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Restricted access to a conical intersection to explain aggregation induced emission in dimethyl tetraphenyl silole

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SUPPORTING INFORMATION

COMPUTATIONAL DETAILS

Calculation of the energy barrier between S_1-Min^{sol} and (S_1/S_0)-CI^{sol}. To estimate the barrier between these structures we have carried out two sets of calculations based on CASSCF and TD-DFT relaxed scans on S_1, freezing the C_1-C_2-C_3-C_4 [φ] and/or C_{16}-C_2-C_3-C_{27} [ϕ] angles in steps of 10°. The S_0 and S_1 energies in both cases are recomputed at the CASPT2 level (CASPT2//CASSCF and CASPT2//TD-DFT, respectively). One of the TD-DFT constrained optimizations on S_1 (φ=60° and ϕ=71°) gives a point with an S_1/S_0 gap of 0.25 eV (3.17 ± 0.125 eV) at the CASPT2 level. This structure is taken as the approximation to the conical intersection for the CASPT2//TD-DFT energy profile. The reaction paths between **S_1-Min^{sol}** and **(S_1/S_0)-CI^{sol}** are obtained connecting contiguous points on the φ/ϕ grid to get the lowest energy profile.

The resulting energy profiles are plotted in Figure ESI-3a-c, where we also present the CASSCF energy profile along the CASSCF optimized path. The relative energies in eV of **S_1-Min^{sol}** with the three approaches are 3.35 (CASPT2//CASSCF), 3.21 (CASSCF//CASSCF) and 3.10 (CASPT2//TD-DFT). To compare the three energy profiles, the CASPT2//CASSCF and CASSCF//CASSCF energies have been shifted by -0.25 eV and -0.11 eV, respectively, to match the relative CASPT2//TD-DFT energy of the S_1 minimum. The three approaches give similar values for the energy of the conical intersection, namely 3.01 (CASPT2//CASSCF), 3.18 (CASSCF//CASSCF) and 3.17 eV (CASPT2//TD-DFT), with S_1/S_0 energy gaps of 0.10, 0.01 and 0.25 eV, respectively. The barriers to access the intersection are 0.44, 0.38 and 0.40 eV, respectively. The discussion in the paper is based on the CASPT2//CASSCF values (see Table 2).

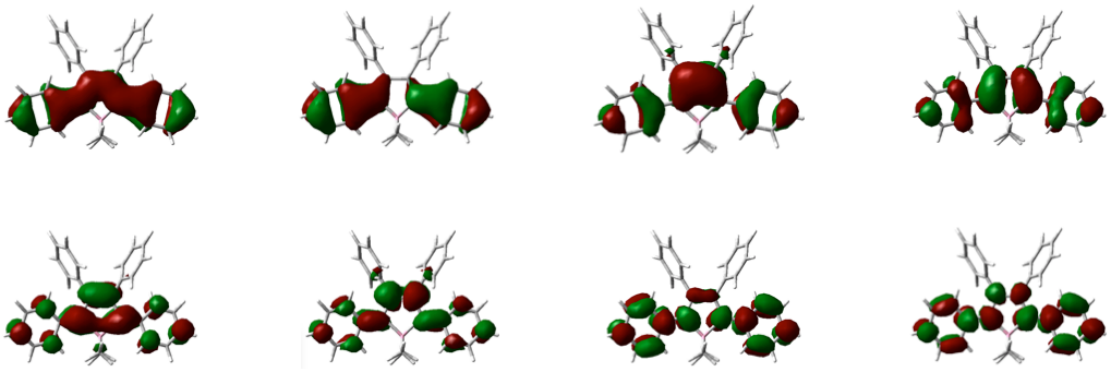


Figure ESI-1. Plot of CASSCF active space orbitals.

