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Interaction Topologies of the S···O Chalcogen Bond: The Conformational Equilibrium of the Cyclohexanol···SO_2 Cluster

Electronic Supplementary Information

Content:

1) Figure of the molecular geometries of the eight predicted isomers.
2) Figure of the interconversion barrier connecting isomers ***Eg*_SO$_2$_1** and ***Et*_SO$_2$_1**.
3) Table of the spectroscopic parameters of the eight isomers.
4) Tables of experimental transitions frequencies of the cyclohexanol-SO_2 cluster.
5) Table of the results of NBO analysis.
6) Table of the results of SAPT analysis.
7) Tables of the final fit of the r_0 structure of four observed isomers.

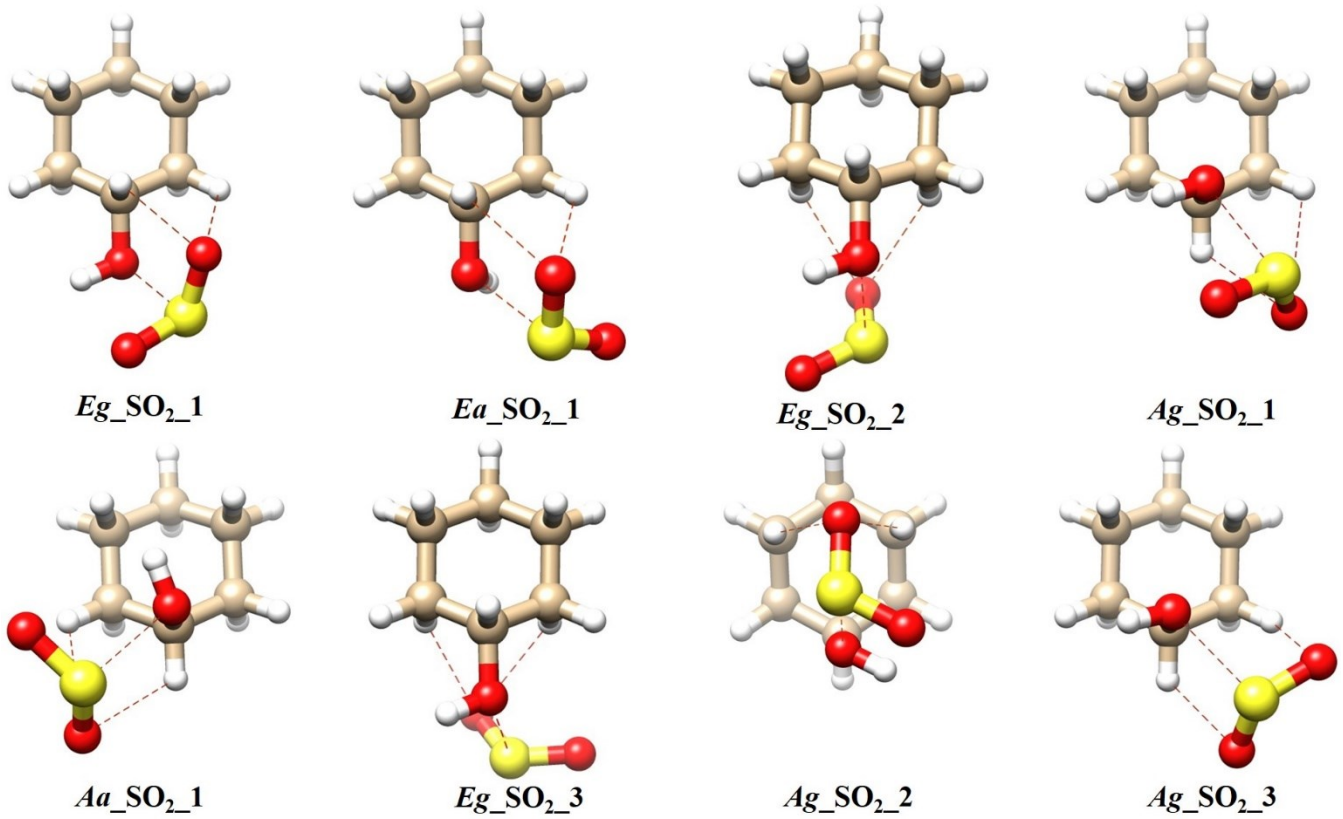

Figure S1. Molecular geometries of the eight predicted isomers of cyclohexanol···SO_2 in a relative energy window of 500 cm^{-1} calculated at the B3LYP-D3(BJ)/def2-TZVP level of theory.

