

The photochemistry of inverse dithienylethene switches understood

SUPPORTINGS

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- **S.2 Figures and Tables**

S.1 Derivation of equations (1) and (2)

As shown on scheme 2, considering the photophysical model, the different relaxation pathways are described as: i) a direct mechanism for photocyclization (k_1) from $S_1(FC)$ already reviewed through transient band Y ; ii) an internal conversion (k_2) to $S_1(opt)$; iii) from the latter, emission (k_3) or internal conversion (k_4) to ground state. iv) a second photocyclization pathway (k_5) from $S_1(opt)$. The relationship between the fluorescence and cyclization quantum yields can be established by analyzing the expression of $\phi(fluo)$ and $\phi(cycl)$:

$$\phi(IC) = \frac{k_2}{k_1 + k_2} \quad (1)$$

$$\phi(fluo) = \frac{k_2}{k_1 + k_2} \times \frac{k_3}{k_3 + k_4 + k_5} \quad (2)$$

$$\phi(cycl) = \frac{k_1}{k_1 + k_2} + \frac{k_2}{k_1 + k_2} \times \frac{k_5}{k_3 + k_4 + k_5} \quad (3)$$

Combining (2), (3) via (1) one gets the expression for both direct mechanism and indirect mechanism:

$$\phi(cycl) = 1 - (1 + \frac{k_4}{k_3})\phi(fluo) \quad (4)$$

Since internal conversions are known to be faster than several hundreds of picoseconds, i.e. less shorter than emission, we have $k_4 \gg k_3$ and thus:

$$\phi(cycl) \approx 1 - \frac{k_4}{k_3}\phi(fluo) \quad (5) \quad \text{Equation (1)}$$

Since k_5 disappears in the course of the equation derivations, it means that based on equation (5), one cannot discriminate between the direct mechanism alone or both mechanisms. Reversly, considering the indirect mechanism alone, i.e. $k_1=0$ et $k_5 \neq 0$ one can obtain a new equation:

$$\phi(cycl) = \frac{k_5}{k_3}\phi(fluo) \quad (6) \quad \text{Equation (2)}$$

S.3 Figures and Tables

Table SI.1 Experimental and PCM-TDDFT maximum of absorption for CF species. Calculated Rcc are listed as well.

CF		Exp (nm)	Theory (nm)	$\Delta E(\text{eV})$	$R_{CC}(\text{\AA})$
	DTE	427	441	0.09	1.45
	DTE-O2	438	473	0.21	1.56
	DTE-O3	453	476	0.13	1.58

Table SI. 2 Maximum absorption wavelength $\lambda_{\text{abs}}^{\text{max}}$ (in nm) for transient bands X, Y and Z: TDDFT vertical excitation from either i) AP or P conformers ii) S_0 or $S_1(\text{opt})$ states.

	DTE	DTE-O2	DTE-O3
Band X (nm)	622	635	616
TDDFT Conformer AP $S_1(\text{opt})$	558	629	671
attribution	$S_1 \rightarrow S_5$	$S_1 \rightarrow S_6$	$S_1 \rightarrow S_7$
TDDFT Conformer AP S_0	812	832	825
Band Z (nm)	573		
TDDFT Conformer P $S_1(\text{opt})$	624		
attribution	$S_1 \rightarrow S_5$		

Figure SI1 Transient Absorption spectra of DTE (ACN/350 nm excitation) for 600 fs and 500 ps pump-probe delay.

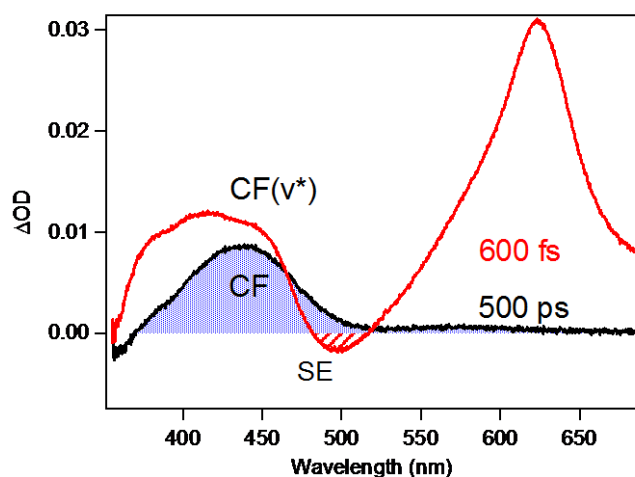
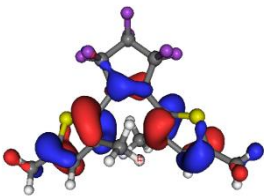
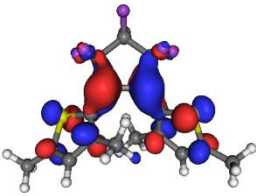
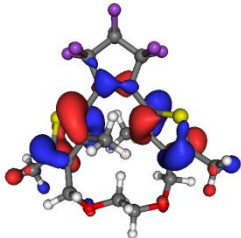
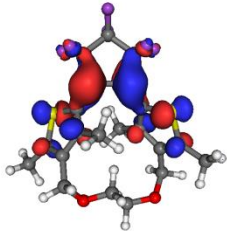
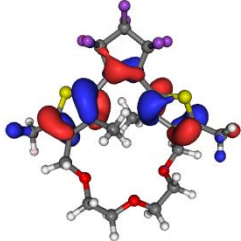
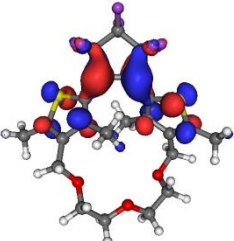


Figure SI2 DFT orbitals for OF and CF.

