

Supporting Information

for

Structural and Solvent Effects on the C-S Bond Cleavage in Aryl

Triphenylmethyl Sulfide Radical Cations

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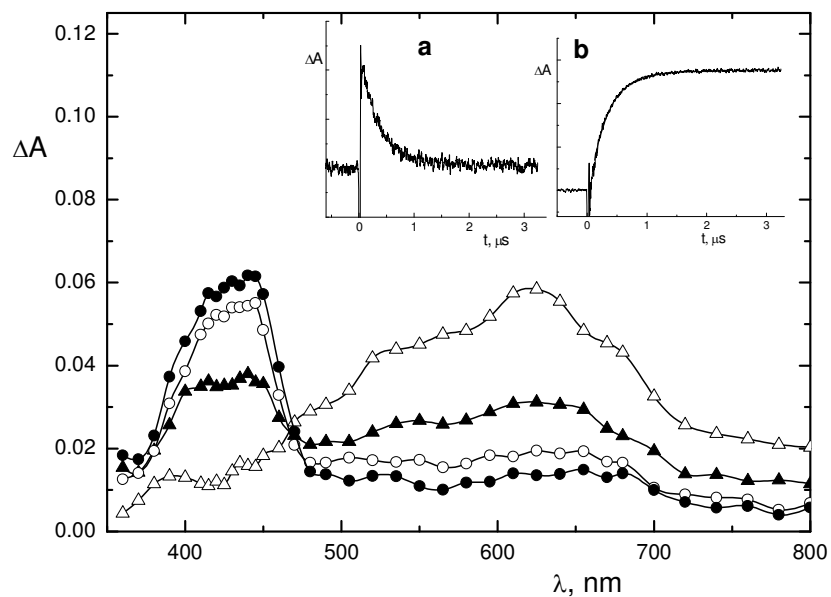


Figure S1. Time-resolved absorption spectra of the MeOP^+ (1.6×10^{-4} M)/3,4- $(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3\text{SC}(\text{C}_6\text{H}_5)_3$ (**1**) (1.0×10^{-2} M) system in N_2 -saturated CH_3CN recorded 0.4 (\triangle), 6.4 (\blacktriangle), 17.9 (\circ) and 32 (\bullet) μs after the laser pulse. Insets: (a) decay kinetics recorded at 600 nm, (b) buildup kinetics recorded at 430 nm.

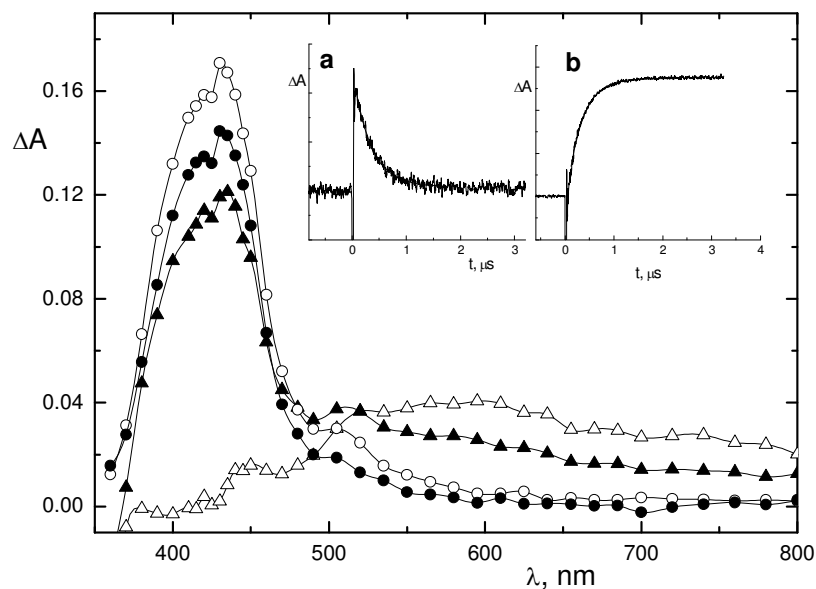


Figure S2. Time-resolved absorption spectra of the MeOP^+ (1.6×10^{-4} M)/4- $\text{CH}_3\text{C}_6\text{H}_4\text{SC}(\text{C}_6\text{H}_5)_3$ (**3**) (1.0×10^{-2} M) system in N_2 -saturated CH_3CN recorded 0.088 (\triangle), 0.3 (\blacktriangle), 1.05 (\circ) and 3.2 (\bullet) μs after the laser pulse. Insets: (a) decay kinetics recorded at 600 nm, (b) buildup kinetics recorded at 430 nm.

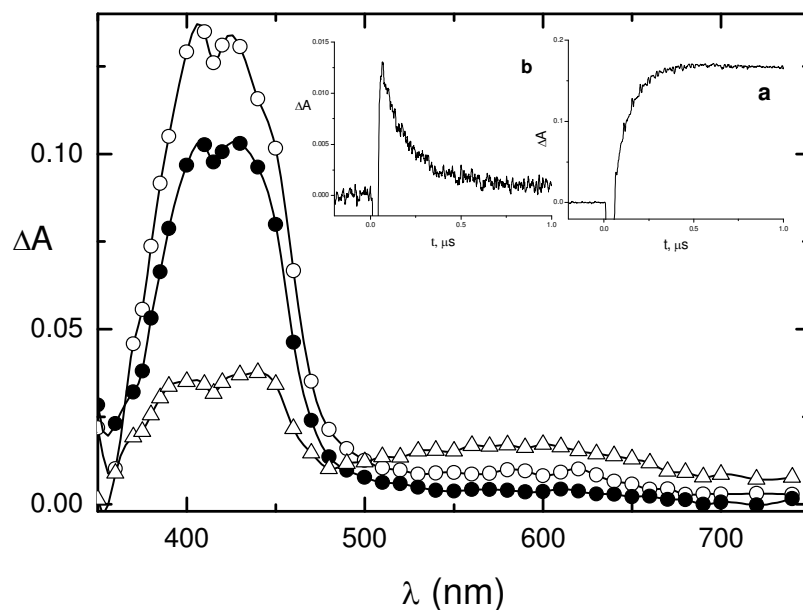


Figure S3. Time-resolved absorption spectra of the MeOP^+ ($1.6 \times 10^{-4} \text{ M}$)/ $\text{C}_6\text{H}_5\text{SC}(\text{C}_6\text{H}_5)_3$ (**4**) ($1.0 \times 10^{-2} \text{ M}$) system in N_2 -saturated CH_3CN recorded 0.088 (\triangle), 0.42 (\circ) and 3.1 (\bullet) μs after the laser pulse. Insets: (a) decay kinetics recorded at 550 nm, (b) buildup kinetics recorded at 430 nm.

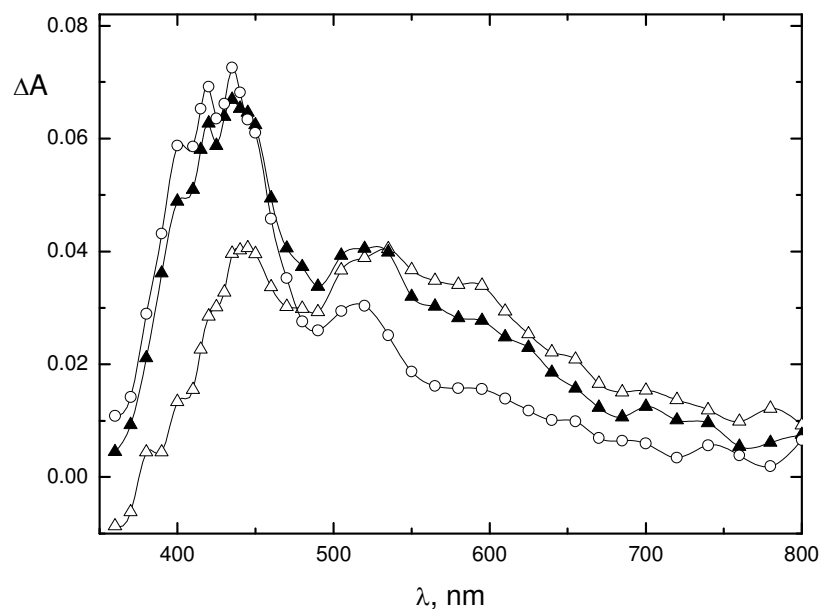


Figure S4. Time-resolved absorption spectra of the MeOP^+ ($1.6 \times 10^{-4} \text{ M}$)/ $4\text{-BrC}_6\text{H}_4\text{SC}(\text{C}_6\text{H}_5)_3$ (**5**) ($1.0 \times 10^{-2} \text{ M}$) system in N_2 -saturated CH_3CN recorded 0.2 (\triangle), 0.5 (\blacktriangle) and 1.5 (\circ) μs after the laser pulse.

