

Supporting Information
Of
Planar Pentacoordinate Sulfur Atom

Complete citation of reference 51

Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

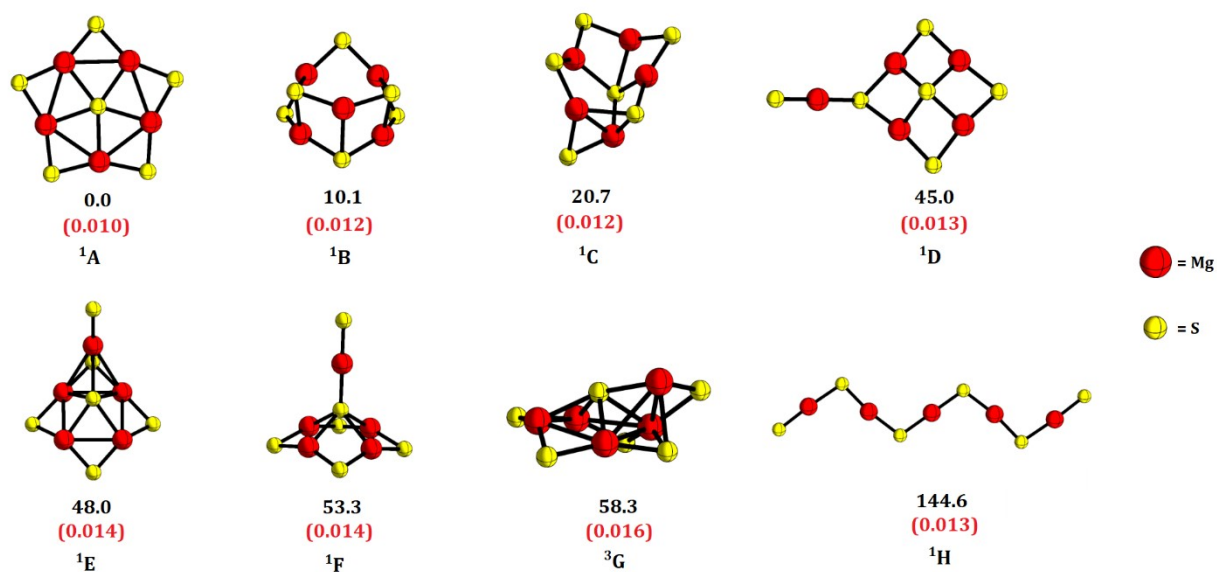


Fig S1. Relative energies (kcal/mol) of the isomers calculated at CCSD(T)/aug-cc-pVTZ//TPSS-D3(BJ)/def2-TZVP level. T_1 diagnostic values are shown in red font and within parenthesis.

Cartesian coordinates of the optimized geometries shown in Fig S1 at TPSS-D3(BJ)/aug-cc-pVTZ level.

¹A

16	0.000141000	-0.000062000	0.000025000
12	-1.920103000	-1.759485000	-0.000253000
12	-2.268122000	1.282697000	-0.000008000
12	0.518397000	2.549003000	0.000228000
12	2.590358000	0.295349000	0.000119000
12	1.079482000	-2.367571000	-0.000183000
16	-0.770484000	-3.789703000	-0.000374000
16	-3.843311000	-0.438400000	-0.000241000
16	-1.603825000	3.519134000	0.000203000
16	2.850957000	2.613787000	0.000415000
16	3.366514000	-1.904751000	0.000045000

¹B

12	1.897052000	1.206314000	0.766924000
12	0.000210000	1.380485000	-1.515527000
12	-1.663130000	-1.506223000	-0.183427000
12	-1.898686000	1.206132000	0.765568000
12	1.663965000	-1.505196000	-0.183994000
16	2.187821000	0.555116000	-1.610992000
16	-2.187752000	0.553114000	-1.611492000
16	2.624191000	-0.698400000	1.866751000
16	0.000720000	-3.027448000	-0.841078000

16	-2.622949000	-0.699787000	1.867393000
16	-0.001590000	2.731270000	0.592261000

¹C

12	1.983913447	-2.068425340	-0.258052355
12	1.298098124	0.633050504	-1.222699224
12	0.134282182	2.107317010	1.255522094
12	-0.853143667	-1.643131363	0.474118235
12	-2.121459870	1.455940658	-0.102707183
16	0.419092708	-3.658391043	0.415144004
16	-0.037159602	2.585225853	-1.145007754
16	1.107514048	-0.115746000	1.190264490
16	-2.003603990	2.541862979	2.047630092
16	2.850440176	-0.894395267	-2.101353616
16	-2.690151250	-0.732544611	-0.669841865

¹D

16	0.795685000	-0.000002000	1.360552000
12	2.591428000	-1.498365000	0.295792000
12	2.591515000	1.498413000	0.295893000
12	-0.327229000	-1.541811000	-0.182501000
12	-0.327112000	1.541747000	-0.182638000
16	1.227460000	-3.229339000	-0.557922000
16	-1.923277000	-0.000019000	-1.193869000
16	1.227559000	3.229316000	-0.557950000
16	4.392463000	-0.000024000	0.161066000

12	-4.050640000	-0.000045000	-0.130408000
16	-6.078362000	0.000115000	0.716019000

¹E

12	-0.420884000	1.539579000	-1.024764000
12	-0.419801000	-1.540261000	-1.024341000
12	2.062373000	-1.498336000	0.617761000
12	2.061489000	1.499238000	0.617158000
16	3.736576000	0.001062000	1.264295000
16	1.251108000	-3.135682000	-0.866533000
16	1.249404000	3.135704000	-0.867656000
16	-4.564630000	0.000333000	1.769377000
12	-2.779448000	-0.000657000	0.462257000
16	-0.040195000	-0.000030000	0.937621000
16	-2.010060000	-0.001059000	-1.973158000

¹F

12	0.843019000	2.176558000	0.069557000
12	0.840853000	-0.067263000	2.176547000
12	0.850565000	-2.174911000	-0.066658000
12	0.853127000	0.068945000	-2.173861000
16	1.353556000	2.207091000	2.350756000
16	1.366342000	2.349619000	-2.202415000
16	1.374426000	-2.203657000	-2.344916000
12	-2.980432000	-0.003449000	-0.005621000
16	-0.589236000	-0.001581000	-0.002638000

16	1.361577000	-2.346257000	2.208208000
16	-5.172014000	-0.005124000	-0.008969000

³G

12	2.589538000	-0.726311000	-0.464851000
12	0.073306000	-1.865183000	0.561258000
12	-2.210881000	-1.257740000	-1.425464000
12	1.329673000	1.947595000	-0.080551000
12	-1.555508000	1.014335000	0.489936000
16	3.583173000	1.388017000	-0.482043000
16	-2.177890000	-1.387862000	1.208190000
16	0.185937000	-0.096747000	-1.199562000
16	-3.630891000	0.594472000	-0.724738000
16	2.226514000	-2.745385000	0.690405000
16	-0.356439000	2.912983000	1.197502000

¹H

12	-7.201926000	0.373576000	0.025029000
12	-3.679437000	0.076517000	0.011750000
12	0.001453000	0.001964000	-0.051224000
12	3.681416000	-0.075402000	0.001173000
12	7.200483000	-0.376734000	0.027140000
16	-5.242447000	1.698178000	0.081393000
16	-8.938023000	-0.974310000	-0.031184000
16	-1.850250000	-1.315252000	-0.048304000
16	1.853873000	1.318255000	-0.064886000
16	5.240712000	-1.700701000	0.073911000
16	8.934644000	0.973889000	-0.021331000

