# New insights concerning the photoswitching mechanisms of normal dithienylethene

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Supporting Information

All documents in supporting information will be notice document S.x (synthesis, MCR-ALS data treatment, derivation of equation…etc); with the same numerotation, table and figure will be notice table S.x and figure S.x.

Document S.0. Synthesis of DTE-m5 molecule.
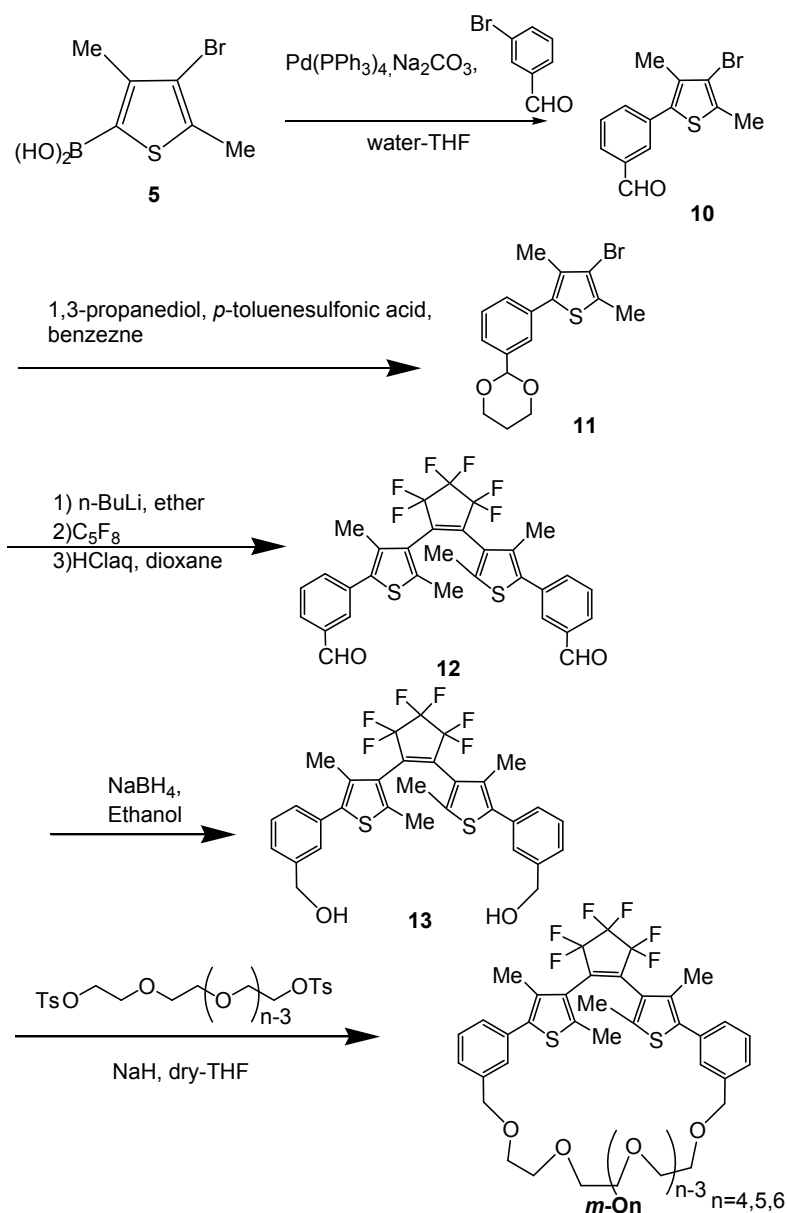
Preparation of compound **10**

A mixture of 17.0 g of 4-bromo-3,5-dimethylthiophene-2-boronic acid (74.0 mmol), 13.7 g of 3-bromobenzaldehyde (130 mmol), 15.0 g of sodium carbonate (140 mmol) , and 1.85 g of tetrakis(triphenylphosphine)palladium (1.6 mmol) in 170 ml of tetrahydrofuran and 85 ml of water was stirred for 12 h at 70 °C. The organic layer was extracted with ethyl acetate, washed with brine, and dried over MgSO₄. The solvents were evaporated and the residue was subjected to silica-gel column chromatography. The hexane/ethyl acetate (10:1) eluate was evaporated and 8.6 g of compound **10** (29 mmol) was obtained in 39% yield as colorless prisms.

10: colorless prisms, mp 38.6-39.2 °C, ^{1}H-NMR (300 MHz, in CDCl₃, TMS) δ (ppm) 2.30 (3H, s, -CH₃), 2.48 (3H, s, -CH₃), 7.57~7.90 (4H, m, Ar-H), 10.08 (1H, s, -CHO).

Preparation of compound **11**

A mixture of 5.6 g of compound **10** (19 mmol), 4.0 g of 1,3-propanediol (53 mmol), and small piece of p-toluenesulfonic acid in 150 ml of benzene was refluxed with Dean-Stark apparatus for 2h. The mixture was cooled to room temperature and brine was added and the organic layer was separated. The mixture was dried over $MgSO_4$ and evaporated in vacuo. The residue was recrystallized from hexane to afford 6.2 g of **11** in 89% yield.

11: colorless prisms, mp 46.3-47.6 °C, ^{1}H-NMR (300 MHz, in $CDCl_3$, TMS) δ (ppm) 1.50 (1H, d, -CH(-O-)$_2$), 2.30 (2H, m, -CH_2-), 2.30 (3H, s, -CH_3),   2.44 (3H, s, -CH_3), 4.00~4.25 (4H, m, -OCH_2), 7.30~7.50 (4H, m, Ar-H).

Preparation of compound **12**

A solution of 3.27 g of **11** (9.25 mmol) in dry-THF was stirred at -78 °C under Ar and 7.0 ml of *n*-BuLi (1.6M) (11 mmol) was added dropwise by 30 min and the mixture was stirred for 1h at same temperature. To the mixture, 0.33 g of octafluorocyclopentene (1.5 mmol) was slowly added three times and the mixture was stirred overnight. To the reaction mixture, 10 ml of 10% of hydrochloric acid was added and the mixture was stirred for 3h. The aqueous phase was neutralized with sodium bicarbonate and ethyl acetate was added. The organic layer was separated, washed with brine, and dried over $MgSO_4$. The solvent was evaporated in vacuo and the residue was subjected to silica-gel column chromatography. Evaporation of ethyl acetate/hexane (4:1) eluate afforded 1.3 g of **12** in 47% yield as blue amorphous.

12: blue amorphous, ^{1}H-NMR (300 MHz, in $CDCl_3$, TMS) δ (ppm) 2.11, 2.13 (6H, d, -CH_3), 2.40 (6H, s, -CH_3), 7.55~7.86 (8H, m, Ar-H), 10.1 (2H, s, -CHO).