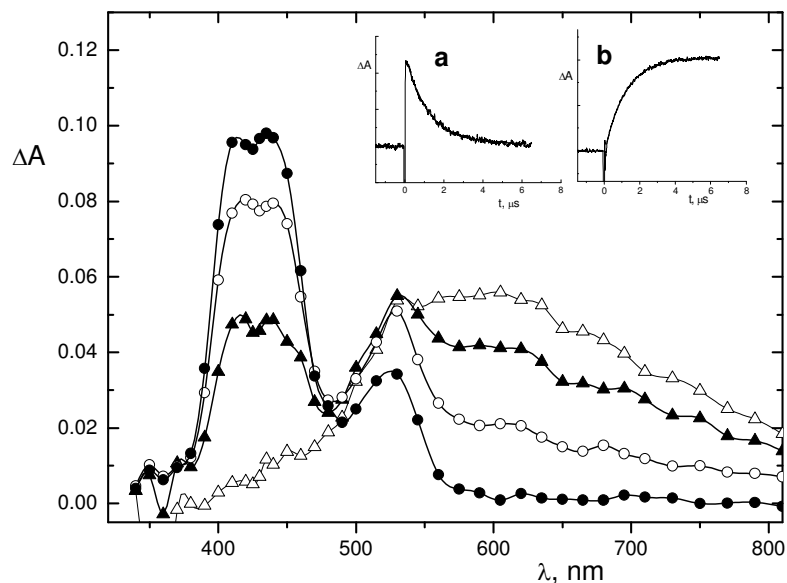


Figure S5. Time-resolved absorption spectra of the MeOP^+ ($1.6 \times 10^{-4} \text{ M}$)/4- $\text{MeOC}_6\text{H}_4\text{SC}(\text{C}_6\text{H}_5)_3$ (**2**) ($1.0 \times 10^{-2} \text{ M}$) system in N_2 -saturated CH_2Cl_2 recorded recorded 0.18 (\triangle), 0.66 (\blacktriangle), 1.9 (\circ) and 6.4 (\bullet) μs after the laser pulse. Insets: (a) decay kinetics recorded at 580 nm, (b) buildup kinetics recorded at 420 nm.

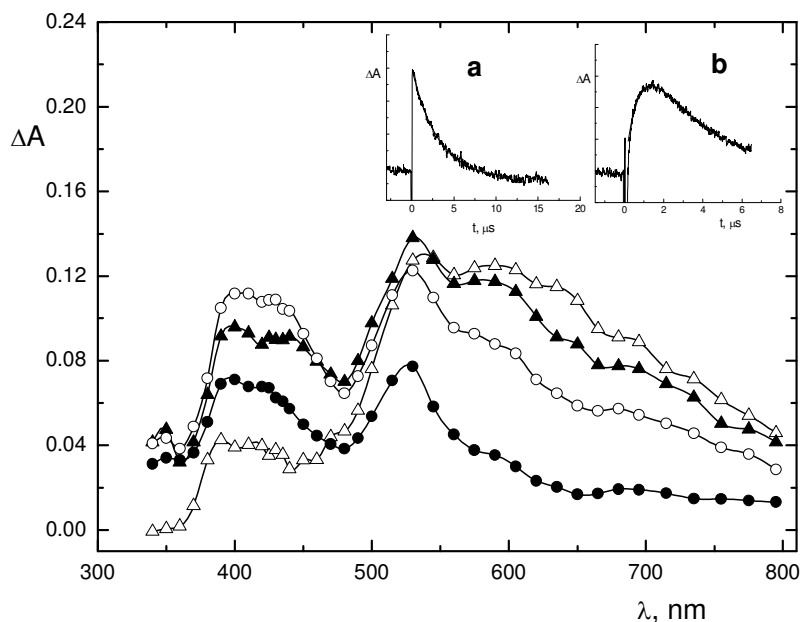


Figure S6. Time-resolved absorption spectra of the MeOP^+ ($1.6 \times 10^{-4} \text{ M}$)/4- $\text{MeOC}_6\text{H}_4\text{SC}(\text{C}_6\text{H}_5)_3$ (**2**) ($1.0 \times 10^{-2} \text{ M}$) system in N_2 -saturated $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$ 1:1 recorded 0.14 (\triangle), 0.30 (\blacktriangle), 0.74 (\circ) and 3.2 (\bullet) μs after the laser pulse. Insets: (a) decay kinetics recorded at 580 nm, (b) buildup kinetics recorded at 420 nm.

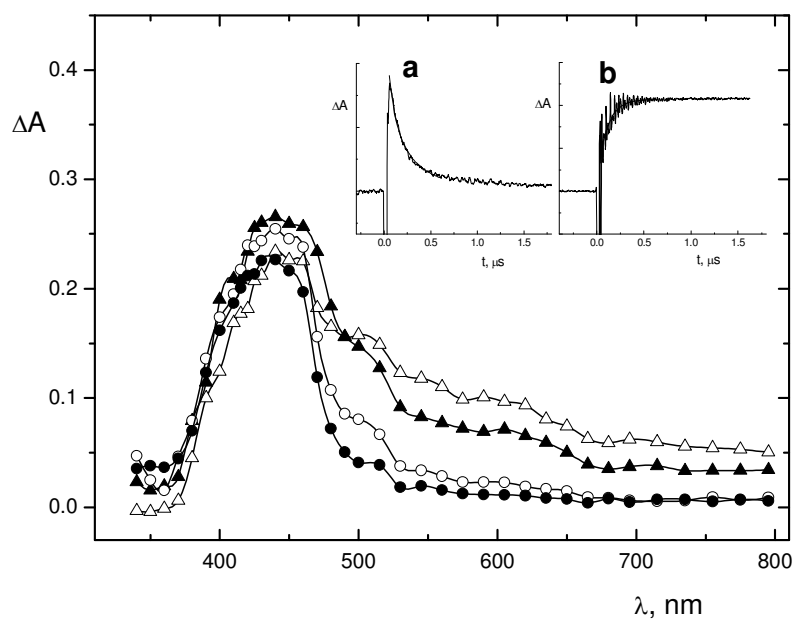


Figure S7. Time-resolved absorption spectra of the MeOP^+ ($1.6 \times 10^{-4} \text{ M}$)/4- $\text{MeC}_6\text{H}_4\text{SC}(\text{C}_6\text{H}_5)_3$ (**3**) ($1.0 \times 10^{-2} \text{ M}$) system in N_2 -saturated CH_2Cl_2 recorded 0.064 (\triangle), 0.16 (\blacktriangle), 0.93 (\circ) and 3.2 (\bullet) μs after the laser pulse. Insets: (a) decay kinetics recorded at 580 nm, (b) buildup kinetics recorded at 430 nm.

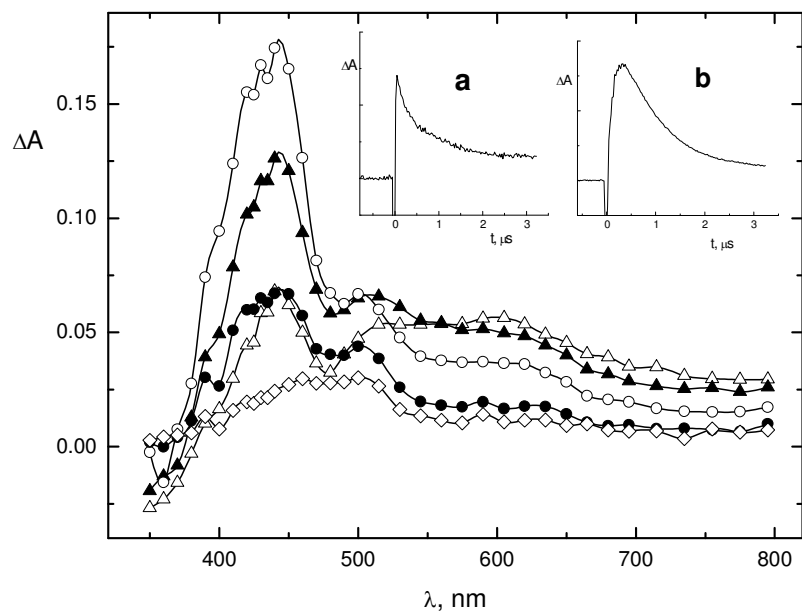


Figure S8. Time-resolved absorption spectra of the MeOP^+ ($1.6 \times 10^{-4} \text{ M}$)/4- $\text{MeC}_6\text{H}_4\text{SC}(\text{C}_6\text{H}_5)_3$ (**3**) ($1.0 \times 10^{-2} \text{ M}$) system in N_2 -saturated $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$ 1:1 recorded 0.04 (\triangle), 0.11 (\blacktriangle), 0.50 (\circ), 1.4 (\diamond) and 3.2 (\bullet) μs after the laser pulse. Insets: (a) decay kinetics recorded at 600 nm, (b) buildup kinetics recorded at 420 nm.

