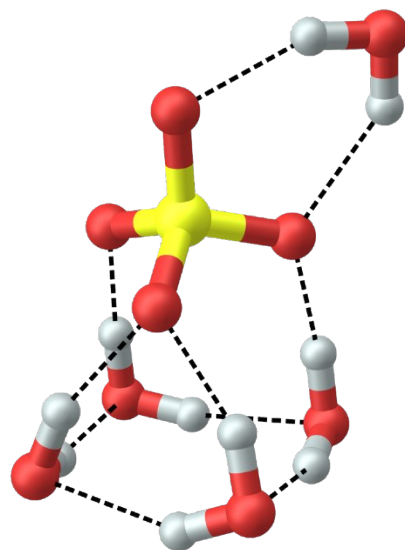


Structures of $\text{SO}_4^{2-}(\text{H}_2\text{O})_5$

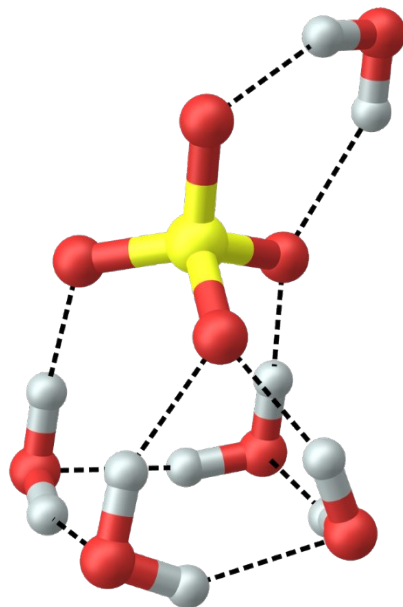
atom	x	y	z
16	-0.850483	-0.581903	-0.076631
8	0.099082	-0.579143	-1.242641
8	-2.150650	-1.156377	-0.486897
8	-1.047296	0.836857	0.377199
8	-0.250616	-1.377956	1.027611
8	2.766072	-1.235527	-0.665856
8	1.995354	1.314596	-1.789663
8	2.081929	-0.353307	1.972890
8	1.242253	2.205882	0.884368
8	-3.889021	0.971759	0.020660
1	2.726243	-0.995559	0.280227
1	1.811391	-1.221752	-0.900960
1	1.141180	0.829912	-1.696014
1	2.598321	0.613116	-1.490405
1	1.926566	0.577793	1.728108
1	1.219223	-0.772295	1.719475
1	1.624274	2.082423	-0.001738
1	0.364644	1.755630	0.779815
1	-3.557826	0.089631	-0.244703
1	-3.023153	1.337259	0.270943

5.6.4-1 (5-IV)



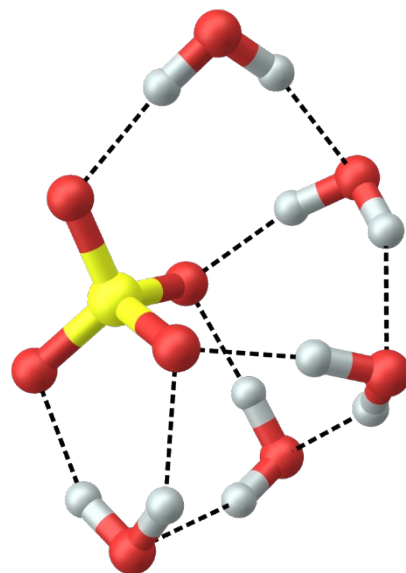
atom	x	y	z
8	-0.244124	-1.286248	1.135761
16	-0.846214	-0.590030	-0.034119
8	0.106526	-0.674215	-1.194353
8	-1.055352	0.859246	0.298671
8	-2.139403	-1.209776	-0.397744
1	0.354269	1.706378	0.890130
8	1.239257	2.076229	1.137884
1	1.701866	1.282509	1.465699
1	1.832560	-1.189615	-1.035100
8	2.810379	-1.056320	-1.038127
1	2.831475	-0.118722	-1.294607
1	-3.561833	0.035574	-0.245236
8	-3.901179	0.932240	-0.048090
1	-3.037870	1.325924	0.165790
1	1.035614	0.885286	-1.623014
8	1.747441	1.562963	-1.635154
1	1.685004	1.912046	-0.725046
1	1.332196	-0.835779	1.645644
8	2.274545	-0.555997	1.789143
1	2.661411	-0.748091	0.917719