Preparation of compound **13**

To a solution of 384 mg of compound **12** (0.636 mmol) in 10 ml of ethanol, 250 mg of sodium borohydride (6.4 mmol) was added portionwise and the mixture was stirred for 1h at room temperature. The mixture was poured to brine and extracted with ethyl acetate. The organic layer was washed with brine and dried over $MgSO_4$. The solvent was evaporated in vacuo and 0.379 g of compound **13** (0.620 mmol) was obtained as colorless amorphous in 98% yield.

13: colorless amorphous, ^{1}H-NMR (300 MHz, in $CDCl_3$, TMS) δ (ppm) 2.06, 2.09 (6H, d, -CH_3), 2.34 (6H, s, -CH_3), 4.71 (4H, s, -CH_2-), 7.20~7.50 (8H, m, Ar-H).

Preparation of *m*-**O5**

To a refluxing mixture of 200 mg of 60% sodium hydride in 10 ml of dry THF a solution of 114 mg of **13** (0.33 mmol) in 10 ml of dry THF was added dropwise for 6 h and the mixture was refluxed overnight. The mixture was allowed to room temperature and poured into brine and extracted with ethyl acetate. The organic layer was washed with brine and dried over $MgSO_4$. The solvent was evaporated in vacuo and the residue was subjected to silica-gel column chromatography. The hexane/acetone (8:3) eluate was evaporated and the residue was subjected to preparative TLC. From one of the bands, 52 mg of *m*-**O5** (0.068 mmol) was obtained in 30% yield.

m-**O5**: blue amorphous, ^{1}H-NMR (300 MHz, in $CDCl_3$, TMS) δ (ppm) 2.00 (*p* , 2.9H, s, -CH_3) 2.02 (*ap*, 3.1H, s, -CH_3), 2.30 (6H, s, -CH_3), 3.52~3.57 (16H, m, -O-CH_2-(CH_2-O-CH_2)$_3$-CH_2-O-), 4.61 (4H, m, -CH_2-), 7.21~7.61 (8H, m, Ar-H).
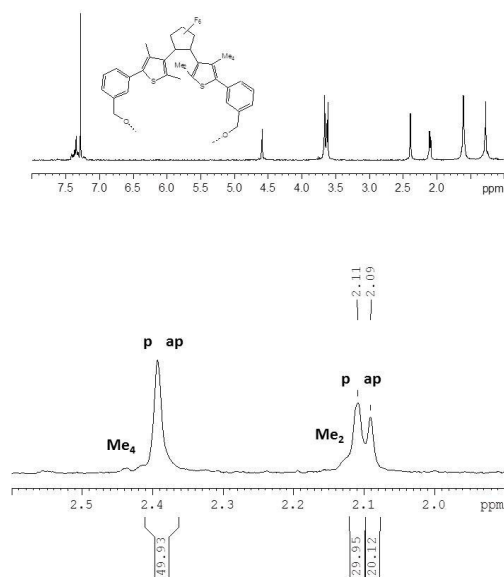
MS (EI) m/z=766 ［M^+］.

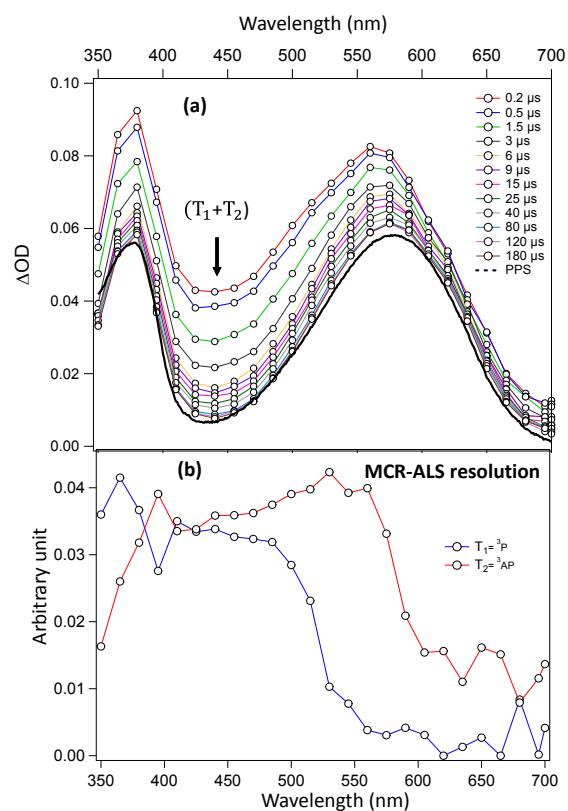**Figure S.1.**[1]NMR methyl signals of DTE-m5 in CDCl$_3$

Figure S.2. (a) Subpicosecond time-resolved spectra of DTE-m5 in chloroform using 355 nm laser excitation. **(b)** Spectra of triplet state of AP and P conformer respectively obtained by MCR-ALS decomposition.
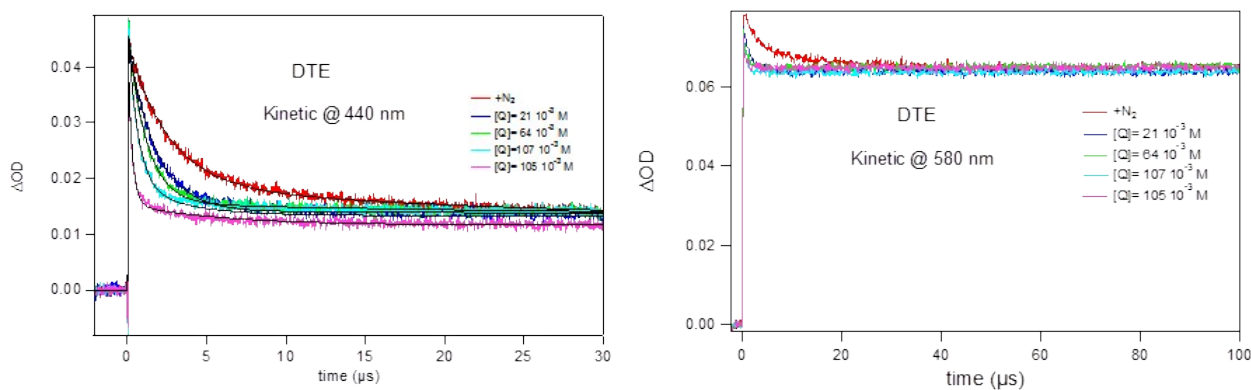
Figure S.3. Kinetics obtained from 355 nm laser flash photolysis excitation at 440 nm (left) and at 580 nm (right) for DTE in chloroform for increasing concentration of 2,5-Dimethyl-2,4-hexadiene quencher
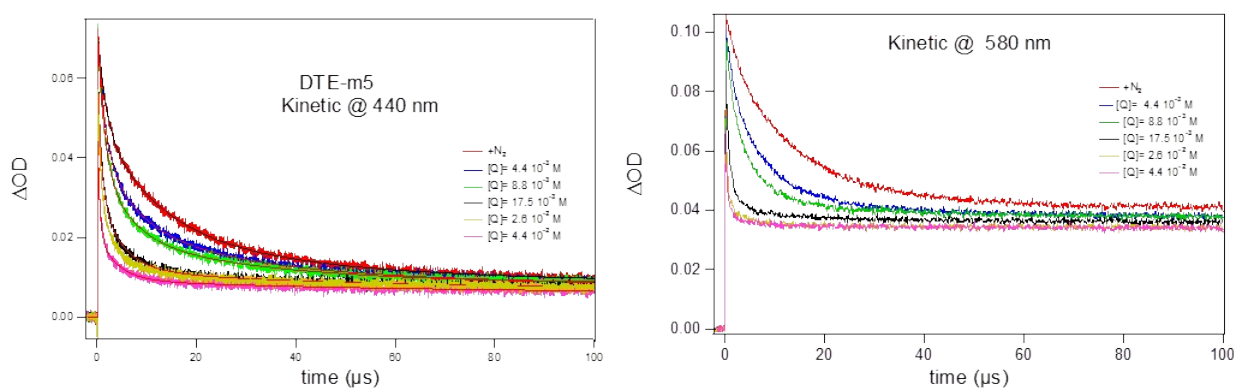

