Supporting Information

Intramolecular S··O Chalcogen Bond as Stabilizing Factor in Geometry of Substituted Phenyl-SF_3 Molecules

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Coordinates and Energies of Optimized Geometries from Figs 1 and 2.

1A E= -929.392255

S	1.50988300	0.15024800	0.34991200
F	2.07340300	-0.36522800	-1.10459300
F	1.57699400	-1.52747200	0.85750000
F	1.50333500	1.77542600	-0.32516300
C	-0.28809300	0.03974900	0.12739300
C	-1.05209600	1.19233400	0.34389500
C	-0.87636700	-1.18272400	-0.21513000
C	-2.44135300	1.10846200	0.21887200
C	-2.26274300	-1.23812500	-0.36408800
C	-3.04520700	-0.09951000	-0.14037000
H	-3.04835200	1.99661700	0.39349700
H	-2.73261600	-2.17955800	-0.64846100
H	-4.12888700	-0.15531300	-0.24662700
H	-0.26301900	-2.06700000	-0.36221900
H	-0.57368600	2.13564500	0.59208400

1A’ E= -929.351041

S	1.36730300	0.38679300	-0.00002500
F	3.16984174	0.48243095	-0.00002732
F	1.52797500	-0.59296300	1.31226400
F	1.52797800	-0.59313000	-1.31218800
C	-0.46954969	0.20483917	-0.00001647
C	-1.18238917	-1.00169792	0.00004622
C	-1.13097601	1.43543403	-0.00008050
C	-2.57570258	-0.96379405	0.00004479
C	-2.53175499	1.46507241	-0.00008296
C	-3.24921302	0.26781392	-0.00001929
H	-0.56093170	2.36697085	-0.00012886
H	-3.14409668	-1.89432020	0.00009415
H	-3.05582845	2.42087951	-0.00013137
H	-4.33937525	0.28821935	-0.00001832
H	-0.65374183	-1.95429881	0.00009564

1B E= -1079.69776

S	-0.88072100	-1.15669600	-0.02508900
F	-0.33465000	-2.55464600	0.65409300
F	-0.42203500	-1.83559000	-1.58273600
F	-1.20181500	-0.58484200	1.63040900
C	0.66661700	-0.19131100	-0.01657200
C	0.61723800	1.20521100	0.10263900
C	1.86976500	-0.88701800	-0.13428400
C	1.83568000	1.89578200	0.10585100
C	3.07032000	-0.17489600	-0.10332300
C	3.05280200	1.21674500	0.01774900
C	-0.68603800	1.95029400	0.22660000
O	-1.63435900	1.32486000	-0.63149100
C	-2.97988200	1.70265500	-0.35659000
H	1.82561900	2.98419600	0.17487400
H	4.01556400	-0.71087500	-0.18610600
H	3.98788600	1.77681700	0.02802500
H	-1.04360200	1.91152100	1.26894700
H	-0.54972700	3.00671600	-0.05812700
H	-3.26007900	1.43028700	0.67352300

H	-3.11733900	2.78685600	-0.49964900
H	-3.61289100	1.16142000	-1.06760700
H	1.86846300	-1.96775500	-0.24884500

1C E= -1079.69170

S	1.35151500	-1.19919100	0.18272900
F	2.77635300	-0.99525900	-0.59901500
F	0.67464000	-1.66680500	-1.37963700
F	2.18427700	-0.66703800	1.62656300
C	0.58451900	0.43487500	0.01505300
C	1.42117300	1.55283100	0.01395300
C	-0.81365200	0.52677300	-0.08032700
C	0.85173300	2.81959500	-0.10896800
C	-1.35611000	1.81636600	-0.17669800
C	-0.53721400	2.94699700	-0.19876600
C	-1.72318600	-0.68481600	-0.09339400
H	1.49271400	3.70072200	-0.12187500
H	-0.98886900	3.93593000	-0.28051800
H	-1.76200100	-1.10621100	-1.11269100
H	-1.32528200	-1.47997600	0.56486400
O	-3.01726400	-0.30826100	0.33736400
C	-3.94260000	-1.38240900	0.26919900
H	-3.63692000	-2.21623700	0.92455600
H	-4.90880500	-0.99321200	0.60781600
H	-4.04178200	-1.75909100	-0.76340300
H	-2.43756700	1.91965100	-0.22548700
H	2.49697500	1.43222900	0.11265700