Table S1. Spectroscopic parameters of the first eight stable isomers of cyclohexanol-SO_2.

B3LYP-D3(BJ)/def2-TZVP								
	*Eg*_SO_2_1	*Et*_SO_2_1	*Eg*_SO_2_2	*Ag*_SO_2_1	*At*_SO_2_1	*Eg*_SO_2_3	*Ag*_SO_2_2	*Ag*_SO_2_3[a]
A/MHz	2451.38	2422.04	2082.99	2524.77	2366.18	1961.37	1722.11	2359.96
B/MHz	534.04	537.58	581.55	544.76	579.03	600.15	716.28	577.63
C/MHz	483.99	503.34	575.47	501.40	540.16	584.42	659.27	525.05
$\|\mu_a\|$/ D	2.21	2.24	1.82	2.36	2.57	1.70	1.73	1.99
$\|\mu_b\|$/ D	0.59	1.11	0.72	0.30	0.41	2.05	1.26	2.10
$\|\mu_c\|$/ D	0.81	0.70	1.09	0.48	0.72	1.47	0.65	1.08
ΔE/cm^{-1}	0	9	96	244	307	418	431	435
ΔE_0/cm^{-1}	36	0	64	252	294	384	428	470
B3LYP-D3(BJ)/ aug-cc-pVTZ								
A/MHz	2479.05	2408.89	2124.13	2517.30	2363.22	1955.05	1736.75	-
B/MHz	527.00	535.48	568.16	538.64	575.52	596.44	705.97	-
C/MHz	479.39	502.14	561.96	500.22	536.64	580.67	648.84	-
$\|\mu_a\|$/ D	2.54	2.40	2.22	2.70	2.75	1.84	2.11	-
$\|\mu_b\|$/ D	0.47	1.16	0.74	0.12	0.47	2.01	1.22	-
$\|\mu_c\|$/ D	0.87	0.74	1.08	042	0.75	1.59	0.73	-
ΔE/cm^{-1}	0	64	131	277	384	458	470	
ΔE_0/cm^{-1}	0	13	94	288	361	378	427	

[a] The geometry optimization of *Ag*_SO_2_3 calculated at the B3LYP-D3(BJ)/def2-TZVP level of theory is converted to *Ag*_SO_2_1.