Figure S.4. Kinetics obtained from 355 nm laser flash photolysis excitation at 440 nm (left) and at 580 nm (right) for DTE-m5 in chloroform for increasing concentration of 2,5-Dimethyl-2,4-hexadiene quencher.
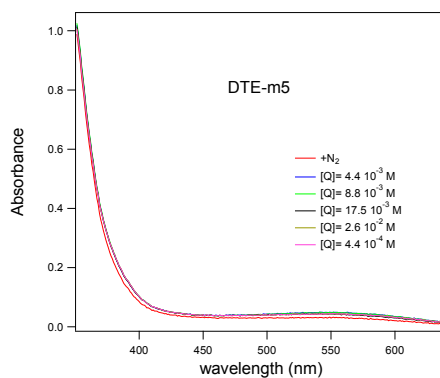

Figure S.5. Stationary absorption spectra of DTE-m5 in chloroform for increasing concentration of 2,5-Dimethyl-2,4-hexadiene quencher showing that no photodegradation occurs after each measurements.
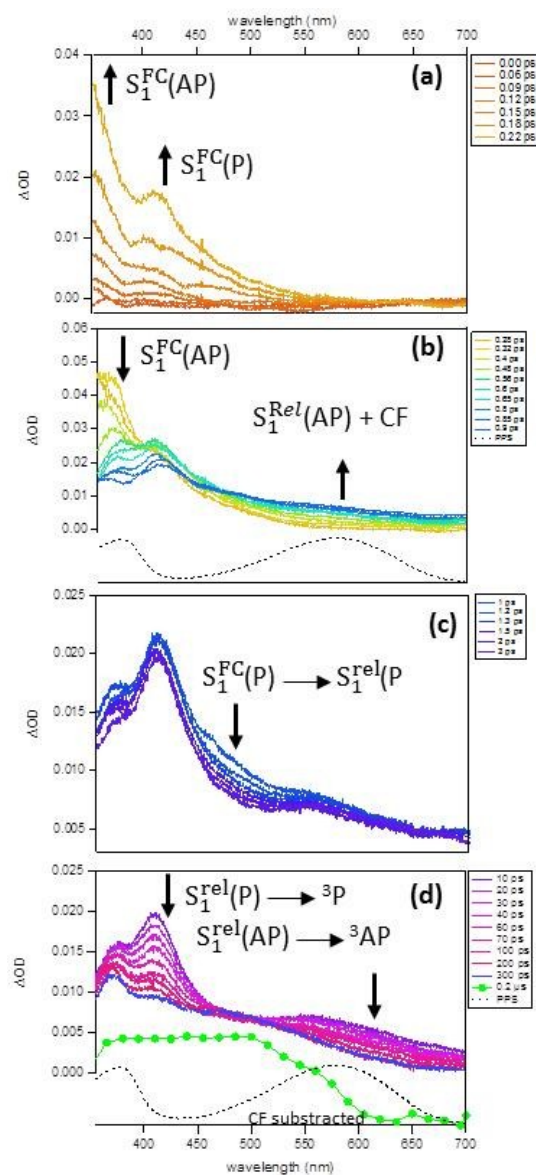
Figure S.6. Subpicosecond time-resolved absorption spectra of DTE-m5 in chloroform using 320 nm excitation wavelengths. All spectra are corrected from the GVD.
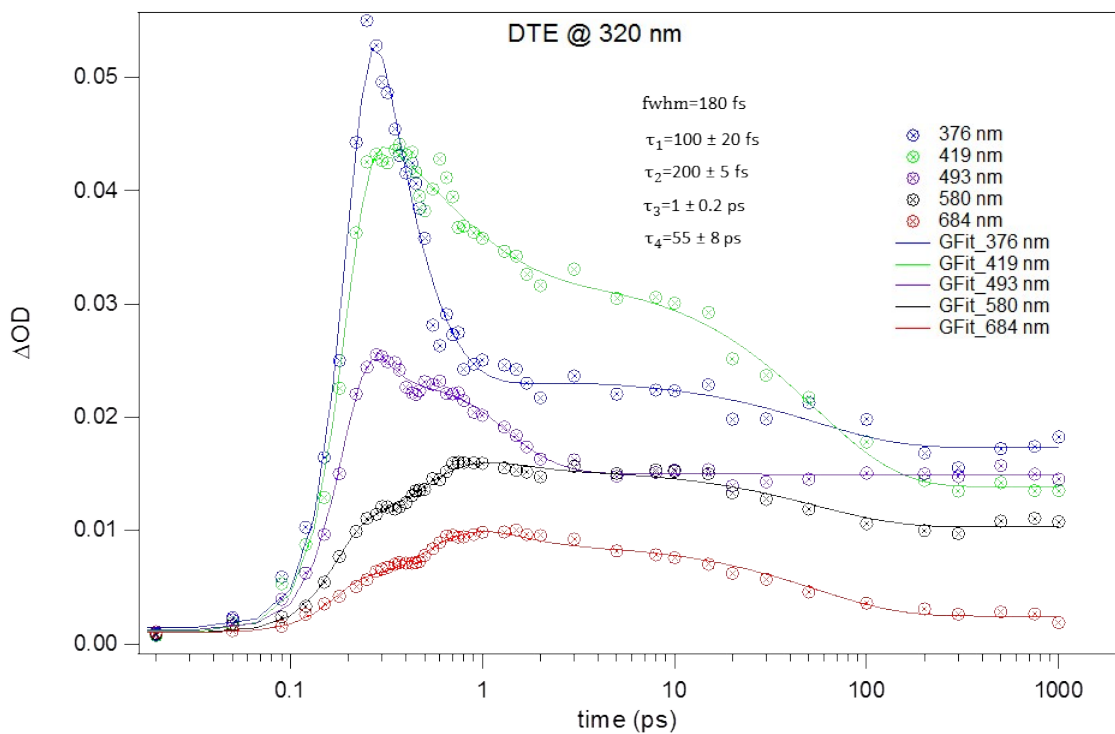
Figure S.7. Characteristics life times for different species of DTE obtained by global fitting convoluted with four exponential functions

