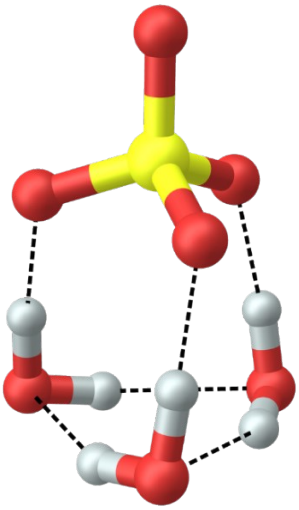
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Structures of $SO_4^{2-}(H_2O)_3$

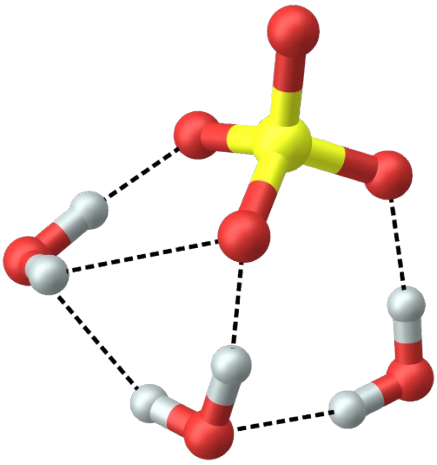
atom	x	y	z
S	0.000000	0.000000	1.185295
O	0.000000	0.000000	2.659275
O	0.000000	1.408657	0.664339
O	1.219932	-0.704328	0.664339
O	-1.219932	-0.704328	0.664339
O	-0.476067	1.658551	-1.957555
H	-0.311684	1.631425	-0.970205
H	-0.950069	0.823199	-2.097035
O	1.674381	-0.416989	-1.957555
H	1.568697	-0.545786	-0.970205
H	1.187946	0.411185	-2.097035
O	-1.198314	-1.241562	-1.957555
H	-1.257013	-1.085639	-0.970205
H	-0.237876	-1.234384	-2.097035

3.3.3-1



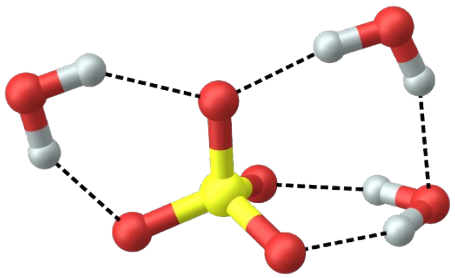
atom	x	y	z
S	-1.032982	-0.274516	0.059785
O	-2.441358	-0.299782	0.495242
O	-0.171976	0.308822	1.158402
O	-0.875399	0.595181	-1.156513
O	-0.553953	-1.650458	-0.255011
O	2.159785	-2.104864	-0.497411
H	1.176629	-2.003704	-0.456511
H	2.445945	-1.244379	-0.152762
O	0.560603	2.728757	-0.538025
H	0.473984	2.512597	0.398759
H	0.018215	1.965802	-0.902381
O	2.410061	0.610745	0.695418
H	2.251732	1.263916	0.001505
H	1.459094	0.390824	0.938023

3.4.2-1



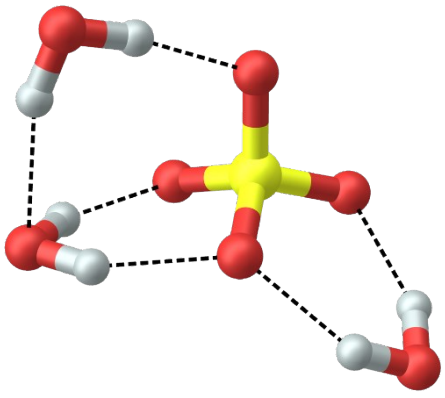
atom	x	y	z
S	0.600821	0.055643	0.000000
O	-0.645223	0.902276	0.000000
O	1.793463	0.947117	0.000000
O	0.600821	-0.811249	1.216674
O	0.600821	-0.811249	-1.216674
O	0.584499	3.447343	0.000000
H	1.279294	2.754652	0.000000
H	-0.163658	2.820224	0.000000
O	-2.884445	-0.777550	0.000000
H	-2.364845	-1.596986	0.000000
H	-2.163014	-0.104289	0.000000
O	-0.738158	-2.901068	0.000000
H	-0.347577	-2.364424	-0.724950
H	-0.347577	-2.364424	0.724950

3.5.1-1



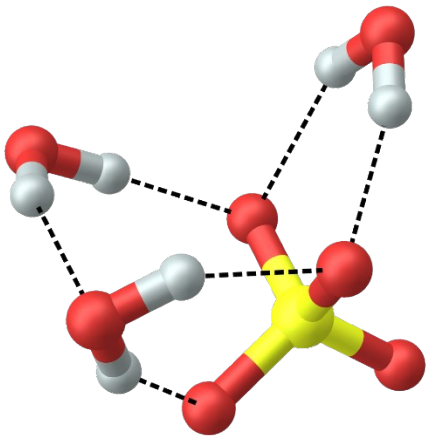
atom	x	y	z
S	-0.331509	-0.467031	0.255778
O	0.360219	-0.099684	1.529043
O	-0.451451	0.773084	-0.596927
O	-1.691252	-1.000578	0.542443
O	0.475023	-1.484946	-0.475428
O	3.038937	-0.516334	-0.966431
H	2.158738	-0.946312	-0.836294
H	2.877163	0.346338	-0.553084
O	1.890179	1.900858	0.430239
H	1.561789	1.235997	1.078539
H	1.136714	1.803282	-0.188291
O	-3.256226	0.896594	-0.767646
H	-3.022483	0.107580	-0.235409
H	-2.331206	1.173658	-0.920246