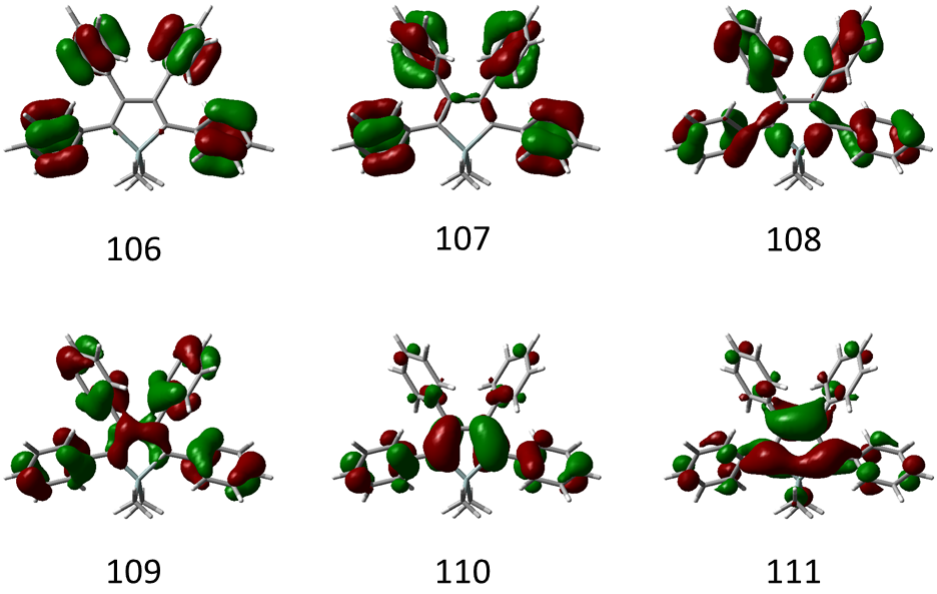
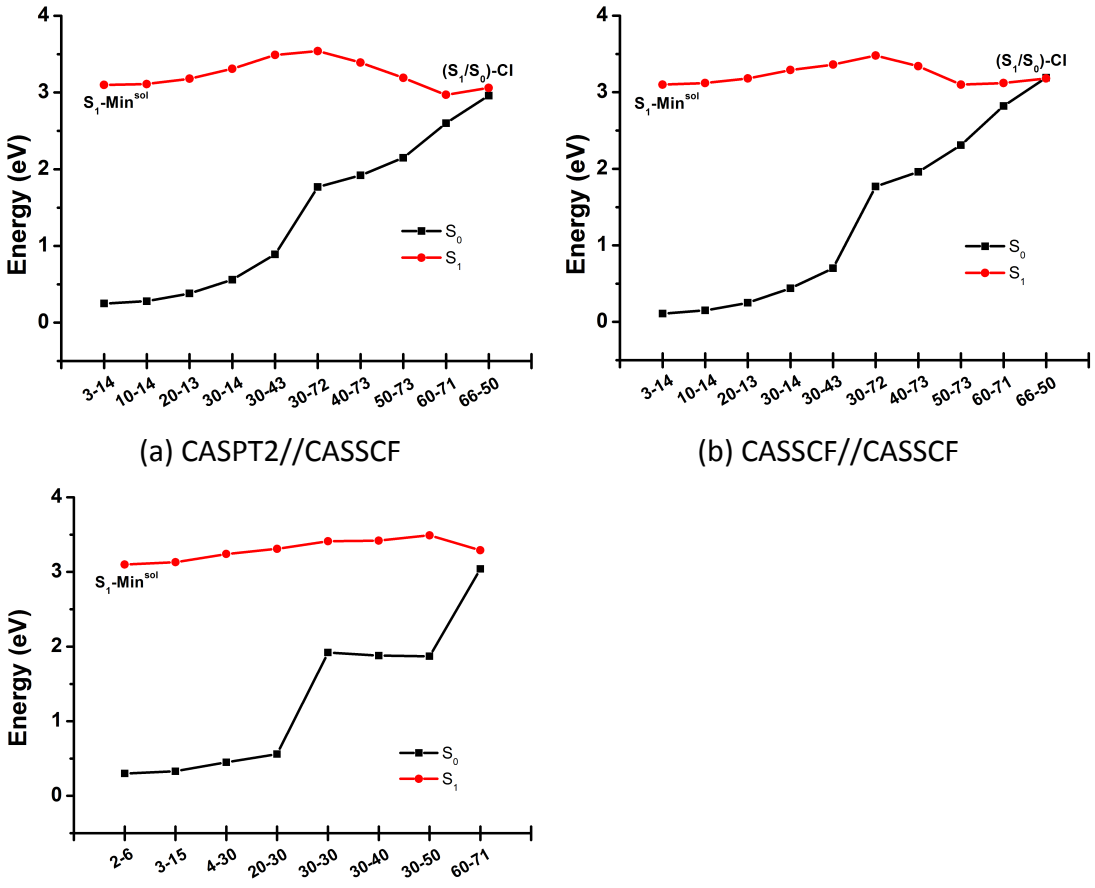