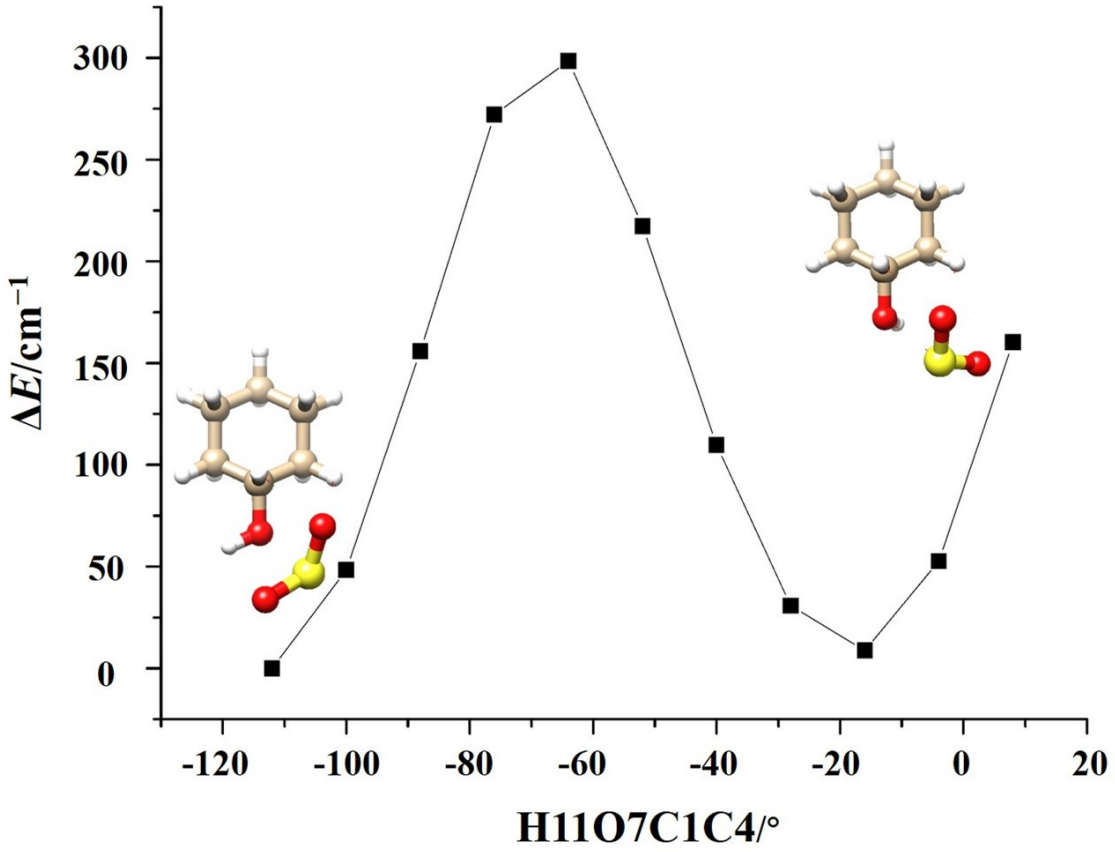

Figure S2. The interconversion potential energy surface calculated at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory. The barrier to intercover isomer ***Ea*_SO$_2$_1** to isomer ***Eg*_SO$_2$_1** is ~298 cm^{-1}.

Table S2. Experimental transition frequencies of the isomer ***Eg*_SO$_2$_1** of cyclohexanol-SO_2 and residuals according to the fit of Table 2.

$J'_{Ka'Kc'}$	$J''_{Ka''Kc''}$	$\nu_{obs.}$/MHz	$\Delta\nu$/MHz
2 1 1	1 1 0	2003.5250	−0.0058
3 1 3	2 1 2	2916.8131	−0.0072
3 0 3	2 0 2	2959.8162	0.0047
3 2 2	2 2 1	2961.1605	−0.0106
3 2 1	2 2 0	2962.5094	−0.0020
3 1 2	2 1 1	3005.0783	0.0044
4 1 4	3 1 3	3888.6808	−0.0056
4 0 4	3 0 3	3944.8272	−0.0044
4 2 3	3 2 2	3947.9460	0.0004
4 2 2	3 2 1	3951.2995	0.0050
4 1 3	3 1 2	4006.3498	0.0031
5 1 5	4 1 4	4860.2054	−0.0050
5 0 5	4 0 4	4928.4957	−0.0048
5 2 4	4 2 3	4934.4818	0.0039
5 2 3	4 2 2	4941.1720	0.0044
5 1 4	4 1 3	5007.2600	0.0064
6 1 6	5 1 5	5831.3075	−0.0081
6 0 6	5 0 5	5910.4895	−0.0051
6 2 5	5 2 4	5920.7060	−0.0015
6 3 4	5 3 3	5924.0359	−0.0050
6 3 3	5 3 2	5924.1860	0.0114
6 2 4	5 2 3	5932.3911	0.0019
6 1 5	5 1 4	6007.6976	0.0037
7 1 7	6 1 6	6801.9258	−0.0051
7 0 7	6 0 6	6890.5032	−0.0053
7 2 6	6 2 5	6906.5713	−0.0028
7 4 3	6 4 2	6910.9841	−0.0010
7 3 5	6 3 4	6911.8742	0.0002
7 3 4	6 3 3	6912.1764	0.0021
7 2 5	6 2 4	6925.2046	0.0055
7 1 6	6 1 5	7007.5612	0.0001
8 1 8	7 1 7	7771.9901	−0.0020
8 0 8	7 0 7	7868.2642	−0.0033
8 2 7	7 2 6	7892.0116	−0.0061
8 4 4	7 4 3	7898.6197	−0.0035
8 3 6	7 3 5	7899.9088	0.0067
8 3 5	7 3 4	7900.5052	0.0029
8 2 6	7 2 5	7919.8091	0.0030
8 1 7	7 1 6	8006.7340	−0.0070
7 2 5	7 1 6	5444.7444	−0.0005
6 2 5	6 1 5	5503.7000	−0.0114
6 2 4	6 1 5	5527.1037	−0.0033
5 2 4	5 1 4	5590.6803	−0.0175
5 2 3	5 1 4	5602.4102	−0.0015