3.5.1-2



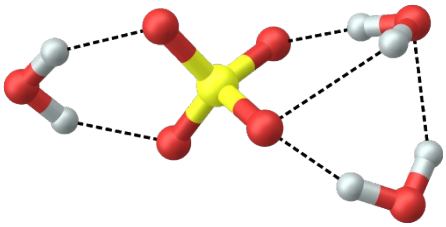
atom	x	y	z
S	-0.682738	-0.614595	-0.160171
O	-0.417719	0.477739	-1.162197
O	0.350448	-1.685690	-0.321969
O	-2.037180	-1.161823	-0.344827
O	-0.534905	-0.020784	1.221186
O	2.309734	1.114146	-1.185900
H	1.345809	0.924113	-1.274529
H	2.513376	0.622575	-0.375107
O	-1.194243	2.612049	0.648690
H	-1.033685	1.768865	1.127180
H	-0.984592	2.265324	-0.235386
O	2.255059	-0.634494	1.281155
H	1.765610	-1.203891	0.635320
H	1.467731	-0.152620	1.596152

3.5.1-3



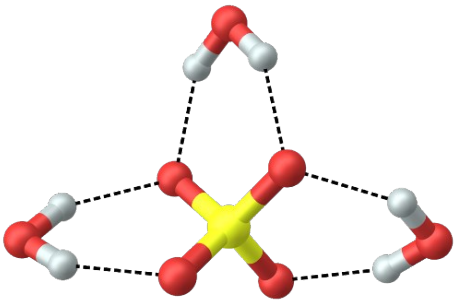
atom	x	y	z
S	0.407717	-0.078393	0.032718
O	1.326799	-0.910445	-0.794752
O	-0.578554	0.609627	-0.865277
O	1.188762	0.928592	0.801560
O	-0.353178	-0.956581	0.983224
O	-2.765341	-1.410463	-0.015040
H	-1.883904	-1.318166	0.458243
H	-2.529654	-0.956999	-0.833486
O	3.759748	0.252597	-0.078136
H	3.132219	-0.352471	-0.525656
H	3.068121	0.736733	0.417252
O	-2.960681	1.611265	-0.034116
H	-3.225772	0.736465	0.279886
H	-2.024925	1.411980	-0.299429

3.5.1-4 (originally 3.4.1-1)



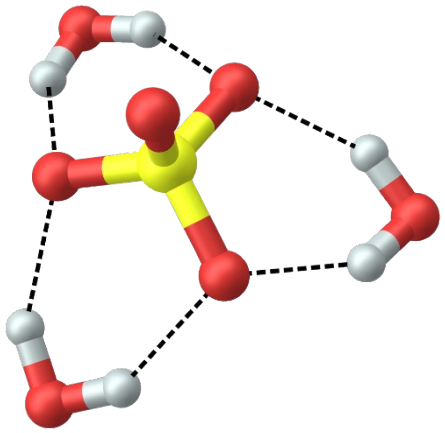
atom	x	y	z
S	0.000000	0.000000	0.370917
O	1.221306	-0.008140	1.221770
O	-1.221306	0.008140	1.221770
O	0.000000	-1.222161	-0.505274
O	0.000000	1.222161	-0.505274
O	-2.268807	2.505734	0.595790
H	-2.163118	1.632134	1.028660
H	-1.493431	2.407434	0.011082
O	2.268807	-2.505734	0.595790
H	2.163118	-1.632134	1.028660
H	1.493431	-2.407434	0.011082
O	0.000000	0.000000	-3.032939
H	-0.002958	0.721978	-2.373611
H	0.002958	-0.721978	-2.373611

3.6.0-1



atom	x	y	z
S	-0.562098	-0.300629	0.000000
O	-0.764944	1.190528	0.000000
O	-1.859614	-0.995141	0.000000
O	0.233441	-0.674696	1.221459
O	0.233441	-0.674696	-1.221459
O	0.233441	1.797367	-2.553049
H	-0.187345	1.948370	-1.683382
H	0.402647	0.845592	-2.405866
O	0.233441	1.797367	2.553049
H	-0.187345	1.948370	1.683382
H	0.402647	0.845592	2.405866
O	2.317088	-2.105801	0.000000
H	1.776296	-1.728644	-0.722149
H	1.776296	-1.728644	0.722149

3.6.0-2



atom	x	y	z
S	-0.204256	-0.678135	0.000000
O	1.006393	-1.545403	0.000000
O	-1.017838	-0.934833	1.220698
O	-1.017838	-0.934833	-1.220698
O	0.234002	0.774970	0.000000
O	-1.017838	1.537666	2.456115
H	-1.190178	0.589327	2.267742
H	-0.487160	1.693771	1.654632
O	-1.017838	1.537666	-2.456115
H	-0.487160	1.693771	-1.654632
H	-1.190178	0.589327	-2.267742
O	3.055367	0.310110	0.000000
H	2.255608	0.865882	0.000000
H	2.571892	-0.544679	0.000000

3.6.0-3