Figure S.8. Figure S.7. Characteristics life times for different species of DTE-m5 obtained by global fitting convoluted with four exponential functions
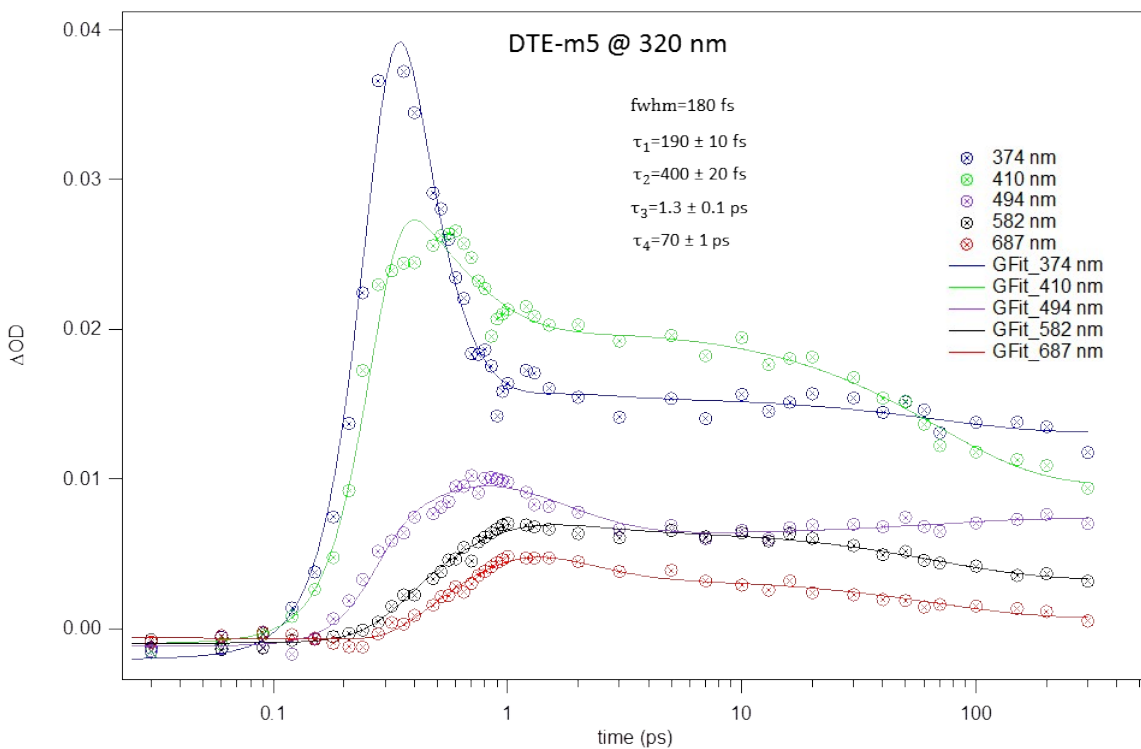
Document S.9: Full kinetic mechanism including the photocyclization via the triplet state.

$$OF + h\nu \xrightarrow{I_{abs}} S\,(FC)$$

$$S(FC) \xrightarrow{k_1} CF$$

$$S(FC) \xrightarrow{k_2} S_1 \qquad\qquad\qquad S_1 \xrightarrow{k_3'} S_0$$

$$S_1 \xrightarrow{k_3'} T_1$$

$$T_1 \xrightarrow{k_4} S_0$$

$$T_1 + Q \xrightarrow{k_4} S_0 + Q^*$$

$$T_1 \xrightarrow{k_5} CF$$

$$CF + h\nu \xrightarrow{k_6} OF$$
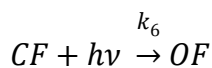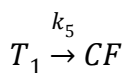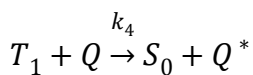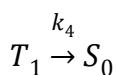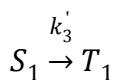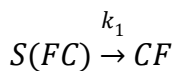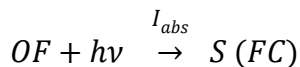
The kinetic equations are:

$$\frac{d[S\,(FC)]}{dt} = I_{abs} - (k_1 + k_2)S\,(FC) \tag{1}$$

$$\frac{d[S_1]}{dt} = k_2\,[S(FC)] - k_3\,[S_1] \tag{2}$$

$$\frac{d[T_1]}{dt} = k_3\,[S_1] - (k_4 + k_5 + k_Q[Q]) \tag{3}$$

$$\frac{[CF]}{dt} = k_1\,[S(FC)] - k_6\,[CF] + k_5\,[T_1] \tag{4}$$

$$\tau_{FC} = \frac{1}{k_1 + k_2} \tag{5}$$

$$\tau_{S_1} = \frac{1}{k_3 + k_3'} \tag{6}$$

$$\tau_T = \frac{1}{k_4 + k_5} \tag{7}$$

The PPS stationary derives:

$$[S(FC)] = \frac{I_{abs}}{k_1 + k_2} \tag{8}$$

$$[S_1] = \frac{k_2}{k_3 + k_3'} [S(FC)] = \frac{I_{abs}k_2}{(k_3 + k_3')(k_1 + k_2)} = I_{abs}k_2 \ \tau_{FC} \ \tau_{S_1} \qquad \textbf{(9)}$$

$$[T_1] = \frac{k_3[S_1]}{k_T + k_Q[Q]} = \frac{k_2k_3I_{abs}\tau_{FC}\tau_{s1}}{k_T + k_Q[Q]} \qquad \textbf{(10)}$$

$$[CF] = \frac{I_{abs}}{k_6} \frac{k_1}{(k_1 + k_2)} + \frac{k_5k_6k_3I_{abs}\tau_{FC}\tau_{s1}}{k_6(k_T + k_Q[Q])}$$

$$= I_{abs} \frac{k_1}{k_6} \tau_{FC} + \frac{k_2k_5k_3I_{abs}\tau_{FC}\tau_{s1}}{k_6(k_T + k_Q[Q])} \qquad \textbf{(11)}$$