4	2	3	4	1	3	5663.4737	0.0002
4	2	2	4	1	3	5668.5001	0.0023
3	2	2	3	1	2	5721.8738	−0.0007
3	2	1	3	1	2	5723.5550	0.0049
4	1	4	3	0	3	5738.5367	−0.0009
2	2	0	2	1	1	5766.1095	−0.0029
4	1	3	3	0	3	6032.6925	−0.0148
8	0	8	7	1	7	6310.6115	0.0031
5	1	5	4	0	4	6653.9102	−0.0062
9	0	9	8	1	8	7382.1571	−0.0016
6	1	6	5	0	5	7556.7244	−0.0070
2	2	1	1	1	0	7769.3271	0.0188
2	2	0	1	1	1	7799.0745	0.0125
2	1	2	1	0	1	3866.6225	0.0063
6	0	6	5	1	5	4185.0817	0.0029
7	0	7	6	1	5	4626.7030	0.0223
3	1	3	2	0	2	4809.6642	0.0015
7	0	7	6	1	6	5244.2761	0.0043
8	2	6	8	1	7	5357.8268	0.0168

Table S3. Experimental transition frequencies of the isomer ***Eg*_SO$_2$_2** of cyclohexanol-SO_2 and residuals according to the fit of Table 2.

$J'_{Ka'Kc'}$	$J''_{Ka''Kc''}$	$\nu_{obs.}$/MHz	$\Delta\nu$/MHz
2 0 2	1 0 1	2133.5007	0.0020
3 1 3	2 1 2	3185.8904	0.0044
3 0 3	2 0 2	3200.1398	0.0145
3 1 2	2 1 1	3214.6754	0.0077
2 1 1	1 0 1	3751.5557	−0.0153
4 1 4	3 1 3	4247.7697	0.0000
4 0 4	3 0 3	4266.6060	0.0013
4 2 3	3 2 2	4267.0247	−0.0102
4 2 2	3 2 1	4267.4622	−0.0031
4 1 3	3 1 2	4286.1495	0.0046
3 1 2	2 0 2	4832.7316	−0.0084
5 1 5	4 1 4	5309.5910	0.0040
5 0 5	4 0 4	5332.8920	0.0041
5 2 4	4 2 3	5333.7007	0.0062
5 3 3	4 3 2	5334.0033	0.0144
5 3 2	4 3 1	5334.0033	0.0119
5 2 3	4 2 2	5334.5610	0.0058
5 1 4	4 1 3	5357.5607	0.0064
7 0 7	6 1 5	5757.9101	0.0127
4 1 4	3 0 3	5822.8092	−0.0117
4 1 3	3 0 3	5918.7482	−0.0114
7 0 7	6 1 6	5959.3718	0.0115
6 1 6	5 1 5	6371.3173	−0.0040
6 0 6	5 0 5	6398.9253	−0.0007
6 2 5	5 2 4	6400.2913	0.0033
6 3 4	5 3 3	6400.7739	−0.0035
6 3 3	5 3 2	6400.7739	−0.0102
6 2 4	5 2 3	6401.7903	−0.0032
6 1 5	5 1 4	6428.8598	−0.0184
5 1 5	4 0 4	6865.7836	−0.0196
2 2 0	1 1 0	6939.7389	0.0318
2 2 1	1 1 1	6949.2548	−0.0032
7 1 7	6 1 6	7432.9481	−0.0088
7 0 7	6 0 6	7464.6650	−0.0059
7 2 6	6 2 5	7466.8009	−0.0011
7 3 5	6 3 4	7467.5716	0.0116
7 3 4	6 3 3	7467.5762	0.0010
7 2 5	6 2 4	7469.2021	−0.0076
7 1 6	6 1 5	7500.0984	−0.0010
6 1 6	5 0 5	7904.2416	0.0049

Table S4. Experimental transitions frequencies of the isomer ***Ag*_SO$_2$_1** of cyclohexanol-SO_2 and residuals according to the fit of Table 2.