OF	HOMO	LUMO
DTE		
DTE-O ₂		
DTE-O ₃		

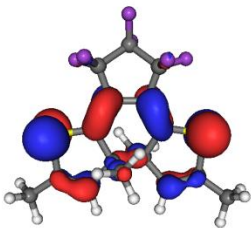
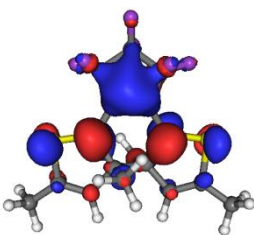
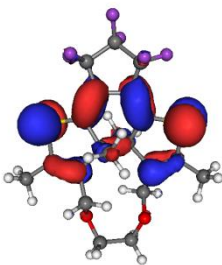
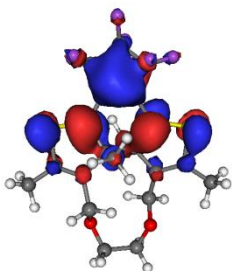
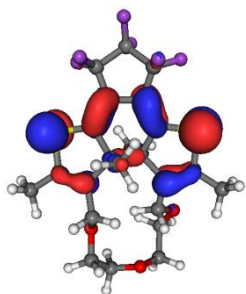
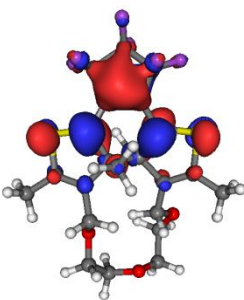
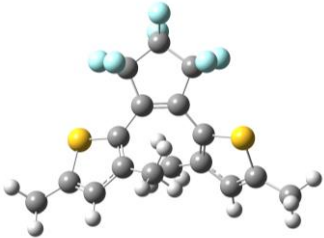
CF	HOMO	LUMO
DTE		
DTE-O ₂		
DTE-O ₃		

Table SI3 Structural informations (Cartesian coordinates; Carbene-Carbene distances and Torsion angles) for the series including Ground and first excited states

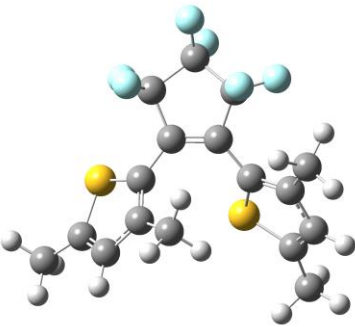
I. DTE

I.A. Ground state S0

1) OF Anti-Parallel OF-AP

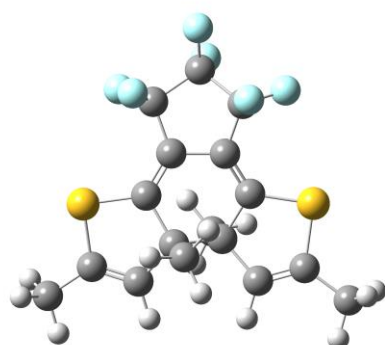
Rcc (Å)	Torsion angle
3.576	46.1 and 46.0
	C,0,-0.0045204981,2.9278912352,0.1924640511 C,0,-1.2301831571,2.0021004987,0.0031490392 C,0,-0.6666931509,0.6035683942,0.0675689344 C,0,0.67542489,0.6168562124,-0.0960582743 C,0,1.1943735923,2.0308504935,-0.2020899766 F,0,-1.8064660973,2.243668697,-1.2125287841 F,0,-2.1764032175,2.2411012724,0.9403330793 F,0,0.0967452828,3.2650075237,1.4977679024 F,0,-0.0784241761,4.0540923329,-0.5363343073 F,0,2.2629878885,2.2655344976,0.6041650282 F,0,1.5897190749,2.3157838959,-1.4724001097 C,0,3.4531894322,-2.1550542268,-0.0911299641 C,0,2.4921952162,-2.5294270443,-0.9839832205 S,0,3.0642804259,-0.6371575099,0.6267971383 C,0,1.4082771682,-1.602303495,-1.1028027428 C,0,1.5773418506,-0.5220754995,-0.2696653733 C,0,-3.4492753971,-2.1543640535,0.1481040183 C,0,-2.4825910479,-2.5189601844,1.0386093623 S,0,-3.0480940641,-0.659931813,-0.612986931 C,0,-1.3877590891,-1.600450632,1.1269035523 C,0,-1.5549326915,-0.5386815298,0.2713116203 C,0,0.2648471184,-1.8175679191,-2.0519503384 H,0,0.6163082336,-2.3183096732,-2.9600702882 H,0,-0.5117257178,-2.4473491583,-1.5990938648 H,0,-0.2059433028,-0.8745035167,-2.3441598325 H,0,5.6033612364,-2.2973322817,-0.0181853666 C,0,4.7180968118,-2.8781703095,0.2630612549 H,0,4.7573917177,-3.8344834177,-0.2667148818 H,0,4.7793158085,-3.0817412154,1.3375849954 C,0,-4.7237026703,-2.8725345808,-0.180323308 H,0,-5.6008569136,-2.2780751828,0.0979533373 H,0,-4.7664935493,-3.8181766416,0.3679822244 H,0,-4.7968592553,-3.0959595536,-1.2501297158 C,0,-0.2368939462,-1.8026188622,2.0695656792 H,0,2.5516002664,-3.446999484,-1.564090179 H,0,-2.5453162463,-3.4233156057,1.6387212458 H,0,0.2324654558,-0.8545345047,2.3478062504 H,0,-0.5784971755,-2.2961841841,2.9852870216 H,0,0.5392228938,-2.4325309741,1.6160697237