Figure ESI-2. Plot of CAM-B3LYP orbitals involved in the vertical excitations.



(a) CASPT2//CASSCF

(b) CASSCF//CASSCF

(c) CASPT2//TD-CAM-B3LYP

Figure ESI-3. Energy profiles along the **S_1-Min^{sol}** - **(S_1/S_0)-CI^{sol}** reaction coordinate obtained with the CASPT2//CASSCF, CASSCF//CASSCF and CASPT2//TD-CAM-B3LYP approaches. The x-axis gives the values of the φ and ϕ angles at the optimized points of the relaxed scan.

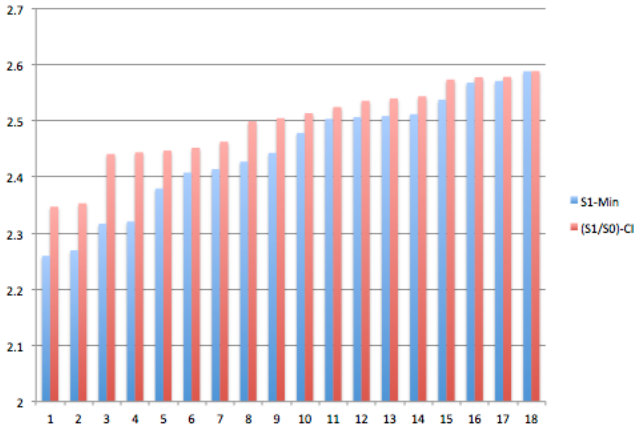


Figure ESI-4. Histogram of 20 closest contacts (in Å) between the active molecule and the surrounding ones for **S_1-Min^{cr}** (blue bars) and **(S_1/S_0)-CI^{cr}** (red bars).

CARTESIAN COORDINATES OF ALL STRUCTURES

S_0-Min^{sol}

Si	-0.00002500	-2.25562500	0.00035300
C	1.35030600	-0.95392400	0.07093900
C	0.75565400	0.26328300	0.02131000
C	-0.75571900	0.26328600	-0.02096400
C	-1.35036900	-0.95394100	-0.07041700
C	2.80106900	-1.23352100	0.01770000
C	3.64234300	-0.62912400	-0.92520200
C	3.36174500	-2.17637200	0.88813300
C	4.99236900	-0.94663600	-0.98384100
C	4.71504500	-2.48754900	0.83670300
C	5.53680700	-1.87418400	-0.10131400
C	1.50592200	1.54966500	0.00764300
C	2.40974900	1.84684400	1.03061100
C	1.34049200	2.47505800	-1.02665900
C	3.13047800	3.03440200	1.02035600
C	2.06785500	3.65828000	-1.04303400
C	2.96394900	3.94324700	-0.01838200
C	-1.50594800	1.54970000	-0.00777000
C	-1.34087500	2.47524800	1.02645400
C	-2.40936500	1.84677400	-1.03113200
C	-2.06821700	3.65848800	1.04238800
C	-3.13006200	3.03435400	-1.02132200
C	-2.96391200	3.94333700	0.01735500
C	-2.80113000	-1.23357800	-0.01717700
C	-3.64241100	-0.62931900	0.92581200
C	-3.36177500	-2.17641100	-0.88764800
C	-4.99241600	-0.94691200	0.98446400
C	-4.71505700	-2.48766800	-0.83620700
C	-5.53682800	-1.87441500	0.10187500
C	-0.17266900	-3.33524300	1.53150100
C	0.17263000	-3.33547900	-1.53062600
H	3.22734500	0.09396300	-1.61884500
H	2.72775300	-2.65843700	1.62687400
H	5.62363100	-0.46682300	-1.72588800
H	5.12690500	-3.21450300	1.53047900
H	6.59333500	-2.11968000	-0.14795900
H	2.54807500	1.13384400	1.83705200
H	0.63470000	2.26549100	-1.82412500
H	3.82645200	3.24837400	1.82586100
H	1.92999400	4.36256300	-1.85785200
H	3.52822500	4.87077300	-0.02879000
H	-0.63540300	2.26577500	1.82422600
H	-2.54739800	1.13367300	-1.83753300
H	-1.93064800	4.36288100	1.85716100
H	-3.82571300	3.24823700	-1.82712900

