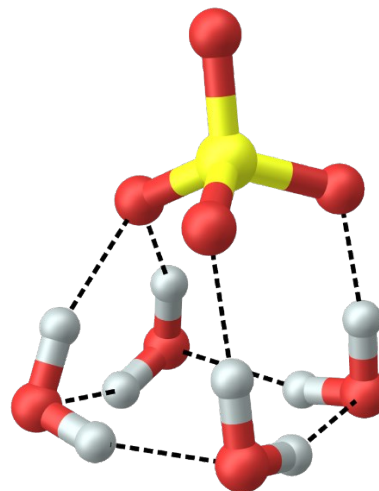


Structures of $\text{SO}_4^{2-}(\text{H}_2\text{O})_4$

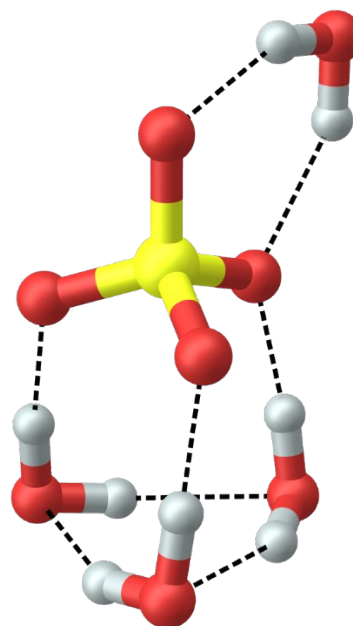
atom	x	y	z
16	-1.361074	-0.061224	-0.039997
8	-1.067887	1.378398	-0.322610
8	-2.768200	-0.373566	-0.330169
8	-1.037535	-0.360394	1.390619
8	-0.454085	-0.902564	-0.913646
8	1.444359	2.116974	0.315964
1	1.623552	1.433292	0.987356
1	0.490709	1.930763	0.093867
8	1.944325	-1.956753	-0.229663
1	2.286415	-1.262633	-0.817120
1	0.976617	-1.763332	-0.322206
8	1.792740	0.378152	-1.946880
1	1.838109	1.073617	-1.262956
1	0.905334	-0.007510	-1.755366
8	1.548702	-0.201135	2.084975
1	0.567159	-0.221540	1.905158
1	1.869934	-0.835962	1.422485

4.4.4-1 (4-V)



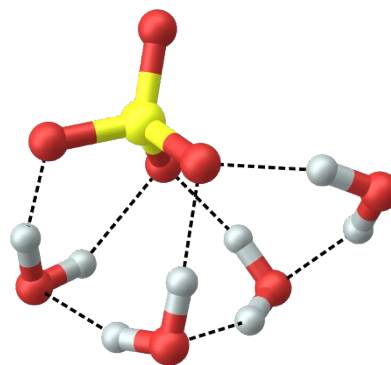
atom	x	y	z
16	-0.666304	-0.581295	0.001275
8	-0.718103	0.925251	-0.001466
8	0.063388	-1.040961	-1.216716
8	-2.049165	-1.117701	0.002861
8	0.064596	-1.037284	1.219896
8	2.722139	-0.576974	-1.214168
1	1.753183	-0.798970	-1.273138
1	2.855821	-0.534688	-0.253448
8	2.450600	0.147500	1.655258
1	2.277571	0.979874	1.186522
1	1.574740	-0.317933	1.566914
8	-3.554525	1.224533	-0.000623
1	-2.636963	1.550840	-0.003389
1	-3.319621	0.273000	0.001663
8	1.681802	2.103864	-0.446424
1	2.102693	1.380205	-0.938107
1	0.767582	1.742569	-0.296363

4.5.3-1 (4-II)



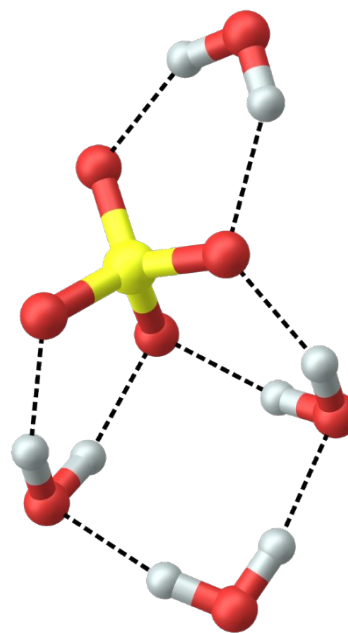
atom	x	y	z
16	0.848834	-0.839682	0.010714
8	2.029944	-0.102467	-0.539694
8	0.382916	-0.122165	1.252010
8	1.191464	-2.234780	0.310512
8	-0.264418	-0.775785	-1.005344
8	-2.914791	-1.304178	-0.283646
1	-1.980007	-1.312921	-0.586781
1	-2.886098	-0.541004	0.315897
8	1.528762	2.374487	0.342387
1	1.883688	1.562056	-0.108690
1	1.008393	1.905801	1.015378
8	-0.867101	1.901063	-1.334811
1	-0.078287	2.242750	-0.879726
1	-0.687682	0.927367	-1.338565
8	-2.054716	1.084188	1.222654
1	-1.883589	1.518927	0.369437
1	-1.214226	0.569025	1.329077