With:

$$A_Q^\infty = \varepsilon_{CF}l[CF] = \varepsilon_{CF}l \ I_{abs} \frac{\tau_{FC}}{k_6} (k_1 + \frac{k_2k_3k_5\tau_{s1}}{(k_T + k_Q[Q])})$$

$$\alpha = \varepsilon_{CF}l \ I_{abs} \frac{\tau_{FC}}{k_6}$$

$$\beta = k_2k_3k_5\tau_{s1}$$

$$\implies A_Q^\infty = \alpha(k_1 + \frac{\beta}{(k_T + k_Q[Q])}) \quad \text{and} \quad A_0^\infty = \alpha(k_1 + \frac{\beta}{k_T})$$

$$A_0^\infty - A_Q^\infty = \ + \frac{\alpha\beta}{k_T} - \frac{\alpha\beta}{(k_T + k_Q[Q])} = \alpha\beta \ . \frac{k_Q[Q]}{k_T(k_T + k_Q[Q])}$$

$$\frac{A_0^\infty}{A_0^\infty - A_Q^\infty} = (1 + \frac{k_1k_T}{\beta}) \ (1 + \frac{k_T}{k_Q}.\frac{1}{[Q]})$$

If: $\dfrac{k_1k_T}{k_2k_3k_5\tau_{s1}} < 1$

$$\frac{A_0^\infty}{A_0^\infty - A_Q^\infty} \approx 1 + \frac{k_T}{k_Q}.\frac{1}{[Q]}$$

Document S.10. Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS)

The underlying bilinear model for time-resolved data can be written as the sum of the contributions of the spectra of k different components related to different absorbing excited state species, weighted by their respective concentration profile.

$$\Delta A(t,\lambda) = \sum_{k} c_k(t)\varepsilon_k(\lambda)l$$

MCR-ALS has been used in order to recover from the time-resolved data the time profiles and the spectra of the transient species. This method is a soft-modelling method since no assumption on the kinetic model is made; the only assumption is that the data can be described by a bilinear model. In matrix form this model can be written as

$$D = C S^T + E$$

where $\mathbf{D}(m{\times}n)$ contains the absorbance value at m different time delay and for n different wavelengths, $\mathbf{C}(m{\times}k)$ contains the concentration profiles of the k contributions, $\mathbf{S}(k{\times}n)$ contains the spectra of the k contributions and $\mathbf{E}(m{\times}n)$ the residuals.

MCR-ALS is an iterative procedure: first initial estimates are furnished and in a second step the concentration and spectra are recalculated iteratively by applying given constraints until convergence. The lack of fit (l.o.f.) is generally used as a global estimator of the fitting error of the experimental data. Here initial concentrations for each contribution have been estimated using EFA or available knowledge. Applied constraints are non-negativity on concentration and spectra and unimodality on the concentration.

Document S.11. MCR-ALS resolution of microsecond time-resolved spectra of DTE in chloroform for 355 nm excitation wavelength.

MCR-ALS resolution for the raw microsecond time-resolved spectra leads to the estimation of two components largely influence by the spectra of the closed form which is the major product and strongly overlap the other transient species spectra. In order to be able to estimate the spectra of the transients species without the influence of the closed form the data have been subtracted from the last spectra where only the closed form is still present taking the hypothesis that the concentration of the closed form is constant in the studied time domain (0.2-180 µs). The corrected spectra are presented in Figure S.12.a). Two contributions are required in order to correctly reproduce the data. The constraints used are non-negativity both on concentration profiles and spectra and unimodality on the concentration. The MCR-ALS results are presented in Figure S.12 b) and c). The lack of fit is 5,31 % and no structure in the residuals are observed. The two contributions (called A and B) appear very quickly and decrease at different rate. Therefore the first contribution A which disappear quickly (red in Figure S.12.b) is attributed to $^3P\,(T_1)$ and the second one B to $^3AP\,(T_2)$.
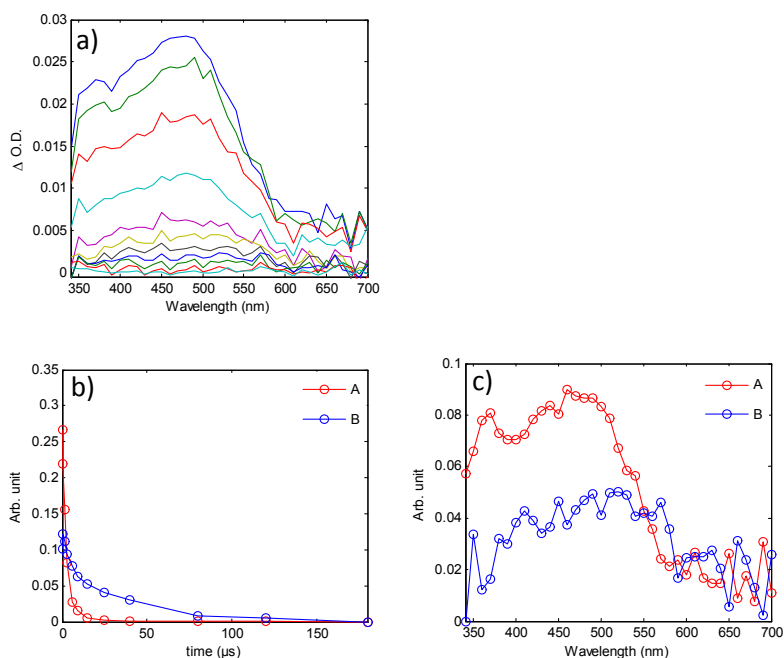

Figure S.12. (a) microsecond time-resolved spectra of DTE with the last spectrum (180 µs) subtracted. Results obtained by MCR-ALS: (b) Concentration profiles and (c) spectra.

Document S.13. MCR-ALS resolution of Subpicosecond time-resolved spectra of DTE in chloroform for 320 nm excitation wavelength.

Due to the strong overlapping of the different species and presence of parallel reactions, MCR-ALS has been realized separately first for the short time delay and in a second step on longer time delay. The constraints used are non-negativity both on concentration profiles and spectra and unimodality on the concentration. To avoid scale indeterminacies during ALS optimization each spectra has been normalized during the MCR-ALS decomposition.

First the 0 - 0.22ps time domain has been used to extract the spectra of $S^{FC}_1(AP)$ and $S^{FC}_1(P)$ (only transient species formed in this time domain). Concentration profile and spectra of this two contributions (called 1 and 2) obtained by MCR-ALS are presented in Figure S.14 a) and b) (l.o.f 4.51 %). These two contributions appear simultaneously with similar time profile.