2) OF Parallel OF-P

Rcc (Å)	Torsion angle
4.386	-144.4 and 48.4
	C,0,-1.5540075208,-2.4592544706,-0.5135533246 C,0,-2.1426762496,-1.111817671,-0.034122187 C,0,-0.9506295849,-0.1832458302,0.0196950665 C,0,0.1961794757,-0.9002666889,0.0659881847 C,0,-0.0759670012,-2.3780620221,-0.0672112748 F,0,-2.6992933989,-1.2995508391,1.2013572391 F,0,-3.1312359841,-0.6799110332,-0.8506042176 F,0,-1.6166002261,-2.5135931598,-1.8630700256 F,0,-2.2004392463,-3.525249848,-0.0125597925 F,0,0.7394669966,-2.9859690149,-0.9677865483 F,0,0.0891701952,-3.0293816384,1.1165721646 C,0,3.9855538789,0.1123456931,0.1595187843 C,0,3.3559094418,0.7418912999,1.1935564839 S,0,2.8800621027,-0.8654627335,-0.7292641596 C,0,1.9575443034,0.4592502393,1.2849947614 C,0,1.5519425928,-0.4006283447,0.2916850344 C,0,-1.1025165402,1.2704108431,-0.0593540702 C,0,-1.859050166,3.4532792344,0.1448414212 S,0,-0.0152209604,2.1813139977,-1.0670372473 C,0,-2.0435422642,2.0865041517,0.5244866125 C,0,-0.816576413,3.6626155029,-0.7106147326 C,0,1.0777130969,1.0492425265,2.348344702 H,0,0.2072436529,0.4181755916,2.5528611376 H,0,1.6364787287,1.1733678134,3.2816916185 H,0,0.7058850829,2.0365393526,2.0444028562 H,0,5.5677308934,0.557051278,-1.2381596354 C,0,5.4350216088,0.1800297666,-0.2182617727 H,0,5.9112027688,-0.8047103538,-0.1599848715 H,0,5.9632975863,0.8531112954,0.463437931 C,0,-0.362177888,4.9566381508,-1.3161674657 H,0,-0.9617737926,5.7810246199,-0.9191579441 H,0,-0.475611124,4.9487807322,-2.4058358148 H,0,0.6900597331,5.1603934581,-1.0905089971 C,0,-3.1349615526,1.6579150576,1.4668875661 H,0,3.8754931744,1.3946600027,1.8905364181 H,0,-2.4966902391,4.2563048828,0.505718034 H,0,-2.7659808845,0.9719885114,2.234964188 H,0,-3.5621280822,2.5313253968,1.9687152393 H,0,-3.9457361948,1.1481312495,0.9349416377

3) CF

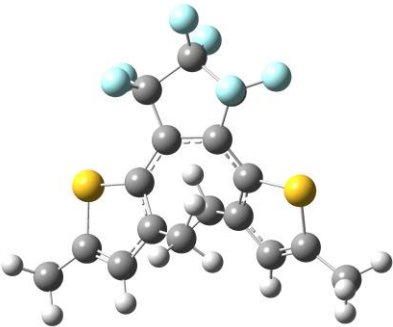
Rcc (Å)	Torsion angle
1.550	5.0 3.5



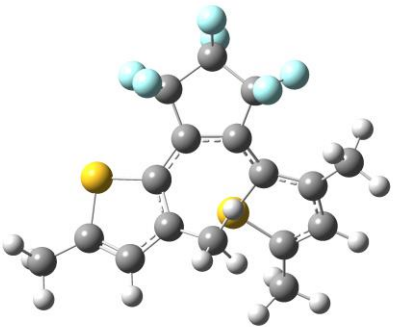
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 C,0,-2.1710857355,1.1958008991,0.2360825314
 F,0,-2.3401605878,-2.2258024067,-0.9166891846
 F,0,-2.5681026174,-1.791127511,1.2109496818
 F,0,-4.2434172188,-0.0568693063,0.2375317623
 F,0,-3.1253658599,0.1227915206,-1.6386016358
 F,0,-2.4935713145,1.3976742153,1.5495876379
 F,0,-2.4580842793,2.3424955479,-0.4248491509
 C,0,2.3691258822,2.9348496214,-0.0082563508
 C,0,2.7595568782,1.6651376947,-0.1242441925
 S,0,0.6010307131,3.1511719581,-0.1138209425
 C,0,1.6676961275,0.6646365552,-0.4242721979
 C,0,0.3649804227,1.4171339726,-0.1325111302
 C,0,2.4406237452,-2.8772458623,-0.0490207234
 C,0,2.8056650501,-1.6000435859,0.0646792507
 S,0,0.684932313,-3.1356125246,0.1349091062
 C,0,1.7077665339,-0.6286025176,0.4292386486
 C,0,0.4075602032,-1.4111823606,0.2099129871
 C,0,1.7007053013,0.3437954341,-1.9381406177
 H,0,1.5796434868,1.266246951,-2.5144986488
 H,0,2.6597931772,-0.1099745809,-2.2094204397
 H,0,0.9011248762,-0.3498025751,-2.2181301032
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 C,0,3.2111874457,4.1576694014,0.1754567281
 H,0,4.2698916005,3.8862717436,0.2207688379
 H,0,2.946037522,4.6804475588,1.1013182115
 C,0,3.3002992509,-4.0769413715,-0.2935116069
 H,0,3.0001777088,-4.5933695428,-1.21220192
 H,0,3.2186588062,-4.793819896,0.5315365819
 H,0,4.3484743022,-3.7790983932,-0.3890815771
 C,0,1.8195936059,-0.3077765874,1.9391071065
 H,0,3.8084931663,1.3753705736,-0.1100109671
 H,0,3.8452906988,-1.2844378617,0.0009923359
 H,0,1.0198189135,0.3645974962,2.2660348399
 H,0,1.75603357,-1.2332969464,2.5197819566
 H,0,2.7808084472,0.1705014378,2.1552233508