Cyclic Voltammetry

Oxidation potentials of 4-methoxyphenyl triphenylmethyl sulfide (**2**) and 4-methylphenyl triphenylmethyl sulfide (**3**) (E_1) have been determined by cyclic voltammetry as the anodic peak potential E_p of the irreversible oxidation wave. Cyclic voltammetry at the steady disk electrode (glassy carbon disk, 1.5 mm in diameter) was carried out at 25 °C in CH₃CN containing Bu₄NBF₄ (0.1 M) as the supporting electrolyte and the substrate (1 mM). A three-electrode circuit was used with a home-made potentiostat with positive feedback ohmicdrop compensation and PLI hardware (Vernier Software & Technology) controlled by a program written in C++ language for Windows 95/98. The auxiliary electrode was a platinum wire (surface 1 cm²) and an Ag/AgCl (KCl 3M) electrode was used as reference; the E_p values are then referred to SCE. The sweep scan was 500 mV/s. In Figure S9 is reported as an example the cyclic voltammogram of 4-methoxyphenyl triphenylmethyl sulfide (**2**) E_1 values are reported in the second column of Table S1.

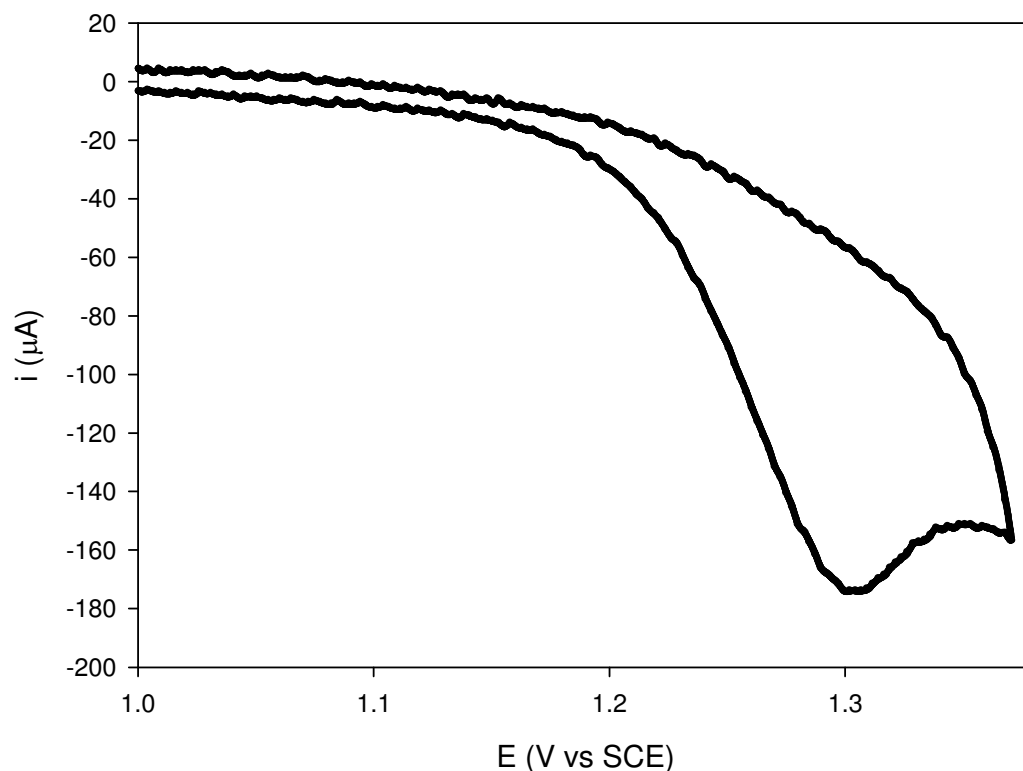
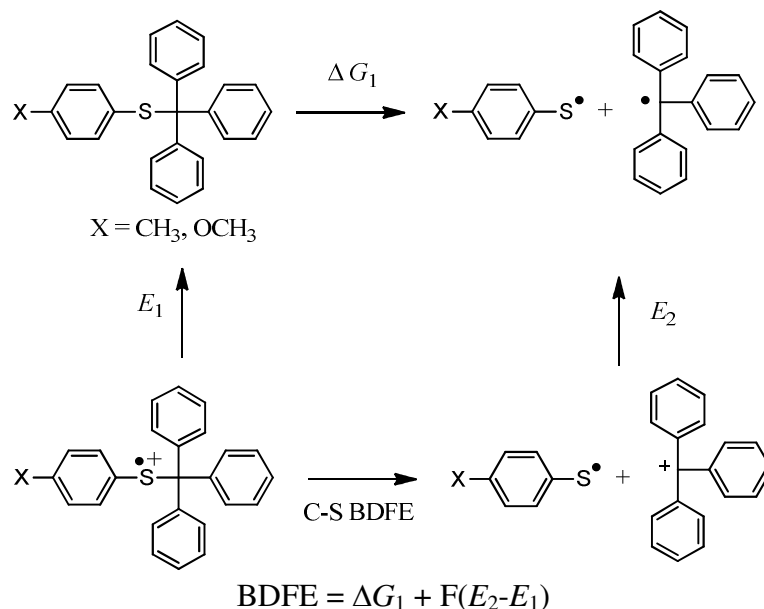


Figure S9. Cyclic voltammogram of **2** (1 mM) in CH₃CN containing Bu₄NBF₄ (0.1 M) as the supporting electrolyte. Voltage sweep rate 500 mV/s⁻¹

C-S BDFEs for the sulfide radical cations

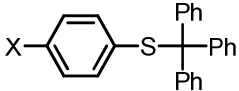
The C-S BDFE values for the sulfide radical cations **2^{•+}**-**3^{•+}** are calculated by using the following thermochemical cycle (Scheme S1):



Scheme S1

E_1 values, the oxidation peak potentials of aryl triphenylmethyl sulfides **2-3**, have been measured by cyclic voltammetry. E_2 , the reduction potential of triphenylmethyl cation (0.21 V vs SCE in MeCN) is available in the literature.^{S1} ΔG_1 , the C-S bond dissociation free energies of the neutral sulfides, have been determined from the C-S BDEs, obtained by DFT calculations, and applying an entropic correction ($T\Delta S^\circ$) of 10 kcal mol⁻¹. The latter value is the entropy change associated with the homolytic C-S bond cleavage of thioanisole.^{S2} The E_1 , C-S BDE and C-S BDFE values are reported in Table S1.

Table S1. Peak Oxidation Potentials (E_p) and C-S BDE of Sulfides **2-3** and C-S BDFEs of Sulfide Radical Cations **2^{•+}**-**3^{•+}**.

	E_1^a	C-S BDE (neutral substrates) ^b	C-S BDFE (radical cations) ^b
2 X=OCH ₃ Y=H	1.30	24.9	-10.2
3 X=CH ₃ Y=H	1.48	26.1	-13.2

^a Peak oxidation potentials E_p (V vs SCE in MeCN) from cyclic voltammetry. ^b kcal mol⁻¹.

Cartesian Coordinates, energies, ZPVE from DFT calculations for neutral sulfides 2-3

Sulfide 2

conformer 1, E = -1481.3494047 a.u., ZPVE = 0.404646a.u.

H	1.71450000	-2.32834800	-1.42839400
C	2.25490300	-1.40893300	-1.23718000
C	3.62903300	0.95731300	-0.73425100
C	1.56489800	-0.19093200	-1.27665500
C	3.60721300	-1.44772500	-0.95492700
C	4.30250400	-0.26403100	-0.69447200
C	2.27104700	0.98526000	-1.03436100
S	-0.14602100	-0.16793300	-1.74369100
H	4.14873800	-2.38581400	-0.92492800
H	-4.57963500	-1.81820500	-2.77468300
H	1.75538000	1.93684700	-1.07427900
H	4.14816700	1.88819600	-0.54630900
H	-5.66133600	1.24169400	0.02420900
C	-1.14359700	-0.01598400	-0.12051400
C	-0.89042200	1.34927600	0.52459300
C	-0.77506500	-1.18177100	0.79269400
C	-2.59846500	-0.09651500	-0.60713900
C	-0.03488200	-3.32469800	2.46508900
C	0.46709300	-1.20070100	1.44123400
C	-1.64012800	-2.25537300	1.01585300
C	-1.27422100	-3.31469700	1.84000500
C	0.83342700	-2.25783600	2.26288500
H	1.15266400	-0.37321000	1.31120200
H	-2.61741700	-2.26664800	0.55111000
H	-1.97033400	-4.13173400	1.99625300
H	1.80299400	-2.24373100	2.74872100
H	0.24946600	-4.14959500	3.10910600
H	-6.31687700	-0.37199800	-1.74489000
O	5.62189200	-0.40048300	-0.41953300
C	-0.62772200	3.89749200	1.68993800
C	-0.82217200	2.50113600	-0.26571500
C	-0.84754300	1.50514100	1.91105300
C	-0.71256600	2.76557800	2.48790900
C	-0.69071600	3.75835200	0.30661900
H	-0.87411500	2.40081100	-1.34362600
H	-0.92974300	0.63721500	2.55323000
H	-0.67831800	2.85603500	3.56827800
H	-0.64006000	4.63422500	-0.33141400
H	-0.52028500	4.87893800	2.13857600
C	-5.28302600	-0.29830800	-1.42605500
C	-3.58739600	0.70705300	-0.03617000
C	-2.98558000	-1.00992100	-1.59444500
C	-4.31003000	-1.10588200	-2.00251900
C	-4.91480300	0.60492300	-0.43792000
H	-3.32271300	1.42320000	0.73156500

H	-2.24196100	-1.65542100	-2.04610800
C	6.37256100	0.76642800	-0.15244900
H	7.38922200	0.43013300	0.04341700
H	5.99076200	1.29503500	0.72774700
H	6.37604100	1.44529100	-1.01205700

Sulfide 2

conformer 2, E = -1481.3494254 a.u., ZPVE = 0.404702 a.u.