H	-3.52816400	4.87088200	0.02741600
H	-3.22743200	0.09371800	1.61951600
H	-2.72777300	-2.65839300	-1.62643500
H	-5.62368200	-0.46720200	1.72657500
H	-5.12689400	-3.21459800	-1.53002100
H	-6.59334000	-2.11997700	0.14853200
H	0.63158800	-4.07473700	1.59784300
H	-0.16219000	-2.73507700	2.44602400
H	-1.12249700	-3.87989500	1.50182900
H	1.12237300	-3.88026900	-1.50077100
H	-0.63172900	-4.07486200	-1.59696300
H	0.16234700	-2.73543300	-2.44523000

S_1-Min^{sol}

Si	-0.00095300	-2.24909800	0.00118900
C	1.32259700	-0.93428800	0.05224900
C	-1.32333800	-0.93312400	-0.05157900
C	0.70912700	0.36541500	0.04165700
C	-0.70880900	0.36597200	-0.04097400
C	2.73382300	-1.21176700	-0.08598400
C	3.65763300	-0.35415500	-0.73263000
C	3.24013500	-2.44695700	0.38802900
C	4.98698900	-0.71250800	-0.88170400
C	4.57231800	-2.79091400	0.25188300
C	5.45904600	-1.92465000	-0.38565400
C	1.49390800	1.61374400	0.15668600
C	2.39367800	1.77677800	1.21844200
C	1.38717900	2.64395300	-0.78665200
C	3.14712400	2.93636200	1.34270200
C	2.15299800	3.79585000	-0.66999000
C	3.03288900	3.94977500	0.39711400
C	-1.49248100	1.61508200	-0.15574700
C	-1.38590600	2.64424800	0.78870500
C	-2.39080200	1.77992800	-1.21841700
C	-2.15053100	3.79697000	0.67225400
C	-3.14306200	2.94031300	-1.34244000
C	-3.02901600	3.95270900	-0.39573700
C	-2.73499600	-1.20951100	0.08510800
C	-3.65892500	-0.35111000	0.73048000
C	-3.24162000	-2.44444600	-0.38917900
C	-4.98871300	-0.70848900	0.87810000
C	-4.57422100	-2.78741900	-0.25453300
C	-5.46107400	-1.92039100	0.38176400
C	-0.19442800	-3.38374300	1.50589400
C	0.19148100	-3.38610700	-1.50187100
H	3.31389000	0.58098600	-1.15400300
H	2.56752200	-3.12523100	0.90404100

H	5.66406000	-0.03742600	-1.39681400
H	4.92517700	-3.74003700	0.64430800
H	6.50417100	-2.19521400	-0.49964300
H	2.49323600	0.98347700	1.95229400
H	0.70292200	2.53288500	-1.62079300
H	3.83104700	3.04556800	2.17896900
H	2.06133600	4.57847600	-1.41706200
H	3.62799600	4.85314200	0.48887600
H	-0.70267300	2.53174100	1.62350000
H	-2.49021600	0.98740300	-1.95313100
H	-2.05902100	4.57881300	1.42016300
H	-3.82590300	3.05095400	-2.17940300
H	-3.62318500	4.85670900	-0.48734300
H	-3.31503300	0.58387500	1.15207100
H	-2.56889500	-3.12336100	-0.90419800
H	-5.66588400	-0.03280900	1.39229400
H	-4.92728000	-3.73639100	-0.64714600
H	-6.50652500	-2.19017900	0.49460000
H	0.53407700	-4.20209100	1.49857400
H	-0.08055900	-2.83290400	2.44362100
H	-1.19278200	-3.83550200	1.50574000
H	1.19066100	-3.83602600	-1.50291900
H	-0.53550800	-4.20576800	-1.49165600
H	0.07480600	-2.83714800	-2.44036000