I.B. Excited State S1

1) OF Anti-Parallel OF-AP

Rcc (A)	Torsion angle
2.816	22.4 and 23.5
	C,0,-0.0363707668,3.023297586,0.2356985333 C,0,-1.2182333648,2.1325556627,-0.2408727766 C,0,-0.7152493215,0.750246028,-0.0067686053 C,0,0.7034578441,0.7539916875,-0.0942775682 C,0,1.2309289186,2.1437914413,0.0178279381 F,0,-1.4576890466,2.3981907259,-1.5699374151 F,0,-2.3664256673,2.4345651305,0.4168375632 F,0,-0.1907749391,3.2725217809,1.5581668165 F,0,0.0301209178,4.2010128067,-0.4093995103 F,0,2.126423676,2.3149512487,1.0404222318 F,0,1.8838556847,2.5555458184,-1.1108845042 C,0,3.0884926191,-2.2940083011,-0.0551612376 C,0,1.9602319744,-2.6578006212,-0.7362278668 S,0,3.0685807801,-0.6084475987,0.3754399465 C,0,1.0307773446,-1.6048705987,-0.9517695623 C,0,1.4729539893,-0.3973578687,-0.3239756156 C,0,-3.0839276505,-2.3039527047,0.0973808275 C,0,-1.9528388633,-2.6303941159,0.7929628335 S,0,-3.0800459221,-0.6343647058,-0.3927755823 C,0,-1.0306150692,-1.5636380846,0.9660012974 C,0,-1.4811299415,-0.3863006155,0.2870117154 C,0,-0.0122049038,-1.6866733269,-2.0297825975 H,0,0.4545771149,-2.0394712615,-2.9578595217 H,0,-0.8137484263,-2.3953973338,-1.7766338941 H,0,-0.466692571,-0.7151803317,-2.2338886607 H,0,5.1863531637,-2.7371725231,-0.1853449956 C,0,4.2759329363,-3.1405421452,0.2734597977 H,0,4.1254177407,-4.1590244594,-0.0960053471 H,0,4.4469055608,-3.1890166122,1.3553013811 C,0,-4.2650772571,-3.1721154813,-0.1952122562 H,0,-5.1787312584,-2.7563024865,0.2457903892 H,0,-4.1072523802,-4.1725737393,0.217968292 H,0,-4.4351748564,-3.2687145343,-1.2739623681 C,0,0.0081640609,-1.5927523677,2.0508839955 H,0,1.8203782151,-3.6586888691,-1.1378947947 H,0,-1.8063481346,-3.6132966348,1.2347961075 H,0,0.4735580846,-0.6163769322,2.1993502193 H,0,-0.4653829869,-1.8844995694,2.996769387 H,0,0.8023157018,-2.3240740932,1.8430734074

2) OF Parallel OF-P

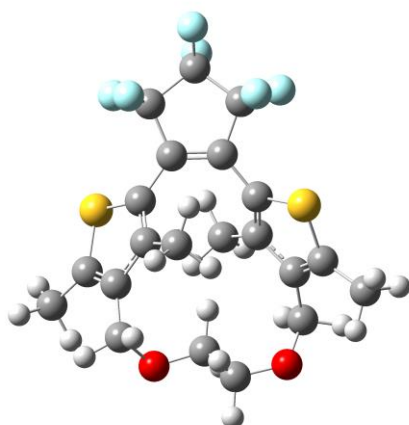
Rcc (A)	Torsion angle
4.351	-159.8 and 28.40
	C,0,-1.5666321473,-2.4691310732,-0.4361330376 C,0,-2.1170966655,-1.2144531907,0.2973326447 C,0,-1.0125511882,-0.2158180614,0.1663040238 C,0,0.2238610684,-0.9190901923,0.0175032405 C,0,-0.0245189932,-2.354961631,-0.3080510606 F,0,-2.3853309999,-1.5562574258,1.6034216483 F,0,-3.3001910652,-0.8306129682,-0.246765836 F,0,-1.91719805,-2.391706453,-1.7416037429 F,0,-2.0495641816,-3.6215822246,0.0613780184 F,0,0.5913233715,-2.7837844487,-1.453039239 F,0,0.4125960874,-3.1995388583,0.6773826267 C,0,3.9624394909,0.1332182515,0.148508248 C,0,3.2778880075,0.9528021658,1.0053393596 S,0,2.9140498553,-1.0276826688,-0.593871304 C,0,1.8931289107,0.6733549711,1.1139340068 C,0,1.511112651,-0.400609335,0.2594772394 C,0,-1.1748982834,1.1642843593,0.0004157395 C,0,-1.8733613436,3.378960447,0.1059163718 S,0,0.086928172,2.0635507829,-0.8891147628 C,0,-2.1780734286,2.0579467609,0.4505080715 C,0,-0.6882244229,3.5537211815,-0.6068713315 C,0,1.0537398178,1.2750333119,2.204457022 H,0,0.1298959562,0.7165512903,2.3692956226 H,0,1.6215791013,1.2755167407,3.1421430105 H,0,0.783993312,2.3184460979,1.9864168992 H,0,5.604382314,0.340421217,-1.2260367082 C,0,5.4241331362,0.1462772417,-0.1617976933 H,0,5.8902563125,-0.8162186342,0.0796591351 H,0,5.924683218,0.9273097653,0.4178054105 C,0,-0.1138191749,4.8443226852,-1.0995453563 H,0,-0.749118842,5.6787131595,-0.7879801516 H,0,-0.0412000615,4.8632133794,-2.1939002389 H,0,0.8936248123,5.0158733679,-0.7008428915 C,0,-3.3581944412,1.6701177358,1.2913465045 H,0,3.7697214117,1.7266233174,1.5898530331 H,0,-2.5006657264,4.2222889472,0.38573114 H,0,-3.0883862216,0.9110040259,2.0345996523 H,0,-3.7472691595,2.5446954393,1.822583655 H,0,-4.1699026099,1.2523885232,0.6861830305