4.5.3-2



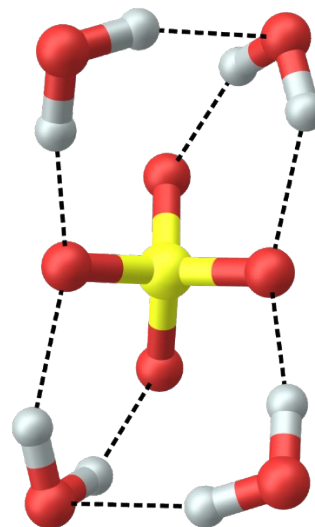
atom	x	y	z
16	-0.715630	-0.498872	0.039872
8	0.244862	-0.304993	1.187621
8	-2.016221	-0.993877	0.554746
8	-0.128732	-1.472449	-0.920017
8	-0.914955	0.825767	-0.639962
8	2.418224	-1.619642	0.068376
1	1.890267	-1.178189	0.765188
1	1.666008	-1.723021	-0.556633
8	1.240041	2.163003	0.464500
1	0.514615	1.991814	-0.171524
1	1.071892	1.363136	1.008064
8	-3.724174	1.043218	-0.301089
1	-3.424677	0.209120	0.114938
1	-2.838442	1.324870	-0.596085
8	3.673896	0.924968	-0.484627
1	2.888784	1.454114	-0.244381
1	3.338112	0.012147	-0.393904

4.6.2-1 (4-IV)



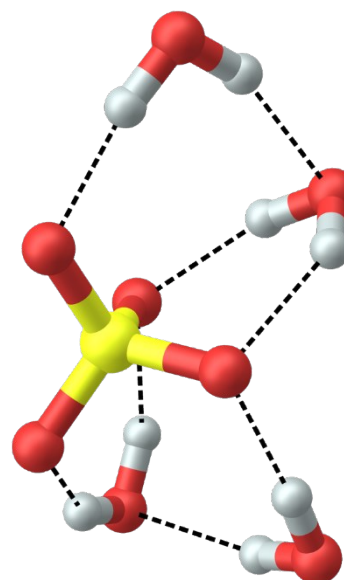
atom	x	y	z
16	0.000000	0.000000	0.734035
8	0.000000	1.219632	-0.143448
8	0.000000	-1.219632	-0.143448
8	-1.224204	0.012163	1.578164
8	1.224204	-0.012163	1.578164
8	2.818968	-1.328189	-0.244452
1	1.914903	-1.559419	-0.533707
1	2.545562	-0.820336	0.551897
8	-2.818968	1.328189	-0.244452
1	-1.914903	1.559419	-0.533707
1	-2.545562	0.820336	0.551897
8	-2.399708	-1.316578	-1.620698
1	-1.537763	-1.380423	-1.150820
1	-2.721968	-0.461147	-1.296181
8	2.399708	1.316578	-1.620698
1	2.721968	0.461147	-1.296181
1	1.537763	1.380423	-1.150820

4.6.2-2 (4-III)



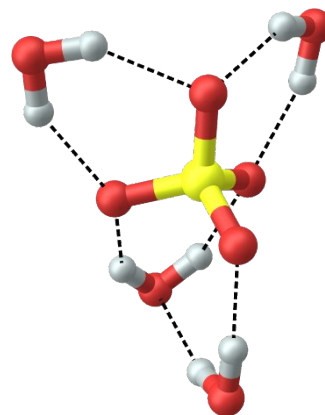
atom	x	y	z
16	-0.060522	-0.710992	-0.205826
8	-0.004806	-0.153598	1.194384
8	-0.010175	0.445159	-1.163899
8	-1.322288	-1.464919	-0.397061
8	1.115593	-1.595722	-0.422020
8	-1.498847	2.101839	0.610128
1	-1.044016	1.400576	1.127015
1	-1.108792	1.867497	-0.253121
8	-3.608693	0.078336	0.082178
1	-3.102533	0.877510	0.301274
1	-2.874841	-0.549246	-0.110038
8	2.820499	-0.284202	1.280699
1	2.487940	-0.909042	0.596860
1	1.939872	0.006036	1.587721
8	2.535093	1.656029	-1.004675
1	2.823279	1.133982	-0.239700
1	1.636446	1.285174	-1.154681

4.6.2-3 (originally 4.8.0-3)