(S_1/S_0)-CI^{sol} (optimized with CASSCF)

Si	-0.30134000	-2.36319900	0.00575700
C	1.12544700	-1.22121400	0.39640000
C	0.47236700	0.16933300	0.39450800
C	-0.71601900	0.04804000	1.16691400
C	-1.41716000	-0.87191900	0.21606900
C	2.45294000	-1.48412400	0.90779200
C	3.01356300	-2.77290700	0.69799000
C	3.28227700	-0.53276900	1.53089400
C	4.30219900	-3.06948000	1.05648700
C	4.58438900	-0.84278700	1.88990300
C	5.10795800	-2.09920200	1.65183500
C	1.05554000	1.36379500	-0.24794700
C	2.11948100	1.23125100	-1.13666100
C	0.55314800	2.65001600	-0.00911300
C	2.68212000	2.34402400	-1.74174400
C	1.11107900	3.75717300	-0.61848800
C	2.18378000	3.61010900	-1.48429500
C	-1.26645500	0.78653900	2.30255800
C	-2.62618400	0.70122700	2.61078100
C	-0.44110600	1.51656200	3.16346600
C	-3.14710100	1.35848700	3.70982700

C	-0.96298200	2.16672200	4.26530500
C	-2.31960900	2.09651100	4.54110100
C	-2.49813800	-0.40286300	-0.66609200
C	-2.90962900	0.93837100	-0.75143700
C	-3.23875100	-1.34191100	-1.41671700
C	-3.98213600	1.31175400	-1.53807800
C	-4.30950600	-0.96537100	-2.19029600
C	-4.69503900	0.36871300	-2.25819200
C	-0.63237700	-3.73484300	1.25954300
C	-0.20837300	-3.09355400	-1.73480100
H	2.41639100	-3.53328000	0.22552800
H	2.92201400	0.45939800	1.71924500
H	4.69415100	-4.05394300	0.86922200
H	5.19428100	-0.08877300	2.35647100
H	6.12281300	-2.32690200	1.92474200
H	2.52701200	0.25766700	-1.33945500
H	-0.27365600	2.78183500	0.66211300
H	3.50963700	2.21833300	-2.41750400
H	0.70974700	4.73463700	-0.41547900
H	2.62239600	4.47194300	-1.95575900
H	-3.27462000	0.12620600	1.97725900
H	0.61402600	1.56715700	2.96965600
H	-4.19952700	1.28885700	3.92021900
H	-0.30964100	2.72350000	4.91346500
H	-2.72454800	2.60376600	5.39838800
H	-2.38671900	1.69295500	-0.19829300
H	-2.97056600	-2.38133400	-1.37039000
H	-4.26662800	2.34772000	-1.58292300
H	-4.85442000	-1.71045500	-2.74252700
H	-5.53376000	0.66316300	-2.86151200
H	0.14914200	-4.48922000	1.24582400
H	-0.68902000	-3.33571800	2.26755900
H	-1.57269300	-4.23824100	1.04685100
H	0.70036900	-3.67775400	-1.85540200
H	-1.04553500	-3.75436800	-1.94399000
H	-0.20246800	-2.31452400	-2.49039900

(S_1/S_0)-CI^{sol} (approximate point from TD-DFT relaxed scans)