1D E= -1079.65361

S	1.06481400	-0.83647600	-0.27074300
F	2.82522400	-1.36651700	-0.11460500
F	1.30929400	-0.33649900	1.28629600
F	0.73500600	-2.43432100	-0.08413100
C	-0.76895900	-0.41280700	-0.04948700
C	-1.76273800	-1.39034500	-0.16899000
C	-1.12534500	0.94642200	0.08811400
C	-3.11425000	-1.03015400	-0.13863600
C	-2.48287900	1.28785300	0.10604900
C	-3.47557700	0.30995200	0.00136900
C	-0.08609300	2.02743600	0.24994100
O	1.02873600	1.70628800	-0.57665400
C	2.20128600	2.46479700	-0.28237300
H	-3.87951500	-1.80139400	-0.22848400
H	-2.76759700	2.33678000	0.20163500
H	0.23943500	2.09109500	1.30304800
H	-0.49956800	3.00784500	-0.03827100
H	2.98694200	2.10688600	-0.95508400
H	2.02006200	3.53681700	-0.46024400
H	2.51405000	2.31115400	0.76213600
H	-4.52683800	0.59782500	0.01935100
H	-1.49228000	-2.43658300	-0.28293200

2A E= -1237.08592

S	-0.78653400	-1.34139200	0.07332200
F	0.41365000	-2.17853100	0.83296900
F	0.04858000	-1.66321000	-1.44734600
F	-1.45996300	-1.04114700	1.69600400
C	-0.11552200	0.37084900	0.08126800
C	-1.08087600	1.39756000	0.09434000
C	1.26964900	0.64244700	0.06122100
C	-0.64379000	2.72502300	0.09403000
C	1.65378900	1.99264300	0.08605400
C	0.71644800	3.02229500	0.10403800
C	-2.56395600	1.12184900	0.11080600
O	-2.83176100	0.05656400	-0.79655100
C	-4.12430000	-0.51749600	-0.62890300
H	-1.38248300	3.52658700	0.08021800
H	2.71604100	2.21949900	0.07368200
H	1.05038700	4.05993400	0.10932600
H	-2.88620000	0.83755300	1.12538400
H	-3.11573600	2.02607700	-0.19273900
H	-4.24262200	-0.92751800	0.38691500
H	-4.91037900	0.23252600	-0.81419000
H	-4.21198700	-1.32257600	-1.36607000
C	2.36352600	-0.41133500	0.03639600
H	2.41661900	-0.91541700	1.01618900
H	2.13999700	-1.17333100	-0.72230000
O	3.61098500	0.20627800	-0.24548000
C	4.67113800	-0.73407400	-0.27479400
H	5.58774100	-0.17692600	-0.49785000
H	4.78289300	-1.24255300	0.69902700
H	4.50943500	-1.49688300	-1.05587800

2B E= -1237.08241

S	-0.17886600	-1.73405600	0.13131700
F	1.20553500	-2.33201300	-0.50860800
F	-0.84454000	-1.84245000	-1.49999100
F	0.67738400	-1.65837900	1.66224200
C	-0.06409700	0.07399800	-0.04769000
C	1.16449700	0.76723700	-0.08150600
C	-1.31428800	0.72275300	-0.10068000
C	1.09833200	2.16296600	-0.18054200
C	-1.32180300	2.12009100	-0.17885000
C	-0.12519200	2.83046700	-0.22133700
C	2.52551500	0.09736700	-0.04002200
C	-2.63572600	-0.02465100	-0.09858700
H	2.03092000	2.71917100	-0.21304100
H	-2.27825300	2.63636300	-0.19470900
H	-2.87337000	-0.35610500	-1.12445300
H	-0.14334100	3.91873600	-0.28507500
H	2.57477800	-0.61010800	0.80071100
H	2.68783300	-0.47463500	-0.96976300
H	-2.57798300	-0.93658400	0.52487500
O	3.53669200	1.08283000	0.09243200
O	-3.65665000	0.82034000	0.39698100
C	4.83354000	0.51099700	0.12920200
H	5.54493300	1.33743800	0.23371400
H	4.94455400	-0.17584200	0.98597200
H	5.05368800	-0.04259000	-0.80045600
C	-4.93620900	0.20875900	0.34316600
H	-5.65456300	0.93767900	0.73341100
H	-5.20957100	-0.05507200	-0.69306800

