726	0.000001
8	-1.216420	-1.767008	-0.008502
8	0.005607	-0.040476	-1.216897
8	-0.005607	-0.040471	1.216895
1	3.004947	0.512711	1.200264
8	2.442865	1.158486	1.658370
1	1.548172	0.747973	1.589909
1	1.321748	1.152155	-1.301388
8	2.100174	1.754292	-1.223066
1	2.170062	1.871656	-0.261692
1	-1.321747	1.152161	1.301382
8	-2.100173	1.754298	1.223058
1	-2.170062	1.871657	0.261684
1	-3.004948	0.512704	-1.200262
8	-2.442867	1.158477	-1.658372
1	-1.548174	0.747965	-1.589911
1	2.802072	-1.107939	-0.274348
8	3.639380	-0.599093	-0.408266
1	3.320580	0.171633	-0.907402
1	-2.802071	-1.107937	0.274355
8	-3.639379	-0.599091	0.408274
1	-3.320577	0.171637	0.907405



atom	x	y	z
8	0.862502	0.862502	0.862502
16	0.000000	0.000000	0.000000
8	-0.862502	-0.862502	0.862502
8	0.862502	-0.862502	-0.862502
8	-0.862502	0.862502	-0.862502
1	-0.515434	2.823248	-0.515434
8	0.000000	3.465619	0.000000
1	0.515434	2.823248	0.515434
1	2.823248	-0.515434	-0.515434
8	3.465619	0.000000	0.000000
1	2.823248	0.515434	0.515434
1	0.515434	-2.823248	-0.515434
8	0.000000	-3.465619	0.000000
1	-0.515434	-2.823248	0.515434
1	-2.823248	-0.515434	0.515434
8	-3.465619	0.000000	0.000000
1	-2.823248	0.515434	-0.515434
1	0.515434	0.515434	2.823248
8	0.000000	0.000000	3.465619
1	-0.515434	-0.515434	2.823248
1	0.515434	-0.515434	-2.823248
8	0.000000	0.000000	-3.465619
1	-0.515434	0.515434	-2.823248

6.12.0-1 (6-II)