5.6.4-2



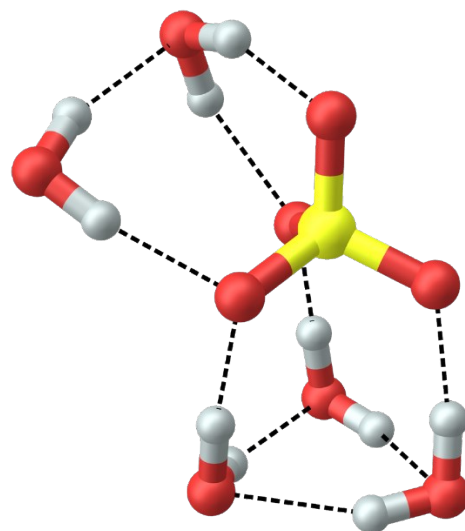
atom	x	y	z
8	1.214177	-1.854231	0.067608
16	-0.014355	-1.054486	-0.101747
8	-0.349227	-0.336442	1.177158
8	-1.165089	-1.914742	-0.484768
8	0.197897	-0.018098	-1.176649
1	-0.203559	1.400496	1.290679
8	-0.273091	2.382521	1.191348
1	-0.877260	2.436695	0.431668
1	1.459586	1.191697	-0.911334
8	2.019713	1.934748	-0.581075
1	1.435934	2.291023	0.109669
1	2.819496	-0.950821	0.315981
8	3.606588	-0.369141	0.382566
1	3.232515	0.493317	0.137951
1	-2.546935	1.106086	-0.593997
8	-1.974821	1.687495	-1.123418
1	-1.187887	1.107374	-1.267116
1	-2.362933	-0.146275	1.194201
8	-3.134557	-0.386642	0.649689
1	-2.672010	-1.061558	0.100592

5.6.4-3



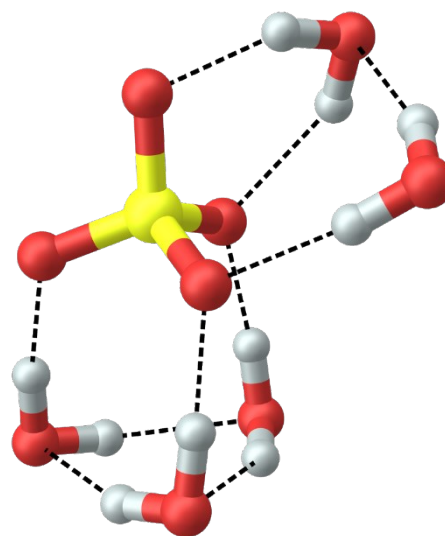
atom	x	y	z
8	1.593520	-1.416124	-0.692820
16	0.320885	-0.730511	-0.363011
8	-0.840057	-1.586628	-0.713148
8	0.236035	0.564763	-1.118965
8	0.295699	-0.420512	1.108228
1	-1.123883	1.598289	-0.701730
8	-1.929424	2.076744	-0.381394
1	-1.969939	1.800625	0.548352
1	-2.696274	-0.064324	1.376875
8	-2.140390	0.372033	2.042590
1	-1.231816	0.074543	1.781564
1	2.984084	1.382812	0.045662
8	2.655270	2.019173	-0.608524
1	1.804668	1.606486	-0.866147
1	-2.453766	-0.964972	-0.644912
8	-3.320577	-0.494881	-0.545322
1	-3.056656	0.428068	-0.698707
1	2.241119	-0.125959	1.619818
8	3.137864	-0.271445	1.267851
1	2.864779	-0.792379	0.479434