II . DTE-O2

II.A.Ground State S0

1) OF-AP

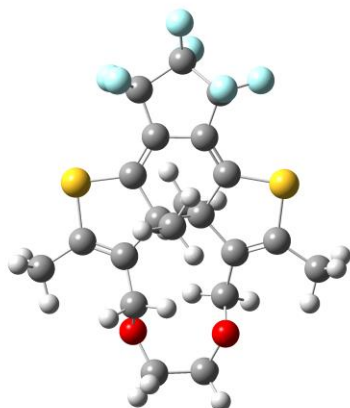
Rcc (A)	Torsion angle
3.479	47.8
	49.6



S,0,0.332053965,2.9527968522,-0.7854176764
C,0,-1.2285770866,3.3040663928,-0.1561168385
C,0,-2.0487166826,4.4335179817,-0.7105046292
H,0,-2.1561052479,5.2388461843,0.0255169467
H,0,-1.5917700703,4.861377145,-1.6074801443
H,0,-3.0505647582,4.0794820606,-0.9750271603
C,0,0.5211378198,1.5958989053,0.2784908967
C,0,-0.5466266222,1.47350548,1.1336206117
C,0,-0.6168306041,0.4881983241,2.2678805143
H,0,0.3547447828,0.0202610856,2.446433709
H,0,-1.3411170941,-0.3140696159,2.086468042
H,0,-0.9118818698,0.99748319,3.1922810458
C,0,-1.5734775172,2.4386694764,0.8497999505
C,0,-2.9587577065,2.4095248034,1.4463904778
H,0,-3.3659494681,3.4193439165,1.5475241475
H,0,-2.9497048535,1.9487230994,2.4454620977
O,0,-3.8831911837,1.7181780587,0.6090018755
C,0,-3.6338787477,0.3284078421,0.5307857792
H,0,-2.5768975742,0.140221614,0.3164369694
H,0,-3.8827490611,-0.1626010041,1.4857928104
C,0,-4.4828367026,-0.2590392302,-0.5879844238
H,0,-5.5435652215,-0.0840080362,-0.3824607921
H,0,-4.2348300266,0.2331084767,-1.5411380379
O,0,-4.3190938483,-1.6622917129,-0.6928662429
C,0,-3.2351942091,-2.1164935773,-1.4961008231
H,0,-3.5210320281,-3.1290903841,-1.7995317077
H,0,-3.1747699613,-1.5052645851,-2.4076047415
C,0,-1.8980771784,-2.1542645285,-0.790294198
C,0,-1.619208514,-3.0760491633,0.1841881781
S,0,-0.0460639179,-2.8477950121,0.8393225782
C,0,-2.50815896,-4.1844681515,0.6690607247
H,0,-2.1540991361,-4.6020204794,1.6161685109
H,0,-2.5451675175,-5.001486548,-0.0618468387
H,0,-3.5270118173,-3.8129988711,0.8156073498
C,0,-0.8107571289,-1.2417677404,-1.0252657426
C,0,-0.8452352972,-0.1746125372,-2.0821836319
H,0,-1.4751545561,0.6732028525,-1.7807878413
H,0,-1.2459657665,-0.5707172693,-3.021363197
H,0,0.153835068,0.2158743108,-2.2897070672
C,0,0.2523168135,-1.4811086678,-0.1877092144
C,0,1.4873711068,-0.7015719097,-0.0539691316
C,0,1.6130312982,0.6337687463,0.1116220169
C,0,3.0605273778,1.04656514,0.167823753
F,0,3.3354943247,2.1022174272,-0.6419239064
F,0,3.4188356352,1.411392724,1.4287906464
C,0,3.8498131606,-0.2160061113,-0.2629993074
F,0,4.9912830413,-0.381034031,0.4251085797
F,0,4.1469241518,-0.1315844356,-1.5791254381
C,0,2.8386951678,-1.3714968294,-0.0459659724
F,0,2.9656923315,-2.3240856388,-0.9978964566
F,0,3.08010489,-1.9752200194,1.1558519496

2) CF

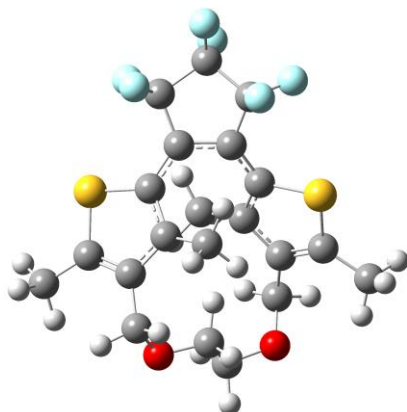
Rcc (A)	Torsion angle
1.568	6.012
	4.249



O,0,-0.0531600488,-0.0084565591,-0.0246746239
 C,0,-0.0556729167,0.0686809766,1.4006009447
 H,0,0.9901613122,0.1392328687,1.7400562848
 H,0,-0.5613039537,0.9859688501,1.7138839036
 C,0,0.2207885472,1.2524351935,-0.6147944573
 H,0,0.7445095437,1.0659273143,-1.5595380186
 H,0,0.8941606174,1.8288027466,0.0365607252
 C,0,-1.0578329508,2.0476521001,-0.8898687023
 H,0,-1.5807844725,1.6358059631,-1.7654821284
 H,0,-0.7999349304,3.0898090514,-1.1113249797
 O,0,-1.9301018185,2.0551877443,0.2290876211
 C,0,-2.8513284145,0.966152898,0.1839250016
 H,0,-2.3332308464,0.0654004109,-0.155394777
 H,0,-3.62284965,1.2028809946,-0.5662370016
 C,0,-3.5062064949,0.6997445972,1.5163927199
 C,0,-4.5221174053,1.4541477755,1.9543876915
 C,0,-5.0279210779,2.7406882806,1.3799520478
 H,0,-4.3621725973,3.0984110081,0.5906613301
 H,0,-5.0742469677,3.5154107993,2.1535481671
 H,0,-6.0395599699,2.617082222,0.9748917737
 S,0,-5.4250724238,0.7741964874,3.3220903744
 C,0,-4.3817597401,-0.6190870757,3.370675765
 C,0,-4.3621807747,-1.5940448813,4.2908300364
 C,0,-5.3251548808,-1.9058167386,5.3948734397
 F,0,-5.576719093,-0.8579105147,6.2244222002
 F,0,-6.5343445052,-2.3245581409,4.9214994358
 C,0,-4.6492062702,-3.0808547326,6.170569614
 F,0,-5.5363425181,-3.9491034426,6.6812211507
 F,0,-3.9132031458,-2.5667253161,7.1852881599
 C,0,-3.6759813795,-3.7313502913,5.1449716764
 F,0,-4.365332706,-4.6860075521,4.4467305882
 F,0,-2.6438280349,-4.3567175888,5.7591125783
 C,0,-3.2795975524,-2.5800299866,4.2815337091
 C,0,-2.149776694,-2.3350190777,3.6050121183
 S,0,-0.8225353894,-3.4289886279,3.3210130191
 C,0,-0.0711444632,-2.2833592275,2.1940930251
 C,0,1.2392189107,-2.6872515778,1.5930455504
 H,0,1.140319836,-3.6421050005,1.0645338926
 H,0,2.0024422301,-2.8176456752,2.3698267024
 H,0,1.5803594523,-1.9413062544,0.8710686023
 C,0,-0.7191907051,-1.1202397344,2.0495492832
 C,0,-1.9660538957,-0.964857921,2.9213315373
 C,0,-1.6302030739,0.0748071177,4.0234598687
 H,0,-1.5792597241,1.0830405541,3.5987321263
 H,0,-2.3803367973,0.0847277477,4.8177182336
 H,0,-0.6613985059,-0.1643752666,4.4737217504
 C,0,-3.3381835647,-0.6391811677,2.2348220483
 C,0,-3.7443534206,-1.7537748065,1.2344222829
 H,0,-2.9754693153,-1.8803311208,0.4647265708
 H,0,-3.8821198139,-2.7178479645,1.7295962103
 H,0,-4.6871720769,-1.4859894787,0.7465639574