H	1.97558000	-2.03368700	-1.40993900
C	2.40213500	-1.05752500	-1.21179000
C	3.48215200	1.44268900	-0.68636200
C	1.57793300	0.06459200	-1.25205500
C	3.75725100	-0.94566100	-0.91763600
C	4.30036600	0.30932600	-0.64625900
C	2.14088000	1.32140200	-0.99597800
S	-0.11905900	-0.11788700	-1.73330800
H	4.37023200	-1.83732700	-0.89754800
H	-4.31249400	-2.31296900	-2.75632900
H	1.51684800	2.20569100	-1.03564800
H	3.92615000	2.41008700	-0.48295000
H	-5.78080500	0.65615600	-0.03697200
C	-1.14347300	-0.05072800	-0.12160200
C	-1.06307300	1.34926200	0.49335400
C	-0.64592000	-1.14293300	0.82076300
C	-2.57336600	-0.31716600	-0.61619000
C	0.32730300	-3.14177400	2.55170100
C	0.58274400	-0.99754300	1.47914600
C	-1.37808800	-2.30746900	1.06311600
C	-0.89701000	-3.29565700	1.91594200
C	1.06345500	-1.98326300	2.33021200
H	1.16537900	-0.09662500	1.33593500
H	-2.34209400	-2.44678200	0.59141600
H	-1.49213300	-4.18623800	2.08694900
H	2.01746400	-1.83976500	2.82588600
H	0.70045000	-3.91045500	3.21956300
H	-6.22079100	-1.06390800	-1.77235300
O	5.60166100	0.53075200	-0.34223100
C	-1.11884100	3.93557700	1.60098100
C	-1.12552000	2.48303100	-0.32308700
C	-1.05345300	1.53972800	1.87606000
C	-1.07585500	2.81971400	2.42442800
C	-1.15096800	3.75930500	0.22088100
H	-1.15332200	2.35376600	-1.39878400
H	-1.03746200	0.68272400	2.53768100
H	-1.06268400	2.93767600	3.50257800
H	-1.19786900	4.62056400	-0.43695800
H	-1.13286600	4.93254700	2.02738700
C	-5.20639500	-0.85914400	-1.44830600
C	-3.65718700	0.37395400	-0.07090000

C	-2.83850700	-1.29240800	-1.58450100
C	-4.13789100	-1.55634900	-1.99910300
C	-4.95881000	0.10362400	-0.47897900
H	-3.48787000	1.13408500	0.68134000
H	-2.01844800	-1.85339600	-2.01625500
C	6.47448100	-0.57947500	-0.29852400
H	7.45420400	-0.18045600	-0.04167400
H	6.53193100	-1.08129900	-1.27046500
H	6.16621500	-1.30087300	0.46602800

Sulfide 2

conformer 3, E = -1481.3480872 a.u., ZPVE = 0.404341 a.u.

H	-1.42688500	2.34776500	-1.01169900
C	-2.06794600	1.47619400	-0.97035500
C	-3.73433000	-0.75170200	-0.87538500
C	-1.54393200	0.21188500	-1.26278000
C	-3.39739000	1.62531400	-0.62270000
C	-4.23991400	0.51148400	-0.57250500
C	-2.39261400	-0.89058000	-1.21395100
S	0.13927100	-0.01225100	-1.78717500
H	-3.81112300	2.59992200	-0.39182400
H	2.50118100	2.65157200	3.35910400
H	-1.99618600	-1.87350000	-1.43877700
H	-4.36634300	-1.62961900	-0.84635800
H	1.46392200	4.61136800	-0.30808500
C	1.12032900	-0.08788300	-0.16492800
C	2.51268800	-0.60738800	-0.55140100
C	0.34326300	-1.04050300	0.73140600
C	1.35664900	1.29899600	0.45246300
C	-1.21640800	-2.82199300	2.24867900
C	0.39062100	-2.41969600	0.49755400
C	-0.52850200	-0.57317500	1.71530700
C	-1.29697300	-1.45475800	2.46994900
C	-0.37202800	-3.30039400	1.25056800
H	1.02763900	-2.80383800	-0.29075400
H	-0.61659700	0.49111000	1.89428100
H	-1.96446200	-1.06314600	3.22976800
H	-0.30866900	-4.36549800	1.05490100
H	-1.81033300	-3.51013600	2.84020200
H	2.25592100	4.74283700	2.04067200
O	-5.52634500	0.75816300	-0.22532100
C	5.13816000	-1.39907900	-1.16810800
C	3.11563200	-0.22416200	-1.75107000
C	3.25889600	-1.37887300	0.34232800
C	4.55681600	-1.77076000	0.03777100
C	4.41027700	-0.62215800	-2.06053300
H	2.57353200	0.39793700	-2.45427100
H	2.82229600	-1.68315000	1.28601200
H	5.11355100	-2.37148200	0.74887000

H	4.85109900	-0.31753300	-3.00341800
H	6.14939800	-1.70822700	-1.40791400
C	2.00864900	3.78435700	1.59803200
C	1.24327700	2.47856300	-0.27987700
C	1.82699300	1.38706800	1.76752500
C	2.14339800	2.61301500	2.33587500
C	1.56284000	3.70914300	0.28601400
H	0.90951500	2.42738900	-1.30937500
H	1.95034200	0.48501900	2.35553800
C	-6.42021100	-0.33400300	-0.16173600
H	-7.38190500	0.08253500	0.13291100
H	-6.10070700	-1.06949700	0.58454500
H	-6.52221100	-0.82461100	-1.13582300

Sulfide 2

conformer 4, E = -1481.3479652 a.u., ZPVE = 0.404343 a.u.

H	-1.76334200	-2.18070400	-1.41409500
C	-2.27213600	-1.24590200	-1.21167600
C	-3.56790000	1.15746100	-0.68154500
C	-1.55250200	-0.04730600	-1.27974900
C	-3.61464500	-1.24756500	-0.88524300
C	-4.27107600	-0.04478200	-0.61302200
C	-2.21832800	1.14717800	-1.02015100
S	0.14868500	-0.07853600	-1.79449000
H	-4.17818900	-2.17133900	-0.83027500
H	0.22739100	-4.49967300	0.98623300
H	-1.68211500	2.08610500	-1.07776200
H	-4.05567900	2.10295500	-0.48285100
H	-1.85493000	-1.45975400	3.17610700
C	1.12207000	-0.06144700	-0.16705700
C	1.18470100	1.33413400	0.47268000
C	2.56989700	-0.40326800	-0.54834900
C	0.46133800	-1.11549600	0.70924900
C	5.27656600	-0.86584000	-1.14872700
C	3.12707800	0.04737300	-1.74652200
C	3.40109400	-1.07399700	0.35187100
C	4.73904400	-1.30309800	0.05564400
C	4.46300200	-0.18814800	-2.04772200
H	2.51630800	0.59452200	-2.45565200
H	2.99985700	-1.42793600	1.29395800
H	5.36182100	-1.82849700	0.77158600
H	4.86774000	0.16535800	-2.98973500
H	6.31958000	-1.04820500	-1.38228800
H	-1.39182800	-3.86206900	2.75968100
O	-5.58500800	-0.14517400	-0.29706900
C	1.52434000	3.86306400	1.65843500
C	0.94721000	2.50264900	-0.24776700
C	1.61938400	1.45865200	1.79703200
C	1.78172500	2.70535200	2.38501000

C	1.11231500	3.75423400	0.33768200
H	0.63913500	2.42681800	-1.28372800
H	1.83665700	0.56943200	2.37723500
H	2.11571600	2.77122800	3.41488000
H	0.92020900	4.64686500	-0.24810800
H	1.65174100	4.83768600	2.11635300
C	-0.88003100	-3.09751800	2.18564000
C	-0.47284600	-0.77368500	1.68744300
C	0.68454500	-2.47470200	0.46080900
C	0.02951700	-3.45349800	1.19369500
C	-1.13352000	-1.75416600	2.42177600
H	-0.69573100	0.26894300	1.87654900
H	1.37390300	-2.76594400	-0.32325000
C	-6.29596400	1.04267900	-0.01584900
H	-7.31502400	0.73518100	0.21247000
H	-6.30707200	1.71646200	-0.87949200
H	-5.87430900	1.56637300	0.84905300

Sulfide 3

conformer 1, E = -1405.9803350 a.u., ZPVE = 0.399415a.u.