In a second step spectra acquired in the 0.43 - 300 ps time domain has been used in order to extract the other transient species taking the hypothesis that both $S^{FC}_1(AP)$ and $S^{FC}_1(P)$ do not exist anymore in this time domain. Furthermore the known spectra of the closed form have been taken into account during the decomposition. Four contributions (called 3, 4, 5 and 6) are necessary to correctly reproduce the data. Concentration profiles and spectra of these three contributions are presented respectively in Figure S.14. c) and d). The lack of fit is equal to 5.11% and observation of the residuals does not show significant structure. The spectra of the extracted transient species with their assignments are presented Figure 7 in the manuscript.
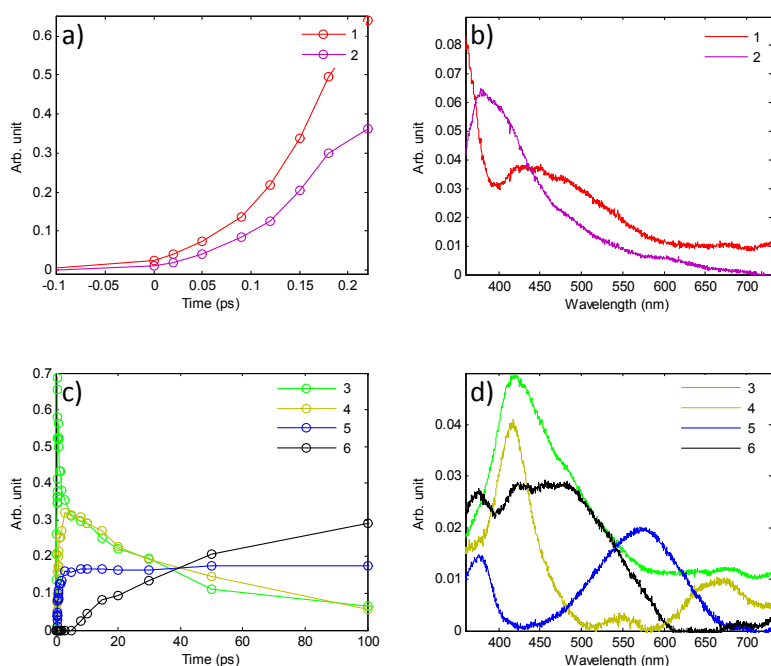
Figure S.14. MCR-ALS results for the transient absorption spectra of DTE in the 0 - 0.22 ps time domain: (a) concentration profiles and (b) spectra. MCR-ALS results for the transient absorption spectra of DTE in the 0.43 - 300 ps time domain: (c) concentration profiles and (d) spectra.

Table S.15. DTE : PCM(chloroform)-uCAM-B3LYP/6-311+G(2d,p) energies at the geometries optimized at the PCM(chloroform)-ωB97XD/6-31G(d) level.

Geometry	r_{cc} (Å)	ϕ_1 (°)	ϕ_2 (°)	Energy (a.u.) (S^2)[a]	Relative energy (eV)[b]
AP	3.781	-60.8	-61.3	-2513.56512509	0.00
^{3}AP	3.684	-19.3	-19.3	-2513.47742114 (2.051)	2.39
P	4.005	116.1	-61.6	-2513.56524036	0.00
^{3}P	3.927	116.1	-63.4	-2513.46624479 (2.003)	2.69
^{1}P	3.979	147.9	-23.5	-2513.42699884	3.76
CF	1.538	-12.2	-3.3	-2513.54030345	0.68
^{3}CF	1.565	-7.5	-18.0	-2513.50804644 (2.062)	1.55
^{1}CF	1.584	-7.2	-16.3	-2513.46824374	2.64
TS(AP-CF)	2.033	-22.4	-28.3	-2513.47901804	2.34
TS(^{3}AP-^{3}CF)	2.433	-20.5	-28.0	-2513.46429757 (2.027)	2.74
TS(AP-P)	3.863	0.4	-110.1	-2513.53799229	0.74

[a] The wavefunction spin-contamination S^2 is reported in brackets.

[b] The reference energies are calculated with the open-ring AP minimum energy as reference.
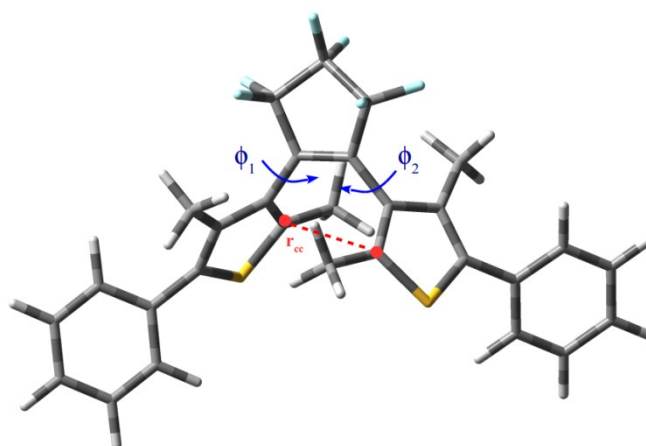
Figure S.16: Representation of the parameters r_{cc} (distance between the two reactive carbon atoms, involved in the bond formation/breaking) and the two dihedral angles ϕ_1 and ϕ_2.

Table S.17. DTE-m5: PCM (chloroform)-uCAM-B3LYP/6-311+G(2d,p) energies at the geometries optimized at the PCM(chloroform)-ωB97XD/6-31G(d) level

Geometry	r_{cc} (Å)	ϕ_1 (°)	ϕ_2 (°)	Energy (a.u.)[a] (S^2)[b]	Relative energy (eV)[c]
AP	3.887	-60.9	-63.8	-2513.56337158	0.00
^{3}AP	3.163	-22.6	-22.3	-2513.47042571 (2.038)	2.53
P	3.958	114.8	-62.1	-2513.56019825	0.09
^{3}P	4.319	154.8	-21.8	-2513.47176487 (2.051)	2.49
^{1}P	3.242	148.5	-24.9	-2513.52584534	1.02
CF	1.538	-5.0	-10.5	-2513.53889722	0.67
^{3}CF	1.581	-16.2	-7.3	-2513.50696551 (2.053)	1.53
^{1}CF	1.565	-15.2	-10.5	-2513.52340861	1.09
TS(AP-CF)	1.920	-10.6	-30.3	-2513.45934099	2.83
TS(^{3}AP-^{3}CF)	2.436	-20.4	-29.6	-2513.46244375 (2.028)	2.75
TS(AP-P)	4.085	-5.1	-106.2	-2513.47426716	2.42