5.6.4-4



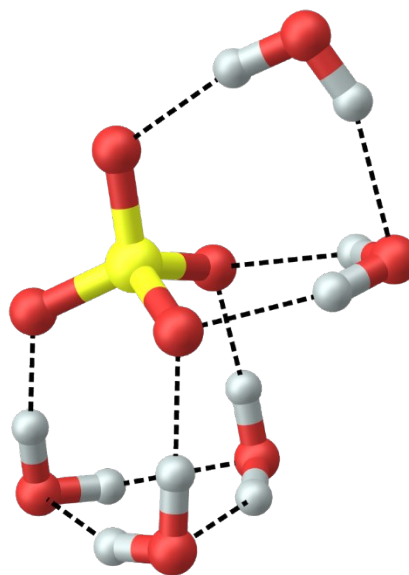
atom	x	y	z
8	-0.239550	0.536407	-1.122313
16	-0.319449	-0.750660	-0.352443
8	-0.289745	-0.425717	1.115773
8	0.843410	-1.605423	-0.699967
8	-1.591555	-1.442527	-0.669853
1	1.324595	1.337973	-1.111734
8	2.238831	1.701805	-1.004035
1	2.759641	0.900275	-0.834859
1	-2.231153	-0.101883	1.616340
8	-3.130535	-0.241923	1.268547
1	-2.865976	-0.778382	0.488204
1	2.426452	-1.179138	-0.142770
8	3.278863	-0.810050	0.202840
1	2.971798	-0.284756	0.960632
1	1.022852	0.567485	1.677869
8	1.822063	1.119388	1.876471
1	1.937838	1.607326	1.045133
1	-2.959267	1.408057	0.037874
8	-2.619300	2.034184	-0.620394
1	-1.775458	1.604452	-0.874154

5.6.4-5



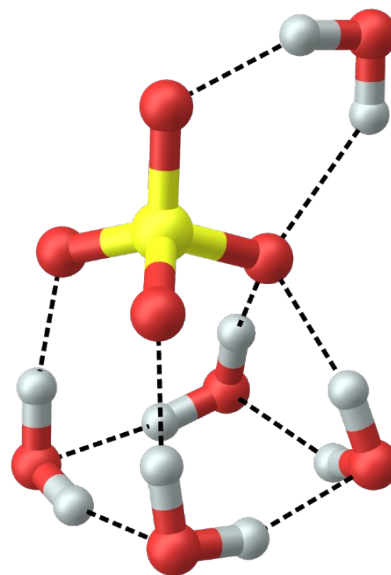
atom	x	y	z
8	0.304867	0.098454	1.203423
16	0.364977	-0.807258	-0.000197
8	0.255850	0.058382	-1.226069
8	-0.771250	-1.761677	0.044220
8	1.650628	-1.534619	-0.013560
1	-1.286446	0.752467	1.551827
8	-2.213732	1.090659	1.632143
1	-2.729231	0.379327	1.218988
1	3.444166	0.898140	-0.002961
8	3.950566	0.070086	-0.017362
1	3.217918	-0.585089	-0.017520
1	-2.407211	-1.279334	-0.193873
8	-3.300384	-0.868637	-0.323309
1	-3.075896	-0.093096	-0.864412
1	-1.183470	1.036911	-1.353591
8	-2.015816	1.572321	-1.297200
1	-2.077092	1.740003	-0.342946
1	1.417207	1.668047	-0.755153
8	1.821527	2.124737	0.004714
1	1.382375	1.601099	0.706791

5.6.4-6 (5-VI) (=5-V)



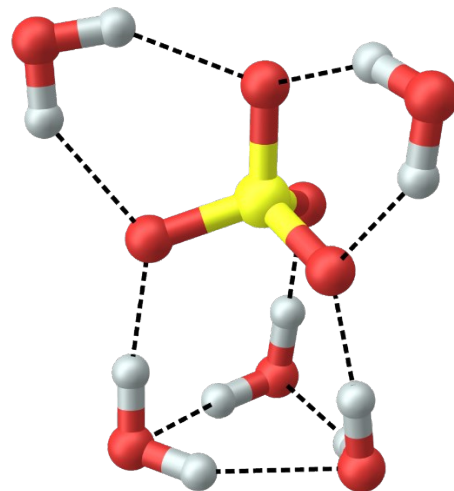
atom	x	y	z
8	-2.280830	-1.092555	-0.040179
16	-0.840568	-0.750937	-0.023272
8	-0.690470	0.758613	0.020370
8	-0.172256	-1.256153	-1.253756
8	-0.183389	-1.321399	1.183807
1	1.487653	-0.896799	-1.521112
8	2.410213	-0.541617	-1.616237
1	2.243133	0.416306	-1.588367
1	2.656199	-0.853685	0.298443
8	2.504134	-0.953635	1.256564
1	1.537352	-1.175393	1.283967
1	-2.591702	1.656568	0.036615
8	-3.524074	1.387504	0.021973
1	-3.358761	0.421060	-0.004072
1	0.570390	1.374438	1.274439
8	1.427272	1.673217	1.650224
1	1.935614	0.838987	1.645401
1	1.668099	2.223562	-0.274152
8	1.355922	2.143112	-1.191781
1	0.528943	1.633260	-1.026693