Si	-0.29188100	-2.24595200	-0.20183600
C	1.09889800	-1.12551800	0.27337500
C	0.56634000	0.25230200	0.25117600
C	-0.68085300	0.14488900	0.92718300
C	-1.42735500	-0.82067500	0.09691000
C	2.32943600	-1.42224900	0.96928400
C	2.82441300	-2.74720000	1.00621700
C	3.10872500	-0.43395900	1.61063200
C	4.01667600	-3.05735800	1.63100400

C	4.29735900	-0.75397800	2.24844000
C	4.76374400	-2.06311300	2.26310600
C	1.14041700	1.39610300	-0.41900700
C	2.34180300	1.25962900	-1.13911400
C	0.51759000	2.65732100	-0.38262200
C	2.90205800	2.34793800	-1.78623500
C	1.07955700	3.73879500	-1.03959100
C	2.27541000	3.59133400	-1.73923000
C	-1.08747200	0.71386500	2.18809100
C	-2.35067400	0.40061700	2.72423600
C	-0.24770500	1.58432000	2.90913700
C	-2.75876400	0.94789800	3.92904900
C	-0.66020400	2.12039100	4.11662700
C	-1.91860000	1.81028300	4.62969400
C	-2.59168400	-0.39689100	-0.64320000
C	-3.13336500	0.90387900	-0.54439300
C	-3.27375900	-1.30913800	-1.48318300
C	-4.27281400	1.26587800	-1.24658100
C	-4.41747200	-0.94665800	-2.16746500
C	-4.92654800	0.34793200	-2.05975200
C	-0.62965700	-3.69202100	0.95319300
C	-0.15875900	-2.85080800	-1.97824900
H	2.25793700	-3.53435600	0.51917300
H	2.77139900	0.59637900	1.60445000
H	4.37031600	-4.08415100	1.63382300
H	4.86720000	0.03115500	2.73670600
H	5.69619600	-2.31097100	2.75975900
H	2.81826400	0.28647800	-1.18148800
H	-0.41129900	2.77627100	0.16478700
H	3.82952600	2.22811500	-2.33749000
H	0.58417900	4.70414900	-1.00812600
H	2.71551300	4.44213400	-2.24964400
H	-2.99682800	-0.27775900	2.17815500
H	0.73176700	1.82876600	2.51176700
H	-3.73669000	0.69904000	4.32931400
H	0.00136300	2.78390700	4.66480500
H	-2.24125800	2.23715700	5.57401000
H	-2.64919100	1.63425500	0.09444000
H	-2.89279900	-2.32075900	-1.57918800
H	-4.65704500	2.27730100	-1.15145200
H	-4.91971400	-1.67470200	-2.79769900
H	-5.82187300	0.63161000	-2.60340100
H	0.13817500	-4.46931800	0.88224300
H	-0.66966400	-3.35537200	1.99298000
H	-1.59188500	-4.15608300	0.71173600
H	0.75033800	-3.44643100	-2.11422400
H	-1.00925000	-3.47996000	-2.26054800