H	2.11061400	-2.16548000	-1.49764000
C	2.59020700	-1.21645700	-1.28887800
C	3.80345500	1.20979700	-0.72633400
C	1.82363200	-0.05044000	-1.29101000
C	3.95036700	-1.16231800	-1.01315900
C	4.57971300	0.04834400	-0.72339500
C	2.44705800	1.16898800	-1.01736200
S	0.10886700	-0.14039200	-1.74842800
H	4.53095600	-2.07974800	-1.01517000
H	6.61051900	0.34611200	-1.36268400
H	1.86549300	2.08268200	-1.02468400
H	4.27102200	2.16484300	-0.50629200
C	6.05455800	0.10886300	-0.44941400
C	-0.88634600	-0.03433600	-0.12194900
C	-0.71877700	1.35112900	0.50780900
C	-0.44156400	-1.16523900	0.80200800
C	-2.33550700	-0.21310800	-0.60072800
C	0.43238000	-3.23674900	2.49974400
C	-1.24231300	-2.28262300	1.04879700
C	0.80496700	-1.10383100	1.43939200
C	1.23697100	-2.12556300	2.27370800
C	-0.81023000	-3.30682300	1.88533400
H	-2.22119200	-2.35653500	0.59327000
H	1.44202800	-0.24127500	1.29165800
H	2.20761200	-2.04837200	2.75142200
H	-1.45761000	-4.15943900	2.05987100
H	0.76803000	-4.03389800	3.15393800
H	6.43064100	-0.84585900	-0.07623000
H	6.29269100	0.88090000	0.28577200

C	-0.61479400	3.92269000	1.64548400
C	-0.73469100	2.49663000	-0.29451900
C	-0.67322700	1.52346600	1.89203600
C	-0.61657400	2.79608100	2.45519100
C	-0.68152300	3.76551900	0.26420800
H	-0.78841000	2.38225100	-1.37094900
H	-0.69140800	0.65873800	2.54339900
H	-0.57743100	2.89980400	3.53417500
H	-0.69412600	4.63612000	-0.38279100
H	-0.56777900	4.91365300	2.08340800
C	-5.00526400	-0.59517100	-1.40320400
C	-3.37081900	0.53332000	-0.03464300
C	-2.66813200	-1.16222000	-1.57409800
C	-3.98553100	-1.34705200	-1.97424000
C	-4.69082000	0.34209100	-0.42831900
H	-3.14884600	1.27448800	0.72277400
H	-1.88718900	-1.76558400	-2.02101100
H	-4.21274100	-2.08508400	-2.73581500
H	-5.47418900	0.93622500	0.02956700
H	-6.03370200	-0.73820800	-1.71590000

Sulfide 3

conformer 2, E = -1405.9789328 a.u., ZPVE = 0.399055 a.u.

H	-2.19007100	-1.96569500	-1.50564900
C	-2.61805700	-0.99944200	-1.26676300
C	-3.70036800	1.46900800	-0.62977500
C	-1.80072900	0.13098600	-1.28185800
C	-3.96223800	-0.88918700	-0.93847400
C	-4.52694600	0.34460500	-0.61367600
C	-2.35688400	1.37093600	-0.96690600
S	-0.10357700	-0.03843600	-1.79467100
H	-4.58211600	-1.78046500	-0.92832500
H	-6.36444500	-0.44351900	0.19037300
H	-1.73768200	2.25912900	-0.97804900
H	-4.11552200	2.44077300	-0.37998100
C	-5.98741700	0.46373900	-0.28666600
C	0.86498800	-0.07894300	-0.16548800
C	1.06406900	1.31687500	0.44497800
C	2.27244800	-0.56628600	-0.54019800
C	0.10597600	-1.04556000	0.73213200
C	4.92048100	-1.29530200	-1.13615600
C	3.02740900	-1.32494800	0.35692600
C	2.87748800	-0.16354100	-1.73245700
C	4.18341700	-0.53072500	-2.03184000
C	4.33674500	-1.68577500	0.06249600
H	2.58908500	-1.64386100	1.29492300
H	2.32785000	0.44976400	-2.43762900
H	4.62586100	-0.21176800	-2.96920100
H	4.90035200	-2.27731000	0.77586900

H	5.94056900	-1.58045800	-1.36805400
H	-6.57800800	0.62486300	-1.19483700
H	-6.17969900	1.30599600	0.38135800
C	1.64908700	3.82335200	1.58046000
C	0.91444200	2.49027500	-0.29060000
C	1.53659600	1.42238900	1.75801800
C	1.81981300	2.65861800	2.32144200
C	1.20095800	3.73130600	0.27035500
H	0.57863700	2.42644400	-1.31874700
H	1.68823900	0.52597600	2.34805400
H	2.18027800	2.71056300	3.34313500
H	1.07456200	4.62840500	-0.32630200
H	1.87089500	4.78984800	2.01915800
C	-1.41599600	-2.85697200	2.25135300
C	-0.77306600	-0.59508100	1.71714400
C	0.18087100	-2.42359200	0.49866600
C	-0.56305100	-3.31895300	1.25286500
C	-1.52334300	-1.49168400	2.47247700
H	-0.88166500	0.46727600	1.89619200
H	0.82437900	-2.79504400	-0.29047900
H	-0.47930800	-4.38260100	1.05710800
H	-2.19825600	-1.11358700	3.23253500
H	-1.99686100	-3.55636000	2.84255600

Cartesian Coordinates, energies, ZPVE from DFT calculations for triphenylmethyl and arylsulfenyl radicals

Triphenylmethyl radical

conformer 1, E = -735.5298370 a.u., ZPVE = 0.277904 a.u.

C	0.00174900	-0.00022100	-0.00018900
C	1.45592100	-0.06625100	-0.00015700
C	-0.78393400	-1.22649600	0.00067400
C	-0.66939000	1.29241700	-0.00072100
C	-2.30675800	-3.60093500	0.00234600
C	-2.01794400	-1.30404000	0.67645800
C	-0.34042300	-2.38079700	-0.67484800
C	-1.09239600	-3.54477400	-0.67657200
C	-2.76206500	-2.47302500	0.68007600
H	-2.37529800	-0.43781100	1.22124400
H	0.59497800	-2.34445600	-1.22122100
H	-0.73330100	-4.41305600	-1.21855400
H	-3.70085500	-2.50811700	1.22232900
H	-2.89199800	-4.51361700	0.00305900
C	4.27438600	-0.19391800	-0.00012100
C	2.23299300	0.90439400	-0.66374500
C	2.14203800	-1.10313000	0.66352800
C	3.52644500	-1.16122000	0.66609000
C	3.61700300	0.83708100	-0.66629200
H	1.73299900	1.70221200	-1.20062400
H	1.57204000	-1.85241800	1.20057600
H	4.02731700	-1.96237500	1.19890300
H	4.18830900	1.58965800	-1.19906400
H	5.35746800	-0.24300100	-0.00011900
C	-1.97033500	3.79518400	-0.00200600
C	-0.12353700	2.40120100	0.67604100
C	-1.89052200	1.48200500	-0.67761100
C	-2.52546600	2.71374300	-0.68102000
C	-0.76672600	3.62865500	0.67799600
H	0.80426100	2.27972300	1.22311300
H	-2.32438300	0.65210800	-1.22339000
H	-3.45662900	2.83431800	-1.22414900
H	-0.33080300	4.46039600	1.22092800
H	-2.47034100	4.75720900	-0.00259900

p-Methoxyphenyl sulfenyl radical

conformer 1, E = -745.7761379 a.u., ZPVE = 0.123217 a.u.

H	1.06065300	-2.13604900	-0.00009700
C	0.61832300	-1.14682900	-0.00006700
C	-0.48222600	1.41031000	-0.00001700
C	1.48074400	-0.02733900	-0.00000300
C	-0.75606900	-1.00400400	-0.00010200

C	-1.31659400	0.27983500	-0.00006900
C	0.88237900	1.25928400	0.00001800
S	3.18010900	-0.21922800	0.00005100
H	-1.38458300	-1.88502700	-0.00017000
O	-2.63783600	0.53063000	-0.00012000
H	1.52997000	2.12797200	0.00007000
H	-0.94431700	2.39038900	0.00000400
H	-3.41337300	-1.17960700	-0.89491500
H	-4.53574900	-0.12532000	0.00042100
H	-3.41288200	-1.17952700	0.89524300
C	-3.53968600	-0.56296100	0.00017200

p-Methylphenyl sulfenyl radical

conformer 1, E = -670.4048917 a.u., ZPVE = 0.117775 a.u.