H	-4.97092000	-0.70324800	0.96379200

2C E= -1237.04178

S	-0.00492200	-1.19718900	-0.18701000
F	-0.01391200	-3.05343200	-0.42844100
F	-1.21152600	-1.22414600	-1.30045800
F	1.20312800	-1.23473600	-1.29836500
C	0.00227900	0.71707200	-0.21960800
C	1.22502700	1.41202200	-0.12972600
C	-1.21574700	1.42003700	-0.12784300
C	1.21313800	2.81286800	-0.13256100
C	-1.19490000	2.82075500	-0.13060200
C	0.01137300	3.51865300	-0.17884800
C	2.53465100	0.68713700	0.07403600
O	2.29214400	-0.37800200	0.99390700
C	3.37981300	-1.29193100	1.09859000
C	-2.52967300	0.70347900	0.07750500
O	-2.29175500	-0.36587600	0.99371500
C	-3.38470000	-1.27363100	1.09822100
H	2.15756300	3.35479500	-0.06640800
H	-2.13569100	3.36878500	-0.06294800
H	0.01494000	4.60858500	-0.18428400
H	2.93557900	0.28592700	-0.87018500
H	3.28155800	1.38029400	0.49473600
H	3.58714200	-1.76917300	0.12769600
H	4.28713700	-0.77819300	1.45672100
H	3.08320100	-2.05656800	1.82388900
H	-2.93580400	0.30755300	-0.86673000
H	-3.27078900	1.40038300	0.50221700
H	-3.09029300	-2.04312400	1.81923600
H	-4.28750600	-0.75570400	1.46156800
H	-3.59817800	-1.74544200	0.12605900

2D E= -1237.03986

S	0.93378300	-1.14862700	-0.15072800
F	2.00310700	-2.68000200	-0.07544600
F	1.64711200	-0.85193700	1.31027700
F	-0.27218000	-2.10073500	0.42696000
C	-0.08067000	0.45971200	0.08142700
C	-1.49293400	0.54133300	0.05514000
C	0.69853200	1.64010800	0.10232900
C	-2.08387900	1.81485700	0.11882900
C	0.07305100	2.88920100	0.15180000
C	-1.31663600	2.97541900	0.17957700
C	-2.42415100	-0.65900300	-0.04564100
C	2.20644800	1.59094800	0.06911200
O	2.59097000	0.50925300	-0.78208900
C	3.96382000	0.12438600	-0.65958100
H	-3.16812000	1.88098900	0.10296300
H	0.67957000	3.79566700	0.15959800
H	-2.40461800	-1.23753000	0.89265600
H	2.62161000	1.43235000	1.07794300
H	2.61394400	2.53393600	-0.32737400
H	4.10441800	-0.74853600	-1.30364400
H	4.61439400	0.94809700	-0.99115700
H	4.20005300	-0.14611200	0.37993400
H	-1.80575500	3.94863400	0.22386400

H	-2.10125700	-1.33647300	-0.85320600
O	-3.74845300	-0.22149100	-0.30376000
C	-4.66058300	-1.30355600	-0.38504900
H	-5.64888700	-0.87549100	-0.58538900
H	-4.39122000	-1.99469700	-1.20274800
H	-4.69513300	-1.87128200	0.56123300

2E E= -1237.03716

S	0.68211200	-1.15671800	-0.29229700
F	1.49542200	-2.83382700	-0.18379700
F	1.21705100	-1.04189900	1.26492900
F	-0.71778900	-1.92547700	0.05221300
C	-0.08959400	0.59080600	-0.08776800
C	-1.44345700	0.91233100	-0.32906000
C	0.84746600	1.62313300	0.15652000
C	-1.83520600	2.25891100	-0.22979200
C	0.41846500	2.95131600	0.23277300
C	-0.92775200	3.27163100	0.06442000
C	-2.54310400	-0.06413100	-0.69959200
C	2.31843100	1.33053500	0.32832700
O	2.65778200	0.26403200	-0.55951500
C	3.91998800	-0.35000700	-0.28239400
H	-2.88345700	2.50768800	-0.39827000
H	1.14828700	3.74121700	0.41556900
H	2.54709200	1.03688800	1.36579000
H	2.91841000	2.22052600	0.08163600
H	4.02652000	-1.18096100	-0.98583800
H	4.73285200	0.37736300	-0.43116500
H	3.94538200	-0.73732800	0.74662700
H	-1.26095300	4.30710400	0.13298400
H	-2.17031700	-0.90788000	-1.29785500
H	-3.28711700	0.47053600	-1.31770400
O	-3.16809200	-0.53339300	0.48789700
C	-4.18639000	-1.48379200	0.22064400
H	-4.61554100	-1.77333500	1.18624800
H	-4.98094200	-1.05356800	-0.41551800
H	-3.77677100	-2.37944000	-0.27738100