H	-0.11697300	-2.00960200	-2.67561200

S_0-Min^{cr}

Si	-0.12753400	-2.23645100	-0.17338400
C	1.31167900	-1.15975800	0.37811700
C	0.80106500	0.03838100	0.76146400
C	-0.70209800	0.18657800	0.66325700
C	-1.38865200	-0.90953600	0.25245800
C	2.71128700	-1.62158400	0.51593500
C	3.28458900	-2.42830700	-0.47689300
C	3.48127600	-1.34737100	1.65561100
C	4.57352200	-2.93179900	-0.34402200
C	4.76410400	-1.85644400	1.79290300
C	5.31687700	-2.65258400	0.79580700
C	1.63122800	1.16468900	1.27776400
C	1.40789600	1.70168600	2.54891000
C	2.67825100	1.68528900	0.51122700
C	2.22276300	2.70816400	3.04842600
C	3.48581700	2.70280200	1.00673400
C	3.26444000	3.21363900	2.28017600
C	-1.34305400	1.48506700	1.01207100
C	-2.33430800	1.55003300	1.99548100
C	-0.98486100	2.65925900	0.34422800
C	-2.95337400	2.75592700	2.29923700
C	-1.61818900	3.85881700	0.63382000
C	-2.60004500	3.90995200	1.61245300
C	-2.84534600	-1.02298100	0.00853000
C	-3.51764000	-2.19111300	0.39610200
C	-3.58884000	-0.03160700	-0.64770100
C	-4.87615000	-2.35727600	0.15521200
C	-4.94388800	-0.20115600	-0.89838800
C	-5.59480500	-1.36274000	-0.49630100
C	-0.23501700	-3.84753400	0.79346800
C	-0.18536500	-2.61088800	-2.01809600
H	2.71486800	-2.65093900	-1.37490000
H	3.06587300	-0.73142800	2.44393300
H	4.99863600	-3.54485400	-1.13279400
H	5.33868400	-1.62589800	2.68450900
H	6.32221000	-3.04335800	0.90609200
H	0.58996100	1.32786600	3.15456700
H	2.86424600	1.27806100	-0.47787300
H	2.04330900	3.09457000	4.04563600
H	4.29944700	3.09101000	0.40220400
H	3.89776200	4.00130700	2.67423900
H	-2.62515500	0.64401500	2.51724600
H	-0.20230100	2.63197000	-0.40486100
H	-3.72157600	2.79424600	3.06434700

H	-1.36103000	4.76186600	0.09177100
H	-3.07471000	4.85582600	1.83414800
H	-2.96868200	-2.97352400	0.91197700
H	-3.09743300	0.88087800	-0.96380000
H	-5.37350700	-3.26812900	0.47512200
H	-5.49606300	0.57939000	-1.41344700
H	-6.65458300	-1.48979100	-0.68670400
H	0.66987600	-4.43896100	0.61970700
H	-0.32051200	-3.67655400	1.87060500
H	-1.08843500	-4.45335600	0.47284700
H	0.53973400	-3.37821800	-2.30568300
H	-1.18252600	-2.97962600	-2.27853800
H	0.00544800	-1.71817700	-2.62033700

S_1-Min^{cr}

Si	-0.08660300	-2.25438000	-0.27547900
C	1.31219800	-1.19414900	0.35875600
C	0.79099500	0.08539500	0.76496900
C	-0.61768100	0.22938900	0.65470000
C	-1.32169500	-0.92561600	0.17274500
C	2.65860600	-1.67191400	0.57695900
C	3.18414300	-2.66746500	-0.28446900
C	3.49391000	-1.24759200	1.64059500
C	4.46052800	-3.17386200	-0.12094400
C	4.75994200	-1.77976600	1.81528400
C	5.26011000	-2.73197700	0.93150300
C	1.65553000	1.17978000	1.25981900
C	1.42083200	1.77045100	2.50878400
C	2.75764400	1.62295200	0.51555900
C	2.26330600	2.75604400	2.99972300
C	3.58548600	2.62921500	0.99947500
C	3.34703300	3.19437000	2.24690600
C	-1.30009400	1.49050600	1.02025200
C	-2.33665700	1.50277700	1.96273000
C	-0.94147700	2.69739900	0.40735000
C	-2.97833900	2.68865300	2.29431000
C	-1.60457900	3.87403600	0.71802100
C	-2.61832100	3.87386500	1.66605300
C	-2.74230900	-1.01017300	-0.10901500
C	-3.39557300	-2.26042400	0.01530800
C	-3.53038700	0.07610900	-0.56149500
C	-4.74501900	-2.40752900	-0.25458900
C	-4.87240900	-0.08721700	-0.86497800
C	-5.49384800	-1.32155100	-0.70157300
C	-0.18656600	-3.93215200	0.59831000
C	-0.14623800	-2.62460300	-2.13104400
H	2.58062900	-3.00780000	-1.12069200