$J'_{Ka'Kc'}$			$J''_{Ka''Kc''}$			$\nu_{obs.}$/MHz	$\Delta\nu$/MHz
3	1	3	2	1	2	2963.4591	−0.0037
3	0	3	2	0	2	3017.4272	−0.0021
3	2	2	2	2	1	3019.4786	−0.0037
3	2	1	2	2	0	3021.5560	0.0087
3	1	2	2	1	1	3074.8820	0.0079
4	1	4	3	1	3	3950.6809	−0.0002
4	0	4	3	0	3	4020.8276	0.0037
4	2	3	3	2	2	4025.5680	0.0037
4	2	2	3	2	1	4030.7131	−0.0089
4	1	3	3	1	2	4099.2161	0.0076
5	1	5	4	1	4	4937.3995	0.0032
5	0	5	4	0	4	5022.1603	−0.0022
5	2	4	4	2	3	5031.2947	0.0018
5	2	3	4	2	2	5041.5884	−0.0017
5	1	4	4	1	3	5122.9980	0.0031
6	1	6	5	1	5	5923.4962	−0.0024
6	0	6	5	0	5	6020.9596	−0.0035
6	2	5	5	2	4	6036.5822	0.0021
6	3	4	5	3	3	6041.5876	−0.0021
6	3	3	5	3	2	6041.8446	0.0037
6	2	4	5	2	3	6054.5408	−0.0020
6	1	5	5	1	4	6146.0776	−0.0013
7	1	7	6	1	6	6908.8898	0.0000
7	0	7	6	0	6	7016.7819	−0.0034
7	2	6	6	2	5	7041.3386	0.0005
7	3	5	6	3	4	7049.3289	−0.0032
7	3	4	6	3	3	7049.8931	−0.0036
7	2	5	6	2	4	7069.9236	−0.0057
7	1	6	6	1	5	7168.2895	−0.0056
8	1	8	7	1	7	7893.4871	0.0041
8	0	8	7	0	7	8009.2522	−0.0042
8	2	7	7	2	6	8045.4938	0.0144

Table S5. Experimental transitions frequencies of the isomer ***Aa*_SO$_2$_1** of cyclohexanol-SO_2 and residuals according to the fit of Table 2.

$J'_{Ka'Kc'}$	$J''_{Ka''Kc''}$	$\nu_{obs.}$/MHz	$\Delta\nu$/MHz
2 1 2	1 1 1	2274.3212	−0.0177
2 0 2	1 0 1	2313.6983	0.0032
3 1 3	2 1 2	3411.0140	−0.0018
3 0 3	2 0 2	3468.6470	0.0063
3 1 2	2 1 1	3531.3597	0.0002
4 1 4	3 1 3	4547.1170	0.0030
4 0 4	3 0 3	4621.3138	−0.0006
4 2 3	3 2 2	4628.3108	0.0045
4 2 2	3 2 1	4635.7823	−0.0106
4 1 3	3 1 2	4707.5297	−0.0014
5 1 5	4 1 4	5682.4625	0.0021
5 0 5	4 0 4	5770.9946	0.0027
5 2 3	4 2 2	5799.2861	−0.0004
5 1 4	4 1 3	5882.8638	0.0001
6 1 6	5 1 5	6816.9019	0.0026
6 0 6	5 0 5	6917.0072	0.0006
6 2 5	5 2 4	6939.7388	0.0025
6 1 5	5 1 4	7057.1140	0.0003
7 1 7	6 1 6	7950.2947	0.0000
7 0 7	6 0 6	8058.7915	−0.0054
5 2 4	4 2 3	5784.3651	0.0037
6 2 4	5 2 3	6965.7042	−0.0008

Table S6. Experimental transition frequencies of the ^{34}S species of the isomer ***Eg*_SO$_2$_1** and residuals according to the fit of Table 2.