[a]The energies correspond to the energie of the DTE core structure : starting with the geometries of DTE-m5 optimized at the PCM(chloroform)-ωB97XD/6-31G(d) level, the methoxy chain has been replaced by H atoms and a single point calculation has been performed at the PCM(chloroform)-uCAM-B3LYP/6-311+G(2d,p) level.
[b]The wavefunction spin-contamination S^2 is reported in brackets.
[c] The reference energies are calculated with the open-ring AP minimum energy as reference.
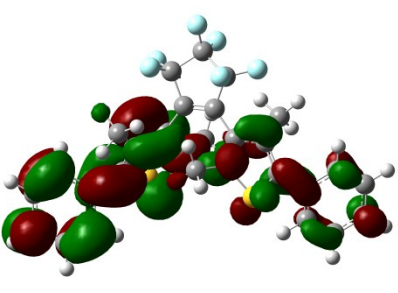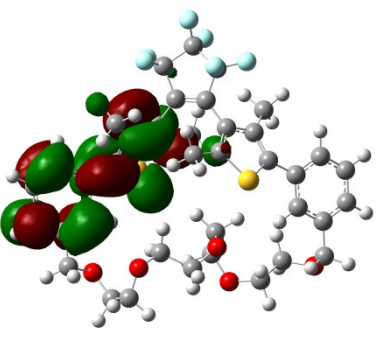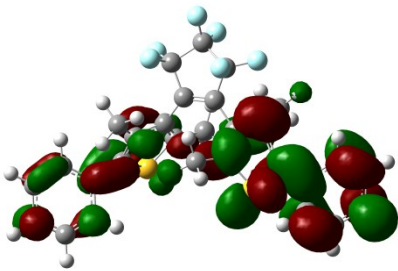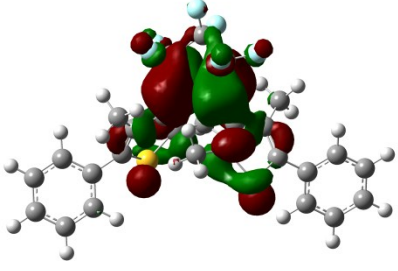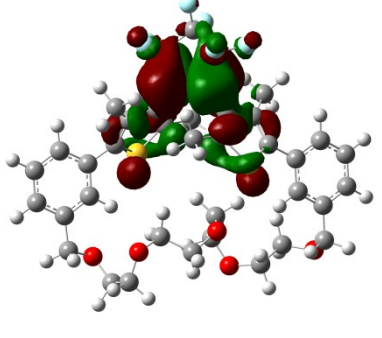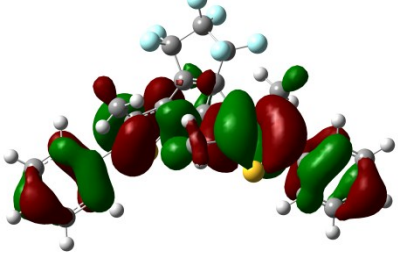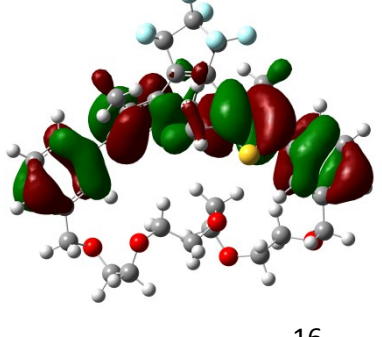
Table S.18. Open-ring AP conformer of DTE and DTE-m5: Computed absorption wavelengths (λ in nm), oscillator strengths f and electronic excitations. For each molecule, the transition with the highest oscillator strength value is highlighted. Only the first five electronic excitations are given.

AP	DTE			DTE-m5		
State	λ (nm)	f	Description	λ (nm)	f	Description
S$_0$ → S$_1$	296.0	0.08	HOMO → LUMO	295.0	0.11	HOMO → LUMO
S$_0$ → S$_2$	270.0	0.03	HOMO-1 → LUMO	**272.1**	**0.62**	**HOMO→ LUMO+1 (maj)** **HOMO-1 → LUMO+1 (min)**
S$_0$ → S$_3$	**266.5**	**0.81**	**HOMO → LUMO+1 (maj)** **HOMO-1 → LUMO+2 (min)**	267.7	0.03	HOMO-1 → LUMO+1
S$_0$ → S$_4$	263.5	0.24	HOMO → LUMO+2 (maj) HOMO-1 → LUMO+1 (min) HOMO-1 → LUMO+2 (min)	252.0	0.41	HOMO → LUMO+2 (maj) HOMO-1 → LUMO+2 (min)
S$_0$ → S$_5$	250.7	0.16	HOMO-2 → LUMO	248.9	0.03	HOMO → LUMO+3 (maj) HOMO-1 → LUMO+3 (min)

Figure S19. Open-ring AP conformer of DTE and DTE-m5: Representation of the frontier orbital contour plot (isovalue : 0.02 a.u.) computed at the PCM(chloroform)-uCAM-B3LYP/6-311+G(2d,p) level.

	DTE	DTE-m5
LUMO+2		
LUMO+1		
LUMO		
HOMO		

16

HOMO-1
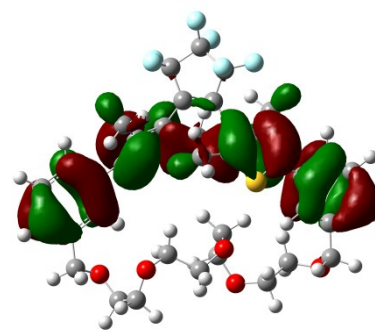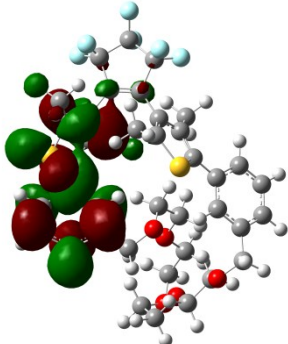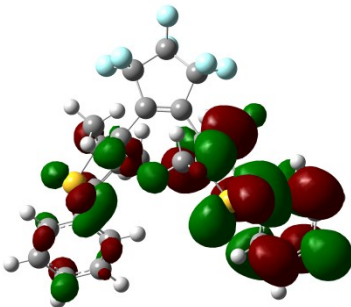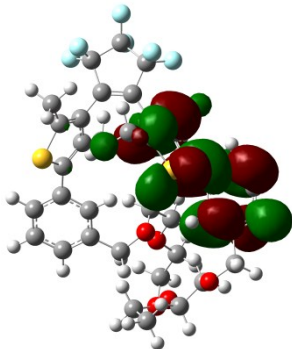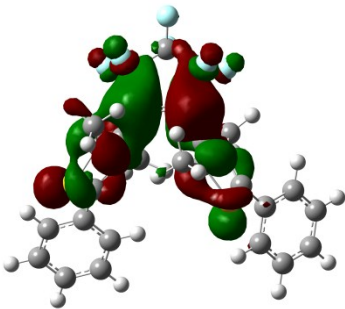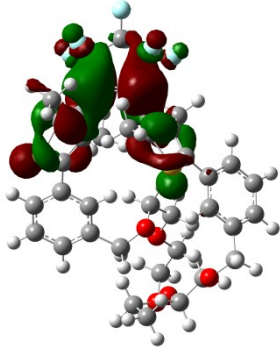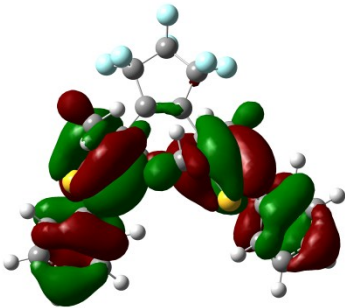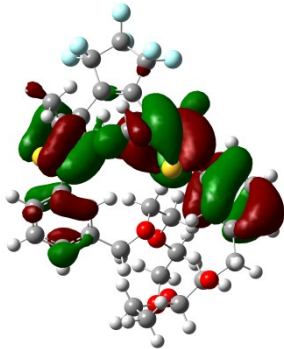
Table S.20. Open-ring P conformer of DTE and DTE-m5: Computed absorption wavelengths (λ in nm), oscillator strengths f and electronic excitations. For each molecule, the transition with the highest oscillator strength value is highlighted.