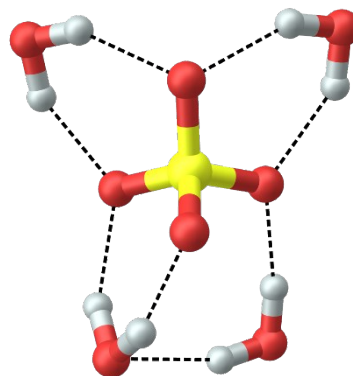
atom	x	y	z
16	-0.342850	-0.188288	0.000000
8	-1.603944	0.589901	0.000000
8	-0.638457	-1.653808	0.000000
8	0.464597	0.155819	1.218157
8	0.464597	0.155819	-1.218157
8	0.464597	-2.343782	-2.516717
1	0.646593	-1.394150	-2.379164
1	0.000803	-2.479825	-1.669484
8	0.464597	-2.343782	2.516717
1	0.646593	-1.394150	2.379164
1	0.000803	-2.479825	1.669484
8	-1.050454	3.347073	0.000000
1	-0.087639	3.228673	0.000000
1	-1.351530	2.409979	0.000000
8	1.770452	2.302856	0.000000
1	1.471052	1.720567	-0.728328
1	1.471052	1.720567	0.728328

4.7.1-1



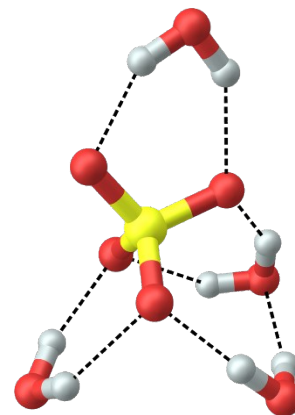
atom	x	y	z
16	0.193948	-0.022611	0.289684
8	-0.168582	-1.113118	-0.675391
8	1.655280	-0.098571	0.597847
8	-0.605561	-0.186594	1.532042
8	-0.109130	1.304385	-0.333357
8	2.278681	-2.501325	-0.769727
1	1.339502	-2.303478	-0.951776
1	2.437740	-1.719564	-0.208748
8	-2.880525	1.459583	-0.874466
1	-3.068946	0.569982	-0.535846
1	-1.910058	1.512805	-0.727758
8	2.434447	2.521443	-0.107838
1	2.519277	1.607302	0.224177
1	1.485883	2.460828	-0.327421
8	-2.802916	-1.310160	0.285703
1	-2.065404	-1.473580	-0.334895
1	-2.254709	-0.897654	0.988818

4.7.1-2



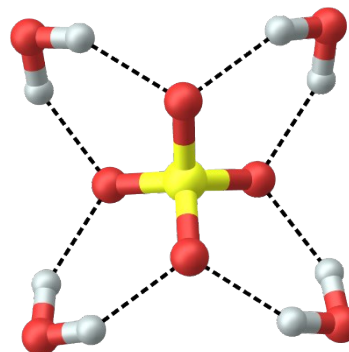
atom	x	y	z
16	-0.411143	-0.379862	-0.030628
8	-1.531197	-1.347420	-0.084278
8	0.355993	-0.537716	1.250592
8	-0.947918	1.021925	-0.093054
8	0.523495	-0.601947	-1.176721
8	2.337935	-2.301980	0.367191
1	1.731019	-1.797363	0.947747
1	2.011094	-1.942478	-0.473482
8	-3.717586	0.394975	-0.212302
1	-3.211470	-0.441669	-0.174996
1	-2.939339	0.981098	-0.185622
8	2.347641	1.554265	-1.357111
1	1.733875	0.788373	-1.404058
1	2.108730	1.926712	-0.494126
8	1.092396	2.216018	1.299239
1	1.180231	1.281969	1.565836
1	0.278079	2.096191	0.760307

4.7.1-3 (new)



atom	x	y	z
16	0.000000	0.000000	0.000000
8	0.865050	-0.865045	0.859579
8	-0.865045	-0.865050	-0.859579
8	0.865045	0.865050	-0.859579
8	-0.865050	0.865045	0.859579
8	-3.417591	0.000000	-0.000013
1	-2.764107	0.514286	0.509998
1	-2.764100	-0.514286	-0.510016
8	0.000000	-3.417591	0.000013
1	0.514286	-2.764100	0.510016
1	-0.514286	-2.764107	-0.509998
8	3.417591	0.000000	-0.000013
1	2.764107	-0.514286	0.509998
1	2.764100	0.514286	-0.510016
8	0.000000	3.417591	0.000013
1	0.514286	2.764107	-0.509998
1	-0.514286	2.764100	0.510016

4.8.0-1 (4-I)



atom	x	y	z
16	-0.156960	-0.436727	0.000000
8	-1.391085	-1.255911	0.000000
8	0.658791	-0.731681	1.218790
8	-0.525281	1.025696	0.000000
8	0.658791	-0.731681	-1.218790
8	2.852065	-2.038789	0.000000
1	2.293328	-1.700115	0.724607
1	2.293328	-1.700115	-0.724607
8	-3.391501	0.674765	0.000000
1	-2.937384	-0.193646	0.000000
1	-2.582536	1.213085	0.000000
8	0.658791	1.771804	-2.492080
1	0.845339	0.825540	-2.335880
1	0.159521	1.914645	-1.668731
8	0.658791	1.771804	2.492080
1	0.845339	0.825540	2.335880
1	0.159521	1.914645	1.668731

4.8.0-2