5.6.4-7 (= 5.6.4-8)



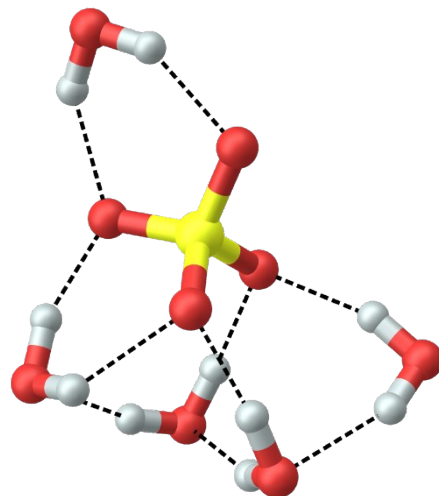
atom	x	y	z
16	-0.503012	0.000591	0.335967
8	0.268930	0.000393	1.603893
8	-1.965586	-0.001921	0.622461
8	-0.157135	1.221868	-0.461016
8	-0.153881	-1.217691	-0.464095
8	-2.682228	-2.534149	-0.421525
1	-1.736695	-2.435879	-0.631445
1	-2.784880	-1.672513	0.024070
8	2.395887	-1.223871	-1.445700
1	2.519626	-0.262055	-1.498551
1	1.455996	-1.292457	-1.142201
8	-2.694680	2.523832	-0.425170
1	-1.747471	2.433886	-0.630865
1	-2.791892	1.660944	0.019410
8	2.527947	1.646774	-0.731456
1	2.819888	1.189684	0.074266
1	1.542794	1.576414	-0.661763
8	2.944337	-0.416097	1.350253
1	2.923289	-0.921885	0.521593
1	1.978805	-0.278708	1.528845

5.7.3-1 (5-III)



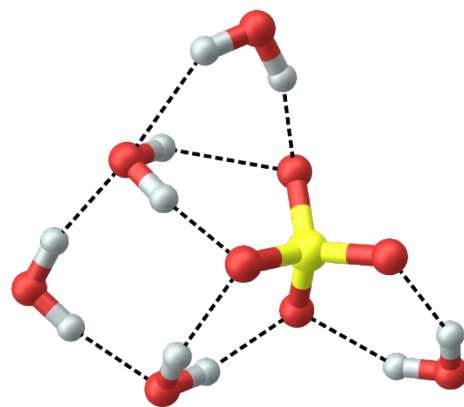
5.7.3-2

atom	x	y	z
8	-1.584977	-1.469615	0.436667
16	-0.679504	-0.358753	0.085035
8	0.096378	0.095239	1.283700
8	-1.475160	0.806864	-0.433361
8	0.286699	-0.785224	-0.977829
1	1.867018	0.030265	1.287069
8	2.835438	0.134089	1.124275
1	2.822323	0.601465	0.270904
1	1.657532	-2.020858	-0.619762
8	2.521085	-2.397126	-0.351384
1	2.844826	-1.685833	0.224912
1	-3.436366	-0.980107	0.134987
8	-4.080051	-0.308210	-0.161796
1	-3.422370	0.375326	-0.383300
1	1.456291	2.026445	-0.915953
8	2.001781	1.374639	-1.389284
1	1.419760	0.578487	-1.377262
1	0.411057	2.196423	1.019540
8	0.127634	2.841045	0.351401
1	-0.578624	2.284824	-0.060811



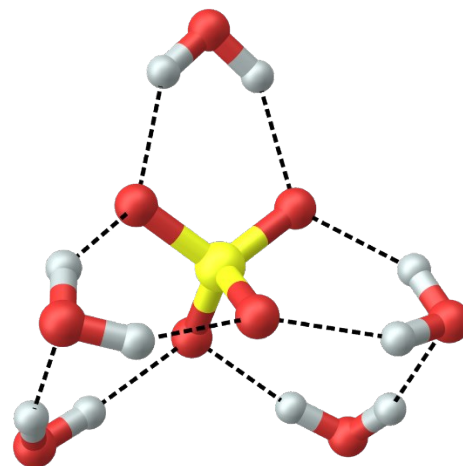
atom	x	y	z
16	-0.779378	0.318455	0.065206
8	0.224534	-0.057965	1.129580
8	-0.142989	1.318589	-0.842356
8	-1.124986	-0.909114	-0.718860
8	-1.991451	0.879749	0.696377
8	1.350739	3.477121	-0.025150
1	2.034993	2.866433	0.274926
1	0.648917	2.834588	-0.284172
8	2.558609	0.647076	0.007568
1	0.629487	-1.928089	1.008989
1	2.033524	0.903731	-0.765499
8	0.604801	-2.725064	0.442544
1	-0.036892	-2.363921	-0.204126
1	1.800593	0.369785	0.589257
8	-3.954868	-0.842277	-0.343899
1	-3.564298	-0.099467	0.156343
1	-3.113354	-1.188089	-0.690783
8	3.284823	-2.143604	-0.419368
1	3.174523	-1.179051	-0.337936
1	2.388854	-2.467300	-0.201772