II.B.Excited State S1 OF-AP

Rcc (A)	Torsion angles
3.088	25.3
	23.9



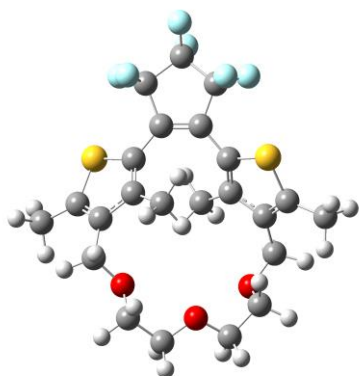
S,0,0.4253442592,3.0576526345,-0.6818876079
 C,0,-1.1984889656,3.2965348391,-0.1318214473
 C,0,-1.9645501302,4.5074177473,-0.566966777
 H,0,-1.8790770968,5.3111408807,0.1764071524
 H,0,-1.590324225,4.8985469424,-1.5178623883
 H,0,-3.0249261729,4.2681556367,-0.6909176776
 C,0,0.5568778327,1.5506814143,0.2044455585
 C,0,-0.6160556915,1.3243734456,0.9858873647
 C,0,-0.6590828434,0.3789253287,2.1551778035
 H,0,0.3093307028,-0.0984990574,2.316783769
 H,0,-1.4098913816,-0.4148091809,2.0443984746
 H,0,-0.9084049598,0.933325934,3.0689966746
 C,0,-1.6084615632,2.3166885859,0.7470440922
 C,0,-2.9758283961,2.3406952347,1.3923852097
 H,0,-3.3275568929,3.3689753948,1.5093587027
 H,0,-2.9315418211,1.8884070539,2.3948417646
 O,0,-3.9697885629,1.6853020286,0.6169640396
 C,0,-3.7781302907,0.2853606755,0.583742699
 H,0,-2.7354612662,0.0581528276,0.34406655
 H,0,-4.0081949877,-0.1575706035,1.5664713376
 C,0,-4.6629927063,-0.3242945417,-0.4908340428
 H,0,-5.7178675997,-0.2841610778,-0.2043310837
 H,0,-4.5396485974,0.2374829176,-1.4294765372
 O,0,-4.3530465639,-1.6932223021,-0.6877619946
 C,0,-3.2038635687,-1.949438739,-1.4831579621
 H,0,-3.3967854553,-2.9163319211,-1.9601260418
 H,0,-3.1378129406,-1.1992136163,-2.2826905244
 C,0,-1.8890903679,-2.0215717784,-0.7285843425
 C,0,-1.6004416682,-3.0671138553,0.1203857957
 S,0,0.0210970697,-2.9983200814,0.7226157697
 C,0,-2.4832073167,-4.2208971,0.4763170775
 H,0,-2.387592258,-4.4834746202,1.5354482269
 H,0,-2.21318682,-5.1116367509,-0.1064930817
 H,0,-3.5300704166,-3.9751204958,0.2802557516
 C,0,-0.8039018084,-1.1134672506,-0.9002534721
 C,0,-0.7773369944,-0.0987495589,-2.0079275739
 H,0,-1.4640314922,0.7424146227,-1.8250390224
 H,0,-1.0813389095,-0.5668588462,-2.9522944675
 H,0,0.2219765366,0.3126641746,-2.1571222883
 C,0,0.3316521361,-1.4929701789,-0.1204813263
 C,0,1.5083584485,-0.7598140246,0.1002410847
 C,0,1.6213539068,0.6580555166,0.003929263
 C,0,3.0367955686,1.0538419585,-0.2439037868
 F,0,3.2217851882,1.7368289112,-1.4191901762
 F,0,3.5389564414,1.869498773,0.7311856982
 C,0,3.8222414771,-0.2929670436,-0.2591139852
 F,0,5.006517883,-0.2087836928,0.3719089278
 F,0,4.0504091229,-0.6708226882,-1.5393700155
 C,0,2.8562995559,-1.3226178038,0.3946252122
 F,0,3.0682989413,-2.5732586035,-0.0876557427
 F,0,3.1295246603,-1.3816520658,1.743538366