$J'_{Ka'Kc'}$	$J''_{Ka''Kc''}$	$\nu_{obs.}$/MHz	$\Delta\nu$/MHz
4 1 4	3 1 3	3833.9788	−0.0252
4 1 3	3 1 2	3948.2213	−0.0058
5 1 5	4 1 4	4791.8840	−0.0096
5 0 5	4 0 4	4858.3464	−0.0037
5 2 4	4 2 3	4863.9730	0.0018
5 2 3	4 2 2	4870.2632	0.0035
5 1 4	4 1 3	4934.6447	0.0013
6 1 6	5 1 5	5749.3849	−0.0026
6 0 6	5 0 5	5826.5260	−0.0056
6 2 5	5 2 4	5836.1440	0.0078
6 2 4	5 2 3	5847.1305	0.0116
7 1 7	6 1 6	6706.4162	−0.0018
7 0 7	6 0 6	6792.8533	0.0064
7 2 6	6 2 5	6807.9546	−0.0037
7 1 6	6 1 5	6906.0502	−0.0077
8 1 8	7 1 7	7662.9370	0.0133
8 0 8	7 0 7	7757.0375	0.0039

Table S7. The NBO analysis (stabilization energy contributions≥0.2 kJ mol^{-1}) for cyclohexanol-SO_2 performed at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory.

Interactions	Donor	Acceptor	***Eg*_SO$_2$_1**	***Eg*_SO$_2$_2**	***Ag*_SO$_2$_1**	***Aa*_SO$_2$_1**
	LP(2)O7	BD*(1)S8-O9	4.8	4.4	4.8	3.8
	LP(2)O7	BD*(2)S8-O9	5.8	3.6	6.1	7.1
	LP(2)O7	BD*(1)S8-O10	6.8	4.7	7.1	7.8
	LP(2)O7	BD*(2)S8-O10	3.6	3.6	3.4	2.6
	LP(1)O7	BD*(2)S8-O9	1.0	1.1	1.0	1.0
	LP(1)O7	BD*(2)S8-O10	0.9	1.1	0.9	1.0
	LP(1)O7	BD*(1)S8-O10	-	0.2	0.2	-
S···O	LP(2)O7	RY*(3)S8	1.9	0.3	2.0	1.3
	LP(2)O7	RY*(4)S8	-	0.5	-	0.3
	LP(2)O7	RY*(5)S8	-	0.2	-	-
	LP(2)O7	RY*(6)S8	0.5	0.2	0.5	-
	LP(2)O7	RY*(7)S8	-	-	-	0.3
	LP(2)O7	RY*(8)S8	0.2	-	-	-
	LP(1)O7	RY*(3)S8	0.3	-	0.3	-
	LP(1)O7	RY*(6)S8	0.3	0.4	0.4	0.6
C1H12···O9	LP(1)O9	RY*(1)H12	0.2	-	-	-
	LP(1)O9	BD*(1)C1-H12	0.6	-	0.3	0.3
C2H13···O9	LP(1)O9	BD*(1)C2-H13	0.3	-	-	-
C2H14···O9	LP(1)O9	BD*(1)C2-H14	-	0.4	-	-
	LP(2)O9	BD*(1)C2-H14		0.3	-	-
C6H22···O9	LP(1)O9	BD*(1)C6-H22	-	0.8	-	-
	LP(2)O9	BD*(1)C6-H22	-	0.8	-	-
C6H21···O9	LP(2)O9	BD*(1)C6-H21				0.3
C6H21···O10	LP(2)O10	BD*(1)C6-H21				0.3
O10···H11	BD*(2)S8-O10	RY*(1)H11	0.2	0.5	0.2	0.2
Total			27.2	22.6	27.0	26.7

Table S8. The SAPT analysis of the cyclohexanol-SO_2 cluster at the SAPT2+(3)δMP2/aug-cc-pVDZ level fo theory (all values of energies are given in kJ mol^{-1}).

	Electrostatic	Dispersion	Induction	Exchange	Charge transfer	Total
***Eg*_SO$_2$_1**	−68.5	−25.8	−31.6	82.8	−17.6	−43.1
***Eg*_SO$_2$_2**	−64.2	−25.6	−27.8	74.6	−14.6	−43.0
***Ag*_SO$_2$_1**	−68.5	−25.6	−31.6	83.2	−17.8	−42.5
***Aa*_SO$_2$_1**	−70.4	−26..8	−32.2	84.4	−17.9	−45.0
***Eg*_SO$_2$_3**	−51.0	−24.8	−25.4	77.2	−11.0	−24.0
***Ag*_SO$_2$_2**	−52.9	−26.5	−24.5	77.9	−9.5	−26.0
***Ag*_SO$_2$_3**	−57.9	−26.0	−30.0	90.2	−13.6	−23.7

Table S9. The final fit of the r_0 structure of isomer *Eg*_SO_2_1. Principal coordinates and estimated uncertainties are given in Å.