H	-0.88664600	-2.14541500	-0.00631100
C	-0.33742200	-1.21121300	-0.00477500
C	1.04238800	1.20399900	-0.01116100
C	-1.06800500	-0.00008600	-0.00029700
C	1.04261900	-1.20356900	-0.01122200
C	1.76063300	0.00046300	-0.01118900
C	-0.33793200	1.21112600	-0.00480900
S	-2.78197800	-0.00014300	0.00746200
H	1.58409300	-2.14432200	-0.01822800
H	3.66671900	-0.87575600	-0.49301500
H	-0.88735800	2.14520500	-0.00635800
H	1.58349400	2.14492700	-0.01822200
C	3.25790500	-0.00003800	0.01514000
H	3.62324900	-0.02257600	1.04804500
H	3.66697900	0.89612500	-0.45542500

Cartesian Coordinates, energies, ZPVE from DFT calculations for radical cations 2⁺-3⁺

Radical cation 2⁺

conformer 1, E = -1477.4396609 a.u., ZPVE = 0.403391 a.u.

H	-1.53294600	0.48593300	1.16080500
C	-2.23929500	0.27363300	0.37259800
C	-4.09331200	-0.30268500	-1.67786200
C	-1.78201900	-0.09152400	-0.92266200
C	-3.58230700	0.35589600	0.62758500
C	-4.53420300	0.07079000	-0.38691100
C	-2.74564900	-0.38286600	-1.93261400
S	-0.14474400	-0.21422000	-1.46268500
H	-3.95255700	0.63673800	1.60541600
H	4.15965600	3.42070000	1.02741600
H	-2.40596800	-0.66987600	-2.92104300
H	-4.80021300	-0.52615500	-2.46445800
H	0.12541600	4.57167600	0.13044700
C	1.20700900	-0.02638400	-0.04261900
C	2.37079900	-0.76444900	-0.72784600
C	0.70048900	-0.70577400	1.22712400
C	1.52204000	1.46554700	0.12754000
C	-0.17738300	-1.98801700	3.57054800
C	0.17970300	-2.00927000	1.18321300
C	0.77674900	-0.06051200	2.46635800
C	0.34328200	-0.69979800	3.62843200
C	-0.25701500	-2.64188400	2.34056500
H	0.12004200	-2.53767500	0.23858000
H	1.18103300	0.94039000	2.53347100
H	0.41876700	-0.18469700	4.57883500
H	-0.65484400	-3.64834000	2.28398300
H	-0.51388200	-2.48289000	4.47383400
H	2.43487700	5.19416900	0.79651700
O	-5.80175000	0.18160900	-0.02251600
C	4.55025000	-2.00265700	-1.99552600
C	2.84634300	-0.29583000	-1.96459300
C	3.01587000	-1.85398900	-0.13323300
C	4.10159400	-2.46236100	-0.76244900
C	3.91801200	-0.91333300	-2.59553800
H	2.38877600	0.56958100	-2.43104800
H	2.69471500	-2.22069200	0.83127900
H	4.59575900	-3.29722900	-0.27987900
H	4.26625300	-0.53901900	-3.55078900
H	5.38975200	-2.48217800	-2.48466800
C	2.17940600	4.15716000	0.61463900
C	0.55917300	2.47364900	0.00593400
C	2.82525200	1.83131500	0.49256300
C	3.14698100	3.16229100	0.74125500
C	0.88539800	3.80756300	0.24335400
H	-0.45463300	2.23831600	-0.28876400

H	3.59248400	1.07400700	0.58880400
C	-6.86750200	-0.08543600	-0.95764700
H	-7.78297700	0.07982700	-0.39718500
H	-6.82167700	-1.12077200	-1.30104100
H	-6.81593300	0.60637300	-1.80067700

Radical cation $2^{+\bullet}$

conformer 2, E = -1477.4392070 a.u., ZPVE = 0.403351 a.u.

H	-1.64674700	0.41171500	0.91402900
C	-2.27667900	0.18415000	0.06718100
C	-3.91634700	-0.43291100	-2.13007700
C	-1.69600500	-0.16353200	-1.18002500
C	-3.64410600	0.23285700	0.21422400
C	-4.48693800	-0.07524100	-0.88053500
C	-2.55840100	-0.47843600	-2.27542700
S	-0.01319700	-0.23838000	-1.56380700
H	-4.06339700	0.50420400	1.17306500
H	4.58538600	-0.40795800	-3.22754700
H	-2.12672600	-0.75290200	-3.23074600
H	-4.58344200	-0.66571500	-2.95011000
H	4.67917300	-3.19441800	0.03465400
C	1.19189700	-0.01908200	-0.02469700
C	0.59140900	-0.72164300	1.19128800
C	1.44625600	1.48032100	0.18088500
C	2.43742000	-0.71709600	-0.60033000
C	1.98035300	4.18613500	0.73669100
C	0.47776800	2.46475700	-0.04428000
C	2.69312800	1.87727900	0.68435200
C	2.95307100	3.21489300	0.96674100
C	0.74339500	3.80582500	0.22745800
H	-0.49100300	2.20599200	-0.44980900
H	3.46426700	1.13876500	0.86175700
H	3.92241500	3.49737200	1.36014400
H	-0.01799700	4.55156300	0.03151200
H	2.18917400	5.22865400	0.94471300
H	5.65626600	-2.33239700	-2.07671100
O	-5.80958200	-0.06179200	-0.84280300
C	-0.45520300	-2.04631900	3.44048200
C	0.11319900	-2.03845900	1.09422500
C	0.53818300	-0.08434900	2.43587600
C	0.02099300	-0.74447200	3.55127100
C	-0.40648000	-2.69227200	2.20466100
H	0.15252100	-2.56095100	0.14529500
H	0.90705300	0.92652900	2.54451200
H	-0.00198500	-0.23518400	4.50756300
H	-0.76790100	-3.70930500	2.10726800
H	-0.85489400	-2.55822200	4.30786800
C	4.76111000	-1.88128300	-1.66544500
C	3.05295300	-1.79583900	0.04314100

C	3.01504300	-0.22134500	-1.78176600
C	4.15863100	-0.80245800	-2.31315200
C	4.21022300	-2.36733800	-0.48505300
H	2.65168600	-2.18282200	0.96894900
H	2.57966700	0.63653500	-2.28213100
C	-6.51577100	0.28661600	0.36584900
H	-7.56836900	0.21683100	0.10754800
H	-6.27262400	1.30718600	0.66794000
H	-6.27932300	-0.42159200	1.16235900

Radical cation **3⁺**

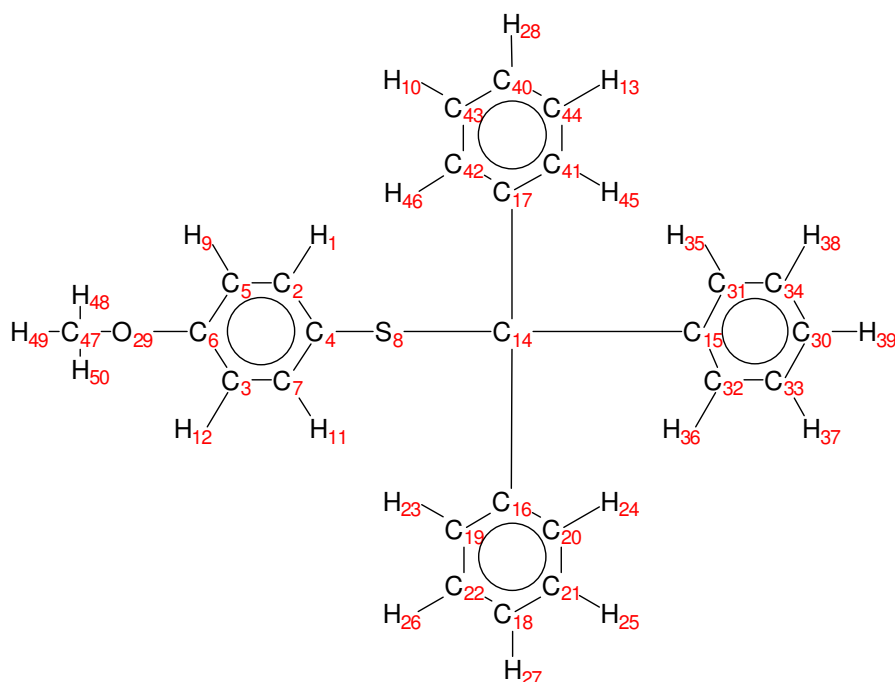
conformer 1, E = -1402.2043135 a.u., ZPVE = 0.397612 a.u.