III. DTE-O3

III.A. S0

1) OF-AP

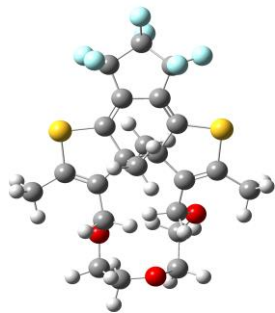
Rcc (Å)	Torsion angle
3.648	43.1 44.1



S,0,2.805013851,2.0895194722,3.6921641849
C,0,1.715750411,2.7824382392,4.825989561
C,0,2.2326481596,3.2719365573,6.1502495237
H,0,3.3093506203,3.4620742963,6.1081990539
H,0,1.7432039705,4.2047781352,6.4478151971
H,0,2.0580965682,2.5311946116,6.9393815486
C,0,1.5252586077,1.763775974,2.5598794143
C,0,0.3099357757,2.1833709246,3.0454700217
C,0,-1.0029526843,2.0479197768,2.3323061604
H,0,-0.9708420505,1.263510695,1.5716608896
H,0,-1.8071337957,1.8067434952,3.0349712732
H,0,-1.2723466302,2.9907801205,1.8390120304
C,0,0.4284502625,2.7642028168,4.3597665394
C,0,-0.7548013902,3.2683625409,5.1438060573
H,0,-1.5803079374,2.552027866,5.0884900674
H,0,-0.4909792496,3.3794071874,6.2071901935
O,0,-1.2826286447,4.4871762752,4.6494298039
C,0,-0.4971853351,5.6116380378,4.9832805078
H,0,-0.5095515601,5.7610299415,6.0768083566
H,0,0.5456249437,5.4750777542,4.6583629597
C,0,-1.0697974684,6.8279452696,4.2933573993
H,0,-2.1682442905,6.7850269409,4.3505565452
H,0,-0.7305507198,7.7460295777,4.8012241895
O,0,-0.6405594263,6.827706364,2.9515347973
C,0,-1.4173177907,7.6404627769,2.1066124933
H,0,-2.4735895857,7.3318566099,2.1487173323
H,0,-1.3513817422,8.6999959695,2.4083543232
C,0,-0.8992832629,7.4905335175,0.6956213849
H,0,-1.438277862,8.1860002227,0.0300290224
H,0,0.1732759275,7.7432695143,0.6661826472
O,0,-1.0939150183,6.1556147465,0.2966214854
C,0,-0.536756653,5.8442050118,-0.9654601446
H,0,0.4417534287,6.3407523193,-1.0720538472
H,0,-1.1825502936,6.2218393202,-1.7731045471
C,0,-0.3751064461,4.3575875946,-1.0505721129
C,0,-1.1592887563,3.5434951255,-1.8193094548
S,0,-0.6992720502,1.8969566721,-1.654155077
C,0,-2.2867895153,3.9262735726,-2.7357663654
H,0,-1.9094662277,4.3548558515,-3.6714051719
H,0,-2.9386351003,4.6652278311,-2.2591128499
H,0,-2.9009045942,3.0582092317,-2.9934789079
C,0,0.6109516588,3.6444123999,-0.2832528213
C,0,1.5758371498,4.3447925485,0.6271351549
H,0,2.4406602622,3.7206993053,0.8648542564
H,0,1.944754496,5.2657015289,0.1612869884
H,0,1.0828804856,4.6305241603,1.5658206133
C,0,0.5508697465,2.2895307002,-0.5073718304
C,0,1.3930205952,1.2325199228,0.0536484224
C,0,1.8365846278,1.0500809097,1.3208648618
C,0,2.8300145899,-0.0890050577,1.3787456177
F,0,4.1126882837,0.3793065652,1.4567568342
F,0,2.6470232945,-0.9065103199,2.4420805049
C,0,2.6403263853,-0.8539598009,0.0508392859
F,0,1.7863816801,-1.8831441855,0.2491069118
F,0,3.7902625187,-1.3426975887,-0.4444253471
C,0,1.9803170016,0.1919264505,-0.8747942969
F,0,2.9149687544,0.7423975551,-1.6968585509
F,0,1.0535120246,-0.3973838512,-1.6760630912