H	3.12305400	-0.52246900	2.35272100
H	4.84063300	-3.91568000	-0.81670200
H	5.36935500	-1.44444500	2.64897000
H	6.26176300	-3.12613000	1.06174700
H	0.57599600	1.44259200	3.10349500
H	2.95902000	1.17465600	-0.45249500
H	2.07449900	3.17770000	3.98051500
H	4.43008900	2.96617800	0.40657500
H	4.00067300	3.96767000	2.63572300
H	-2.63497100	0.57421900	2.43838400
H	-0.13838100	2.70553100	-0.31961800
H	-3.77144600	2.68769000	3.03444000
H	-1.34470500	4.80020900	0.21790400
H	-3.11355600	4.80354700	1.90799400
H	-2.83062700	-3.11421200	0.37599000
H	-3.06863900	1.04263300	-0.71406800
H	-5.22123600	-3.37289000	-0.11259500
H	-5.44433300	0.75811600	-1.23552500
H	-6.54891400	-1.43680900	-0.92254600
H	0.75074400	-4.48073500	0.45587100
H	-0.34764300	-3.82328500	1.67469200
H	-0.99019600	-4.55556400	0.19119800
H	0.57313200	-3.39745600	-2.42147300
H	-1.14600700	-2.98949900	-2.38799200
H	0.04756000	-1.73351200	-2.73409200

(S_1/S_0)-Cl^{cr}

Si	-0.69899500	-2.75501700	0.69795000
C	0.69044400	-1.47345000	0.53011500
C	0.54144900	-0.40225700	1.51975700
C	-0.63918000	-0.07226600	0.89330700
C	-1.54092900	-1.19654000	0.32446800
C	1.92010500	-1.66684100	-0.31085100
C	2.33732000	-0.99135400	-1.44438600
C	2.81389700	-2.64087900	0.25235700
C	3.60623500	-1.27482900	-2.01107000
C	4.03545100	-2.89580000	-0.31036300
C	4.44054400	-2.20311600	-1.46582000
C	1.51604100	0.48952500	2.10610800
C	2.88498900	0.36715600	1.94297300
C	1.05784900	1.60236300	2.83311700
C	3.73993300	1.38802200	2.34082200
C	1.90803900	2.58997400	3.26338000
C	3.26433400	2.50586000	2.99010500
C	-1.08544000	1.38377700	0.71703600
C	-2.13800300	1.83697400	1.51969300
C	-0.48627200	2.27658100	-0.16643900

C	-2.56530100	3.15605600	1.44179000
C	-0.94278500	3.58582300	-0.25867600
C	-1.96489800	4.03500000	0.55600300
C	-2.89662400	-1.10041700	-0.24966400
C	-3.50737200	-0.11418600	-1.00304500
C	-3.72296200	-2.24509300	0.06150300
C	-4.85109600	-0.25198100	-1.42501300
C	-5.01220700	-2.36221700	-0.33161000
C	-5.59894800	-1.34245500	-1.10484900
C	-0.93950600	-3.66012500	2.33457600
C	-0.62568800	-4.07584100	-0.64018200
H	1.73774700	-0.21635100	-1.89472300
H	2.53822300	-3.16680800	1.15454700
H	3.92583300	-0.71607300	-2.86989100
H	4.69643400	-3.61759500	0.14007000
H	5.40466200	-2.40114100	-1.90172900
H	3.30231200	-0.47518200	1.44121500
H	0.01527900	1.68124000	3.04977700
H	4.79021200	1.29144100	2.14976200
H	1.51809500	3.43206900	3.79873600
H	3.93523300	3.28680000	3.29365200
H	-2.62672400	1.16977900	2.21183700
H	0.35497800	1.97664200	-0.76617100
H	-3.36405600	3.49301100	2.07782600
H	-0.47507900	4.26270100	-0.95197700
H	-2.29375100	5.05627000	0.49721300
H	-2.97791800	0.76302400	-1.30051000
H	-3.30785700	-3.02402000	0.67296700
H	-5.28705000	0.52863400	-2.01882200
H	-5.58393700	-3.22825600	-0.05000300
H	-6.61816600	-1.42747000	-1.43243400
H	-0.28267600	-4.51613800	2.37173400
H	-0.75772000	-3.05044200	3.20887300
H	-1.95313800	-4.03494700	2.40592300
H	0.27043000	-4.67725700	-0.53790600
H	-1.47299800	-4.75020900	-0.54545900
H	-0.63961300	-3.65716500	-1.63869300