ATOM	A	dA	B	dB	C	dC
C	-3.53990	0.00100	-0.16951	0.00509	-0.26091	0.00194
C	-2.76711	0.00269	0.99009	0.00449	-0.89226	0.00321
C	-2.62136	0.00405	-1.35893	0.00188	0.02528	0.00308
C	-1.56974	0.00358	1.39460	0.00092	-0.02714	0.00326
C	-1.42399	0.00293	-0.94732	0.00357	0.88503	0.00294
C	-0.66557	0.00041	0.19735	0.00404	0.23622	0.00170
O	0.42279	0.00202	0.54854	0.00917	1.11623	0.00295
S	2.66901	0.00049	-0.35200	0.00047	0.06654	0.00139
O	2.03228	0.00153	-0.98428	0.00540	-1.07998	0.00501
O	3.19546	0.00142	0.99110	0.00155	-0.13461	0.00631
H	-4.35942	0.00231	-0.47369	0.00891	-0.91421	0.00283
H	-3.99357	0.00086	0.16898	0.00423	0.67579	0.00303
H	-3.42134	0.00491	1.85000	0.00665	-1.04261	0.00600
H	-2.41191	0.00307	0.69078	0.00603	-1.88281	0.00211
H	-3.17469	0.00618	-2.15672	0.00233	0.52236	0.00480
H	-2.26026	0.00558	-1.77325	0.00320	-0.92064	0.00433
H	-1.91812	0.00498	1.78447	0.00241	0.93333	0.00446
H	-1.00042	0.00575	2.19113	0.00144	-0.51460	0.00496
H	-1.76430	0.00293	-0.61969	0.00518	1.87122	0.00179
H	-0.74946	0.00519	-1.79022	0.00577	1.03567	0.00571
H	-0.24313	0.00147	-0.15080	0.00307	-0.71321	0.00273
H	0.82663	0.00379	1.36641	0.00952	0.80220	0.00365

Table S10 The final fit of the r_0 structure of isomer *Eg*_SO_2_2. Principal coordinates and estimated uncertainties are given in Å.

ATOM	A	dA	B	dB	C	dC
C	3.05502	0.00642	-0.63604	0.02927	-0.77418	0.01549
C	2.77454	0.00191	-0.99584	0.02342	0.68618	0.03004
C	2.67350	0.00629	0.81551	0.03935	-1.07037	0.03422
C	1.31738	0.00446	-0.71339	0.03881	1.06059	0.02856
C	1.21521	0.00381	1.09094	0.02386	-0.69357	0.03544
C	0.95649	0.00479	0.73321	0.02874	0.76548	0.02110
O	-0.42844	0.00712	0.91801	0.04351	1.12492	0.01951
S	-2.53129	0.00170	-0.42291	0.00039	0.08887	0.01229
O	-1.83599	0.00339	-1.20893	0.02726	-0.91886	0.03542
O	-3.14458	0.00393	0.82001	0.01464	-0.35433	0.02402
H	4.10767	0.00802	-0.80381	0.03910	-1.00849	0.01526
H	2.47679	0.01115	-1.29859	0.05177	-1.42485	0.04265
H	2.83225	0.01217	1.04548	0.07732	-2.12477	0.04340
H	3.32891	0.00243	1.48402	0.01994	-0.50305	0.06204
H	0.54988	0.00817	0.49449	0.04542	-1.32114	0.01014
H	0.96860	0.00361	2.14227	0.02973	-0.86696	0.07163
H	1.56058	0.00943	1.38516	0.05094	1.40838	0.04802
H	-0.70130	0.00697	1.80994	0.03516	0.88135	0.04983
H	0.65693	0.00054	-1.36126	0.01894	0.48024	0.05568
H	1.13720	0.01039	-0.92393	0.07684	2.11570	0.03717
H	3.43670	0.00649	-0.41361	0.04574	1.33482	0.00527
H	3.00435	0.00149	-2.04607	0.02971	0.87069	0.06629

Table S11 The final fit of the r_0 structure of isomer *Ag*_SO_2_1. Principal coordinates and estimated uncertainties are given in Å.