H	-2.46447100	-0.68222100	-3.13786900
C	-2.87948600	-0.41097700	-2.17408800
C	-3.92452800	0.28467800	0.31717300
C	-2.00264700	-0.11278000	-1.09100600
C	-4.24381800	-0.35409400	-1.99887700
C	-4.80188900	-0.00352800	-0.75297600
C	-2.55640300	0.22928600	0.16850800
S	-0.32713500	-0.18546000	-1.51497100
H	-4.89825200	-0.58453200	-2.83128700
H	-6.58304800	-0.22696100	0.43403400
H	-1.91385700	0.44153600	1.00969300
H	-4.33991900	0.55061100	1.28251700
C	-6.28454600	0.08549500	-0.56874300
C	0.95149600	-0.01545300	-0.00741000
C	0.35497600	-0.64613900	1.24341300
C	1.27839700	1.47442800	0.12774600
C	2.12201300	-0.80640700	-0.61338000
C	1.93015300	4.17737300	0.54871000
C	2.58880800	1.85295900	0.44779700
C	0.30318100	2.47521600	0.02004000
C	0.62688800	3.81439200	0.22360400
C	2.90774600	3.19065300	0.66473300
H	3.36312500	1.10261600	0.53818000
H	-0.71951600	2.22537900	-0.22975400
H	-0.14123200	4.57186800	0.12274300
H	3.92583600	3.46061600	0.91900600
H	2.18459000	5.21880300	0.70475400
H	-6.82142600	-0.51517600	-1.30375200
H	-6.61253500	1.12557700	-0.69124900
C	-0.68415800	-1.84215000	3.56430500
C	-0.18429300	-1.94241200	1.20517200
C	0.36915900	0.03568600	2.46525700
C	-0.14413900	-0.56143100	3.61696600
C	-0.70194300	-2.53213100	2.35140300
H	-0.19643800	-2.49828800	0.27443200
H	0.78782100	1.03111400	2.52688800
H	-0.11578800	-0.02015100	4.55524900

H	-1.11458300	-3.53281800	2.30039900
H	-1.08324300	-2.30399900	4.45954800
C	4.32907700	-2.14404200	-1.72345100
C	2.71494900	-1.88279800	0.05706900
C	2.66485300	-0.40311700	-1.84683900
C	3.75019400	-1.06919000	-2.39911500
C	3.81419200	-2.53970500	-0.49345200
H	2.34265900	-2.19874000	1.02099900
H	2.24926500	0.44888000	-2.37328500
H	4.14983400	-0.74535100	-3.35258900
H	4.26755400	-3.36170100	0.04757200
H	5.17839900	-2.66256000	-2.15204100

NPA Charges and Mulliken spin densities for radical cations 2^{•+}-3^{•+}

Figure S10. Numbering of atoms in radical cation 2^{•+}

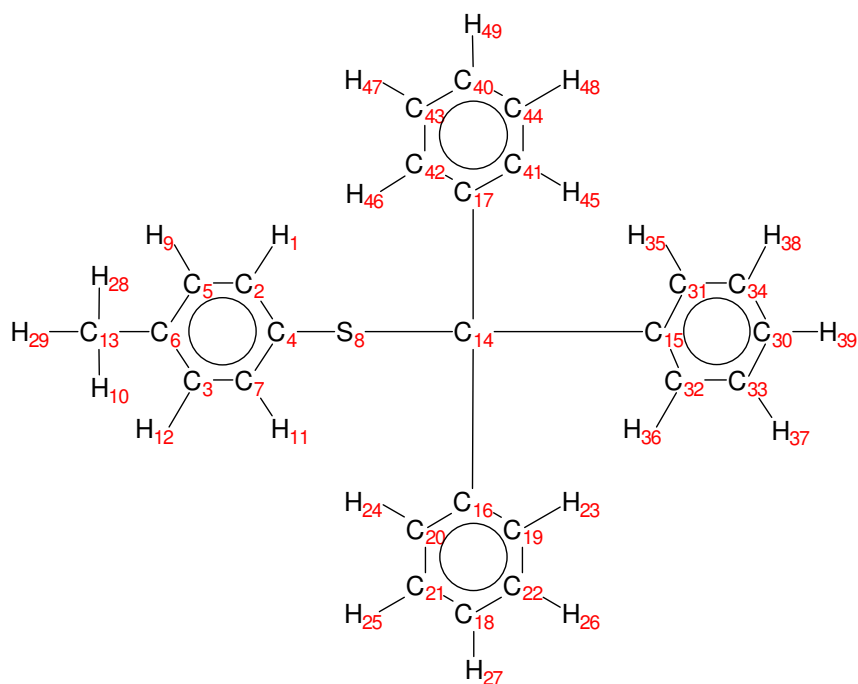


NPA Charges and Mulliken spin densities for radical cation 2^{•+}
conformer 1

		NPA charges	spin pop
1	H	0.2433	-0.0029
2	C	-0.1850	0.0348
3	C	-0.2671	-0.0139
4	C	-0.1921	0.1025
5	C	-0.1912	0.0310
6	C	0.4169	0.1643
7	C	-0.1393	0.1011
8	S	0.5437	0.4307
9	H	0.2396	-0.0026
10	H	0.2161	-0.0004
11	H	0.2313	-0.0061
12	H	0.2338	-0.0004
13	H	0.2125	0.0000
14	C	-0.0799	-0.0143
15	C	-0.0804	0.0061
16	C	-0.0904	0.0000
17	C	-0.0742	0.0178
18	C	-0.1742	0.0023
19	C	-0.2074	0.0045
20	C	-0.1956	-0.0001
21	C	-0.1808	0.0003
22	C	-0.1821	-0.0012
23	H	0.2157	-0.0014

24	H	0.2253	0.0000
25	H	0.2159	0.0000
26	H	0.2147	0.0001
27	H	0.2151	-0.0001
28	H	0.2152	-0.0003
29	O	-0.4510	0.1104
30	C	-0.1660	0.0095
31	C	-0.1993	0.0035
32	C	-0.1903	0.0071
33	C	-0.1784	-0.0033
34	C	-0.1773	-0.0009
35	H	0.2162	-0.0002
36	H	0.2223	-0.0002
37	H	0.2149	0.0002
38	H	0.2153	0.0000
39	H	0.2148	-0.0004
40	C	-0.1736	0.0048
41	C	-0.2035	0.0079
42	C	-0.1912	-0.0046
43	C	-0.1720	0.0105
44	C	-0.1799	-0.0009
45	H	0.2002	-0.0009
46	H	0.2226	0.0003
47	C	-0.2057	-0.0087
48	H	0.2102	-0.0001
49	H	0.1863	0.0071
50	H	0.1863	0.0072

Figure S11. Numbering of atoms in radical cation $3^{+\bullet}$



NPA Charges and Mulliken spin densities for radical cation $3^{+\bullet}$
conformer 1

		NPA charges	spin pop
1	H	0.2297	-0.0075
2	C	-0.1451	0.1354
3	C	-0.1754	-0.0361
4	C	-0.1939	0.0442
5	C	-0.1937	-0.0689
6	C	0.1028	0.2428
7	C	-0.1763	0.0999
8	S	0.5803	0.5013
9	H	0.2274	0.0023
10	H	0.2272	0.0064
11	H	0.2388	-0.0060
12	H	0.2242	0.0009
13	C	-0.6056	-0.0148
14	C	-0.0711	-0.0219
15	C	-0.0952	0.0006
16	C	-0.0763	0.0244
17	C	-0.0812	0.0146
18	C	-0.1685	0.0100
19	C	-0.1898	-0.0073
20	C	-0.1979	0.0160
21	C	-0.1798	-0.0031
22	C	-0.1679	0.0171
23	H	0.2237	0.0004
24	H	0.2015	-0.0014
25	H	0.2144	0.0000

26	H	0.2173	-0.0008
27	H	0.2166	-0.0006
28	H	0.2241	0.0028
29	H	0.2420	0.0199
30	C	-0.1717	0.0030
31	C	-0.2057	0.0041
32	C	-0.1917	-0.0003
33	C	-0.1807	0.0007
34	C	-0.1816	-0.0013
35	H	0.2157	-0.0013
36	H	0.2251	0.0001
37	H	0.2169	-0.0001
38	H	0.2161	0.0000
39	H	0.2161	-0.0002
40	C	-0.1601	0.0175
41	C	-0.1872	0.0083
42	C	-0.1979	0.0073
43	C	-0.1777	-0.0038
44	C	-0.1775	-0.0037
45	H	0.2235	-0.0003
46	H	0.2167	-0.0003
47	H	0.2169	0.0001
48	H	0.2165	0.0002
49	H	0.2161	-0.0008

Cartesian Coordinates and energies from DFT calculations for the Transition State for the C–S bond cleavage in the radical cations 2^{•+}-3^{•+}

Transition State for the C–S bond cleavage in radical cation 2^{•+}
conformer 1, E = -1477.4377912 a.u., 1 imaginary frequency