5.7.3-3 (new)



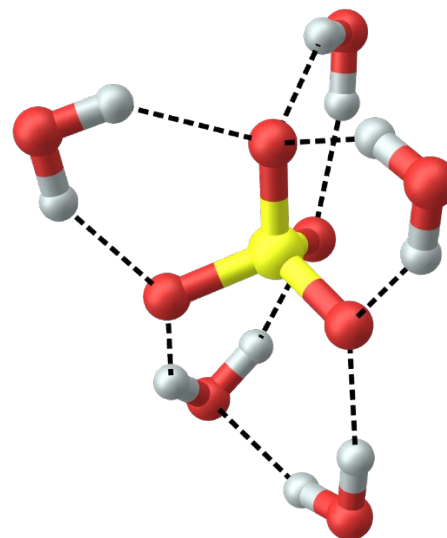
atom	x	y	z
16	0.000000	0.302697	-0.125842
8	0.000000	-0.306553	1.242987
8	-1.222159	1.145378	-0.288658
8	0.000001	-0.785023	-1.145232
8	1.222158	1.145380	-0.288658
8	-2.802636	-0.369685	1.448054
8	-0.000002	3.680515	-0.665946
8	2.802636	-0.369683	1.448054
8	2.436715	-2.268721	-0.847770
8	-2.436713	-2.268723	-0.847770
1	-1.880601	-0.582099	1.692784
1	-2.587657	0.312758	0.780944
1	0.726419	3.038019	-0.569362
1	-0.726421	3.038018	-0.569362
1	1.880601	-0.582097	1.692784
1	2.587657	0.312760	0.780944
1	2.729215	-1.764631	-0.072491
1	1.579792	-1.837153	-1.045383
1	-1.579790	-1.837155	-1.045383
1	-2.729213	-1.764633	-0.072492

5.8.2-1 (new)



atom	x	y	z
16	-0.043081	-0.033949	0.000000
8	-0.484250	-1.467260	0.000000
8	0.781408	0.234768	1.216228
8	0.781408	0.234768	-1.216228
8	-1.238783	0.853613	0.000000
1	-2.502314	-1.572986	0.000000
8	-3.326137	-1.056336	0.000000
1	-2.906776	-0.176174	0.000000
1	1.957818	1.706953	0.730261
8	2.304779	2.256310	0.000000
1	1.957818	1.706953	-0.730261
1	-0.792954	2.685401	0.000000
8	-0.384634	3.576245	0.000000
1	0.558960	3.350520	0.000000
1	0.974704	-1.346929	-2.307307
8	0.781408	-2.291753	-2.458807
1	0.247235	-2.426222	-1.658545
1	0.974704	-1.346929	2.307307
8	0.781408	-2.291753	2.458807
1	0.247235	-2.426222	1.658545

5.9.1-1 (5-II)



atom	x	y	z
8	-1.220672	0.000000	1.143414
16	0.000000	0.000000	0.291360
8	0.000000	1.222656	-0.578304
8	0.000000	-1.222656	-0.578304
8	1.220672	0.000000	1.143414
1	2.274293	-1.617532	0.885108
8	2.394987	-2.468885	0.425001
1	1.605318	-2.405317	-0.137604
1	-2.274293	1.617532	0.885108
8	-2.394987	2.468885	0.425001
1	-1.605318	2.405317	-0.137604
1	0.000000	-0.726984	-2.511875
8	0.000000	0.000000	-3.158730
1	0.000000	0.726984	-2.511875
1	-1.605318	-2.405317	-0.137604
8	-2.394987	-2.468885	0.425001
1	-2.274293	-1.617532	0.885108
1	2.274293	1.617532	0.885108
8	2.394987	2.468885	0.425001
1	1.605318	2.405317	-0.137604

5.10.0-1 (5-I)