2) CF

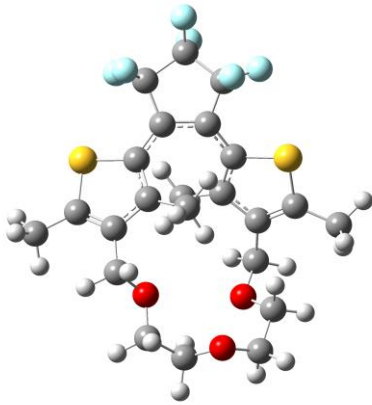
Rcc (A)	Torsion angle
1,576	5.9 4.0



O,0,3.020735652,1.0821416247,1.2598679961
C,0,2.4618355165,-0.0909312288,0.661061777
H,0,2.7831283365,-0.9763347268,1.2284503094
H,0,2.8699401816,-0.1869854014,-0.3448741173
C,0,4.2997719575,1.4288941141,0.7696567173
H,0,4.5182890579,2.416617499,1.1907494037
H,0,4.2659022928,1.5268258063,-0.3283324627
C,0,5.4072000499,0.4658007225,1.1796343293
H,0,5.3471856274,0.2841767066,2.2578064175
H,0,6.388623326,0.9174216181,0.9628332398
O,0,5.2971824418,-0.8058985235,0.5627341245
C,0,5.83074164,-0.9066808799,-0.7436116293
H,0,6.8720577972,-1.2605323125,-0.6913612759
H,0,5.8217640844,0.0649454666,-1.2570637268
C,0,4.9911536452,-1.886568961,-1.5366325618
H,0,5.5455272929,-2.2318043,-2.4220544433
H,0,4.7738603135,-2.7565214491,-0.9016874837
O,0,3.7901242382,-1.2542570709,-1.9560917602
C,0,2.6252776318,-2.0563983695,-1.8158254242
H,0,2.4312942168,-2.252718471,-0.7515982109
H,0,2.801202239,-3.0346272155,-2.2892622955
C,0,1.4402604678,-1.385660279,-2.4723770338
C,0,1.3385424476,-1.407578149,-3.8085437816
C,0,2.3419549423,-1.8962370578,-4.8078080803
H,0,2.5142757388,-1.1369194228,-5.5788739413
H,0,1.9790701212,-2.8006223372,-5.3111463406
H,0,3.3017450967,-2.1073713553,-4.331733041
S,0,-0.2184405622,-0.8771706119,-4.4571241601
C,0,-0.8056170885,-0.53263036,-2.8534657779
C,0,-1.9548017459,0.081968973,-2.5469593961
C,0,-3.1129582265,0.4544730819,-3.4222379472
F,0,-2.7713701667,1.1868769197,-4.515379993
F,0,-3.7810147812,-0.6426409478,-3.8832980639
C,0,-4.0578390156,1.2644920446,-2.4805898494
F,0,-5.3571751464,1.0951062912,-2.7726128331
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C,0,-3.6866043813,0.7964459845,-1.0435498995
F,0,-4.4513829272,-0.297505629,-0.7389585015
F,0,-3.9680678072,1.7461232859,-0.120334937
C,0,-2.2379668596,0.4543088957,-1.1631768449
C,0,-1.2517529986,0.4854997256,-0.2588386431
S,0,-1.4222508675,0.7582263676,1.4533457177
C,0,0.2634590468,0.2835895688,1.7295390935
C,0,0.751469418,0.3283409571,3.1441502788
H,0,0.0582430027,-0.1974673949,3.8106462941
H,0,0.8332670573,1.3654111823,3.4889721611
H,0,1.7399377892,-0.1284321869,3.2302431125
C,0,0.9627876419,0.0250025351,0.6183964574
C,0,0.2054784606,0.2180951794,-0.6954005437
C,0,0.7568530718,1.5061703855,-1.3551035248
H,0,0.1703103215,1.7987594571,-2.2309053618
H,0,0.7403223009,2.3274797204,-0.632410742
H,0,1.7927566124,1.3499737699,-1.6768034322
C,0,0.1614090578,-0.9704199236,-1.7297179503
C,0,-0.4212449013,-2.2487894261,-1.0755700913
H,0,-1.413047682,-2.0726182279,-0.6500958137
H,0,-0.5054128723,-3.0439321583,-1.8233966226
H,0,0.2318676911,-2.5968937909,-0.2674857644

III.B. S1 OF-AP

Rcc (A)	Torsion angle
3.247	22.6
	127.5

	O,0,3.020735652,1.0821416247,1.2598679961 C,0,2.4618355165,-0.0909312288,0.661061777 H,0,2.7831283365,-0.9763347268,1.2284503094 H,0,2.8699401816,-0.1869854014,-0.3448741173 C,0,4.2997719575,1.4288941141,0.7696567173 H,0,4.5182890579,2.416617499,1.1907494037 H,0,4.2659022928,1.5268258063,-0.3283324627 C,0,5.4072000499,0.4658007225,1.1796343293 H,0,5.3471856274,0.2841767066,2.2578064175 H,0,6.388623326,0.9174216181,0.9628332398 O,0,5.2971824418,-0.8058985235,0.5627341245 C,0,5.83074164,-0.9066808799,-0.7436116293 H,0,6.8720577972,-1.2605323125,-0.6913612759 H,0,5.8217640844,0.0649454666,-1.2570637268 C,0,4.9911536452,-1.886568961,-1.5366325618 H,0,5.5455272929,-2.2318043,-2.4220544433 H,0,4.7738603135,-2.7565214491,-0.9016874837 O,0,3.7901242382,-1.2542570709,-1.9560917602 C,0,2.6252776318,-2.0563983695,-1.8158254242 H,0,2.4312942168,-2.252718471,-0.7515982109 H,0,2.801202239,-3.0346272155,-2.2892622955 C,0,1.4402604678,-1.385660279,-2.4723770338 C,0,1.3385424476,-1.407578149,-3.8085437816 C,0,2.3419549423,-1.8962370578,-4.8078080803 H,0,2.5142757388,-1.1369194228,-5.5788739413 H,0,1.9790701212,-2.8006223372,-5.3111463406 H,0,3.3017450967,-2.1073713553,-4.331733041 S,0,-0.2184405622,-0.8771706119,-4.4571241601 C,0,-0.8056170885,-0.53263036,-2.8534657779 C,0,-1.9548017459,0.081968973,-2.5469593961 C,0,-3.1129582265,0.4544730819,-3.4222379472 F,0,-2.7713701667,1.1868769197,-4.515379993 F,0,-3.7810147812,-0.6426409478,-3.8832980639 C,0,-4.0578390156,1.2644920446,-2.4805898494 F,0,-5.3571751464,1.0951062912,-2.7726128331 F,0,-3.7578597952,2.5809802847,-2.5897931257 C,0,-3.6866043813,0.7964459845,-1.0435498995 F,0,-4.4513829272,-0.297505629,-0.7389585015 F,0,-3.9680678072,1.7461232859,-0.120334937 C,0,-2.2379668596,0.4543088957,-1.1631768449 C,0,-1.2517529986,0.4854997256,-0.2588386431 S,0,-1.4222508675,0.7582263676,1.4533457177 C,0,0.2634590468,0.2835895688,1.7295390935 C,0,0.751469418,0.3283409571,3.1441502788 H,0,0.0582430027,-0.1974673949,3.8106462941 H,0,0.8332670573,1.3654111823,3.4889721611 H,0,1.7399377892,-0.1284321869,3.2302431125 C,0,0.9627876419,0.0250025351,0.6183964574 C,0,0.2054784606,0.2180951794,-0.6954005437 C,0,0.7568530718,1.5061703855,-1.3551035248 H,0,0.1703103215,1.7987594571,-2.2309053618 H,0,0.7403223009,2.3274797204,-0.632410742 H,0,1.7927566124,1.3499737699,-1.6768034322 C,0,0.1614090578,-0.9704199236,-1.7297179503 C,0,-0.4212449013,-2.2487894261,-1.0755700913 H,0,-1.413047682,-2.0726182279,-0.6500958137 H,0,-0.5054128723,-3.0439321583,-1.8233966226 H,0,0.2318676911,-2.5968937909,-0.2674857644
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