H	-1.61193000	0.46275300	1.09812400
C	-2.32782800	0.22943100	0.32376600
C	-4.20457300	-0.40603200	-1.68063900
C	-1.87933500	-0.17218500	-0.96641600
C	-3.66750300	0.31712600	0.59602500
C	-4.63027000	0.00279400	-0.39702700
C	-2.85903500	-0.49115000	-1.95240200
S	-0.23568900	-0.30107700	-1.46294300
H	-4.02612700	0.62484400	1.57014000
H	4.43063100	3.52787200	-0.22100700
H	-2.53012100	-0.80277500	-2.93640800
H	-4.92125700	-0.65167200	-2.45180100
H	0.26728100	4.54489300	0.00488600
C	1.41182600	0.00044900	0.09712900
C	2.39548700	-0.93006800	-0.54476100
C	0.81560500	-0.43429100	1.39956300
C	1.72536500	1.46483400	-0.04461900
C	-0.20000800	-1.28707200	3.87797500
C	0.22841600	-1.70576800	1.54041200
C	0.88461800	0.39718700	2.52799900
C	0.38462400	-0.03072300	3.75686000
C	-0.27700400	-2.12446900	2.76242200
H	0.15648000	-2.36137500	0.68060800
H	1.35053300	1.37031800	2.45457800
H	0.46042100	0.62066500	4.61937400
H	-0.73210200	-3.10406300	2.84853500
H	-0.59071200	-1.61697900	4.83334700
H	2.64421600	5.24968600	-0.14392600
O	-5.89691800	0.12312100	-0.02007300
C	4.32334000	-2.58521600	-1.74746300
C	2.81084700	-0.71177100	-1.87426800
C	2.98117600	-1.98832500	0.16954700
C	3.94177700	-2.80035300	-0.42665000
C	3.75353300	-1.53590500	-2.47044800
H	2.39055900	0.10903400	-2.44308000
H	2.71577600	-2.15818300	1.20335900
H	4.39449100	-3.59985100	0.14746200
H	4.04947000	-1.35837300	-3.49735600
H	5.06495400	-3.22477500	-2.21125100
C	2.38958000	4.19705000	-0.11176400
C	0.72813900	2.45237500	0.01530200
C	3.06383500	1.87789100	-0.13625700
C	3.39009900	3.23214400	-0.16044900
C	1.05437100	3.80087300	-0.02536400

H	-0.31395900	2.16625800	0.07521400
H	3.85629800	1.14254300	-0.16348400
C	-6.96715100	-0.16939600	-0.93904800
H	-7.87988700	0.00971400	-0.37799200
H	-6.92439800	-1.21345100	-1.25635100
H	-6.92384100	0.49860100	-1.80185700

Transition State for the C–S bond cleavage in radical cation **3⁺**
conformer 1, E = -1402.2033518 a.u., 1 imaginary frequency

H	-2.56692700	-0.83471400	-3.14499400
C	-2.96973800	-0.52550300	-2.18798700
C	-3.98105900	0.27247900	0.28786700
C	-2.07440400	-0.17728600	-1.13462800
C	-4.33155200	-0.46816000	-1.99204400
C	-4.87224200	-0.06588700	-0.75417100
C	-2.61509600	0.21780600	0.11704000
S	-0.39739800	-0.25831600	-1.52738200
H	-4.99854100	-0.73732800	-2.80287400
H	-6.63410500	-0.17984800	0.47974100
H	-1.95978700	0.47027500	0.93764100
H	-4.38300700	0.57865300	1.24700800
C	-6.35374100	0.02651900	-0.55477100
C	1.09660000	0.00212300	0.10712900
C	0.42734100	-0.44608300	1.37278800
C	1.43272900	1.46962300	0.01050100
C	2.13128400	-0.92439100	-0.47140200
C	2.11745600	4.19686300	0.02360500
C	2.77638200	1.87233400	0.03515600
C	0.44016500	2.46332200	-0.00471100
C	0.77763700	3.81046600	-0.00594200
C	3.11222300	3.22429800	0.05078800
H	3.56362100	1.13140000	0.06486500
H	-0.60590800	2.18587800	-0.02935100
H	-0.00438500	4.55980300	-0.03446900
H	4.15607300	3.51298500	0.07985300
H	2.38145200	5.24763300	0.02181000
H	-6.89290900	-0.65690900	-1.21233700
H	-6.69819700	1.04214200	-0.78677900
C	-0.72958300	-1.32238500	3.77921500
C	-0.16585900	-1.71856100	1.46677300
C	0.43056800	0.37479200	2.51023200
C	-0.13943300	-0.06492300	3.70403200
C	-0.74143300	-2.14909200	2.65346300
H	-0.18441900	-2.36929400	0.60026500
H	0.89753900	1.34950200	2.47276700
H	-0.11427200	0.57832800	4.57555100
H	-1.19911600	-3.12993700	2.70384200
H	-1.17427200	-1.66148400	4.70735300
C	4.14894800	-2.56157800	-1.54429100

C	2.67000300	-1.98399500	0.27615900
C	2.63938800	-0.69489100	-1.76633400
C	3.62710100	-1.50983600	-2.29906800
C	3.67507500	-2.78722100	-0.25545400
H	2.33256800	-2.16301400	1.28705700
H	2.26041600	0.12979900	-2.35837900
H	3.99538800	-1.32278800	-3.30052800
H	4.08975900	-3.58835800	0.34448000
H	4.92484300	-3.19466800	-1.95808200

NPA Charges and Mulliken spin densities of the Transition State for the C–S bond cleavage in the radical cations 2⁺•-3⁺•

Transition State for the C–S bond cleavage in radical cation radical cation 2⁺•

		<u>NPA charges</u>	<u>spin pop</u>
1	H	0.2322	-0.0042
2	C	-0.1848	0.0600
3	C	-0.2721	-0.0280
4	C	-0.2084	0.0668
5	C	-0.2012	0.0087
6	C	0.4106	0.1698
7	C	-0.1355	0.1201
8	S	0.3676	0.5098
9	H	0.2362	-0.0015
10	H	0.2176	-0.0003
11	H	0.2289	-0.0073
12	H	0.2314	0.0004
13	H	0.2146	0.0000
14	C	0.0818	-0.0274
15	C	-0.1091	0.0071
16	C	-0.1145	0.0010
17	C	-0.1035	0.0111
18	C	-0.1619	-0.0020
19	C	-0.1876	0.0007
20	C	-0.1725	-0.0029
21	C	-0.1868	0.0017
22	C	-0.1860	0.0008
23	H	0.2199	-0.0012
24	H	0.2247	0.0003
25	H	0.2179	-0.0001
26	H	0.2165	-0.0001
27	H	0.2160	0.0001
28	H	0.2159	-0.0001
29	O	-0.4605	0.0993
30	C	-0.1510	0.0042
31	C	-0.1777	0.0018
32	C	-0.1668	0.0025
33	C	-0.1844	-0.0009
34	C	-0.1836	-0.0019
35	H	0.2201	-0.0002
36	H	0.2221	0.0000
37	H	0.2172	0.0000
38	H	0.2175	0.0001
39	H	0.2159	-0.0002
40	C	-0.1601	0.0019
41	C	-0.1813	0.0034
42	C	-0.1703	-0.0035
43	C	-0.1805	0.0060
44	C	-0.1829	0.0001

45	H	0.2054	-0.0009
46	H	0.2221	0.0003
47	C	-0.2051	-0.0080
48	H	0.2078	-0.0001
49	H	0.1840	0.0065
50	H	0.1842	0.0066

Transition State for the C–S bond cleavage in radical cation radical cation **3⁺**

		NPA charges	spin pop
1	H	0.2281	-0.0083
2	C	-0.1424	0.1458
3	C	-0.1819	-0.0489
4	C	-0.2048	0.0222
5	C	-0.1954	-0.0753
6	C	0.0968	0.2464
7	C	-0.1745	0.1195
8	S	0.4444	0.5653
9	H	0.2255	0.0027
10	H	0.2238	0.0052
11	H	0.2307	-0.0070
12	H	0.2219	0.0015
13	C	-0.6043	-0.0158
14	C	0.0583	-0.0310
15	C	-0.1138	0.0012
16	C	-0.1012	0.0154
17	C	-0.1064	0.0114
18	C	-0.1601	0.0044
19	C	-0.1737	-0.0054
20	C	-0.1846	0.0081
21	C	-0.1815	-0.0007
22	C	-0.1765	0.0100
23	H	0.2228	0.0004
24	H	0.2050	-0.0011
25	H	0.2155	0.0000
26	H	0.2183	-0.0006
27	H	0.2168	-0.0003
28	H	0.2239	0.0038
29	H	0.2399	0.0196
30	C	-0.1623	-0.0012
31	C	-0.1906	0.0008
32	C	-0.1743	-0.0027
33	C	-0.1853	0.0017
34	C	-0.1847	0.0005
35	H	0.2187	-0.0012
36	H	0.2250	0.0003
37	H	0.2184	-0.0001
38	H	0.2173	0.0000
39	H	0.2166	0.0001

40	C	-0.1500	0.0100
41	C	-0.1692	0.0042
42	C	-0.1809	0.0053
43	C	-0.1824	-0.0039
44	C	-0.1823	-0.0013
45	H	0.2230	-0.0001
46	H	0.2194	-0.0003
47	H	0.2183	0.0001
48	H	0.2180	0.0000
49	H	0.2168	-0.0005

References for Supporting Information

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