ATOM	A	dA	B	dB	C	dC
C	-3.40973	0.00067	-0.36473	0.00203	-0.38291	0.00054
C	-2.93733	0.00109	1.07683	0.00137	-0.18458	0.00113
C	-2.23265	0.00189	-1.29496	0.00084	-0.68217	0.00057
C	-1.87119	0.00173	1.16305	0.00048	0.90964	0.00065
C	-1.16676	0.00126	-1.21342	0.00101	0.41218	0.00104
C	-0.70043	0.00052	0.21428	0.00169	0.66287	0.00046
O	0.04964	0.00041	0.62284	0.00190	-0.50736	0.00059
S	2.58908	0.00015	-0.25055	0.00001	-0.36120	0.00017
O	2.42338	0.00039	-0.92431	0.00063	0.91846	0.00053
O	3.11856	0.00071	1.10592	0.00036	-0.32514	0.00052
H	-4.14413	0.00112	-0.41214	0.00333	-1.18872	0.00087
H	-3.91857	0.00062	-0.70532	0.00210	0.52514	0.00060
H	-2.57791	0.00313	-2.32529	0.00129	-0.78138	0.00098
H	-1.78712	0.00204	-1.01745	0.00087	-1.63982	0.00063
H	-1.57147	0.00124	-1.59708	0.00108	1.35241	0.00106
H	-0.30340	0.00209	-1.83235	0.00187	0.16718	0.00182
H	-0.02392	0.00095	0.23027	0.00296	1.52141	0.00078
H	0.23141	0.00153	1.56792	0.00214	-0.44744	0.00015
H	-1.49880	0.00296	2.18645	0.00097	1.01294	0.00105
H	-2.31105	0.00190	0.89921	0.00053	1.87552	0.00072
H	-2.52531	0.00107	1.45179	0.00143	-1.12455	0.00114
H	-3.77832	0.00197	1.72379	0.00219	0.07001	0.00191

Table S12 The final fit of the r_0 structure of isomer *Aa*_SO_2_1. Principal coordinates and estimated uncertainties are given in Å.

ATOM	A	dA	B	dB	C	dC
C	0.70524	0.00023	-0.34629	0.00526	1.09105	0.00237
C	0.89712	0.00502	1.00739	0.00365	0.40975	0.00060
C	2.36598	0.00571	1.27456	0.00338	0.08634	0.00209
C	3.00150	0.00086	0.13033	0.00712	-0.70721	0.00190
C	2.81736	0.00575	-1.21309	0.00552	0.00218	0.00015
C	1.34115	0.00653	-1.48935	0.00151	0.29483	0.00256
O	0.09469	0.00354	1.11050	0.00601	-0.79211	0.00180
S	-2.54374	0.00072	0.17520	0.00031	-0.26571	0.00016
O	-2.41064	0.00071	0.28786	0.00400	1.17932	0.00050
O	-2.33982	0.00075	-1.14631	0.00226	-0.84262	0.00390
H	0.50715	0.00966	1.79726	0.00611	1.04990	0.00039
H	2.44643	0.00911	2.21680	0.00432	-0.45650	0.00323
H	2.89969	0.00783	1.40092	0.00479	1.03283	0.00310
H	2.55000	0.00268	0.08116	0.00613	-1.70320	0.00111
H	4.06111	0.00037	0.33489	0.01211	-0.86693	0.00385
H	3.37032	0.00414	-1.19847	0.00702	0.94682	0.00107
H	3.24301	0.01040	-2.01978	0.00810	-0.59698	0.00004
H	1.22540	0.00989	-2.42563	0.00262	0.84207	0.00375
H	0.80456	0.00875	-1.63703	0.00293	-0.64999	0.00359
H	1.17518	0.00184	-0.29165	0.00418	2.07647	0.00154
H	-0.35647	0.00061	-0.52545	0.01026	1.25655	0.00430
H	0.15810	0.00110	0.28692	0.00519	-1.28755	0.00258