P	DTE			DTE-m5		
State	λ (nm)	f	Description	λ (nm)	f	Description
$S_0 \rightarrow S_1$	285.6	0.02	HOMO $\rightarrow$ LUMO	289.0	0.06	HOMO $\rightarrow$ LUMO
$S_0 \rightarrow S_2$	284.7	0.13	HOMO-1 $\rightarrow$ LUMO	286.2	0.13	HOMO-1$\rightarrow$ LUMO
$S_0 \rightarrow S_3$	267.0	0.34	HOMO $\rightarrow$ LUMO+1 (maj) HOMO-1 $\rightarrow$ LUMO+2 (min)	277.3	0.36	HOMO$\rightarrow$ LUMO+1
$S_0 \rightarrow S_4$	**262.4**	**0.65**	**HOMO $\rightarrow$ LUMO+2 (maj)** **HOMO-1 $\rightarrow$ LUMO+1 (min)** **HOMO-1 $\rightarrow$ LUMO+2 (min)**	**263.0**	**0.51**	**HOMO-1 $\rightarrow$ LUMO+2**
$S_0 \rightarrow S_5$	250.7	0.10	HOMO-2 $\rightarrow$ LUMO	252.7	0.03	HOMO $\rightarrow$ LUMO+3

Figure S21. Open-ring P conformer of DTE and DTE-m5: Representation of the frontier orbital contour plot (isovalue : 0.02 a.u.) computed at the PCM(chloroform)-uCAM-B3LYP/6-311+G(2d,p) level.

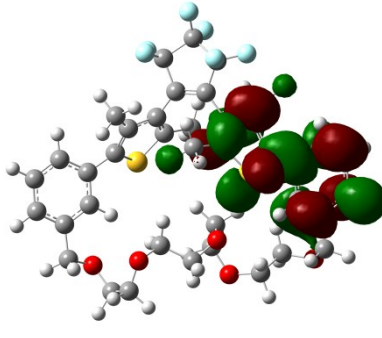|	DTE	DTE-m5
LUMO+2		
LUMO+1		
LUMO		
HOMO		

| HOMO-1 | | |
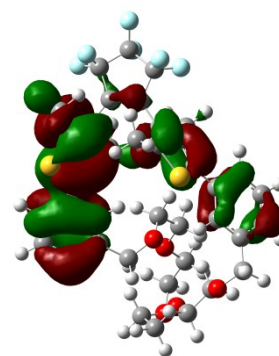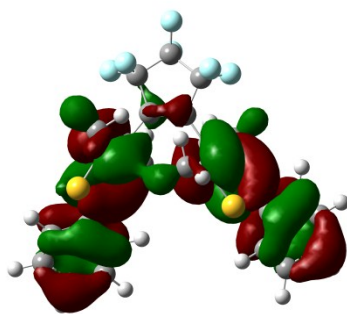
Table S.22. Closed-Form CF conformer of DTE and DTE-m5 : Computed absorption wavelengths (λ in nm), oscillator strengths f and electronic excitations. For each molecule, the transition with the highest oscillator strength value is highlighted.

P	DTE			DTE-m5		
State	λ (nm)	f	Description	λ (nm)	f	Description
$S_0 \rightarrow S_1$	**525.4**	**0.33**	**HOMO $\rightarrow$ LUMO**	**512.8**	**0.30**	**HOMO $\rightarrow$ LUMO**
$S_0 \rightarrow S_2$	348.1	0.24	HOMO-1 $\rightarrow$ LUMO	345.7	0.23	HOMO-1$\rightarrow$ LUMO
$S_0 \rightarrow S_3$	299.5	0.10	HOMO$\rightarrow$ LUMO+1 (maj) HOMO$\rightarrow$ LUMO+2 (min)	296.7	0.07	HOMO$\rightarrow$ LUMO+1 (maj) HOMO$\rightarrow$ LUMO+2 (min)
$S_0 \rightarrow S_4$	290	0.12	HOMO $\rightarrow$ LUMO+1 (min) HOMO$\rightarrow$ LUMO+2 (maj)	284.3	0.15	HOMO $\rightarrow$ LUMO+1 (min) HOMO$\rightarrow$ LUMO+2 (maj)
$S_0 \rightarrow S_5$	268	0.16	HOMO $\rightarrow$ LUMO+3	267.7	0.15	HOMO-2 $\rightarrow$ LUMO

Figure S.23. Closed Form CF conformer of DTE and DTE-m5: Representation of the frontier orbital contour plot (isovalue : 0.02 a.u.) computed at the PCM(chloroform)-uCAM-B3LYP/6-311+G(2d,p) level.
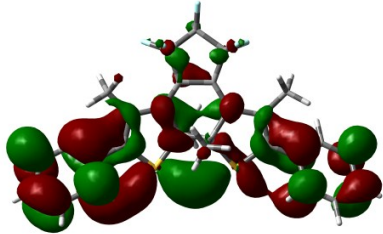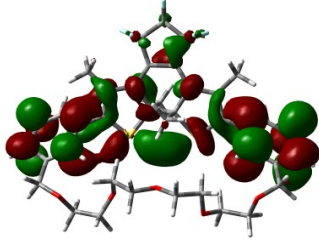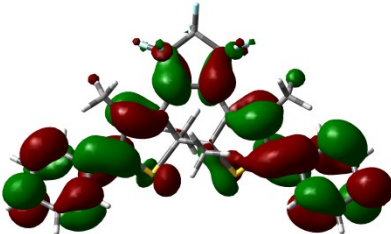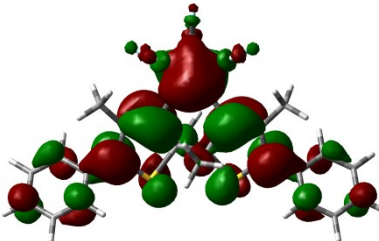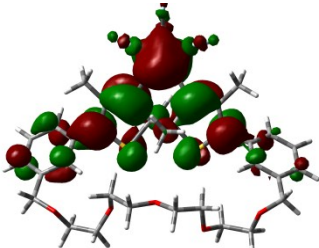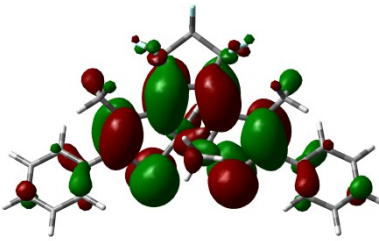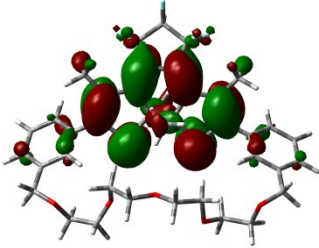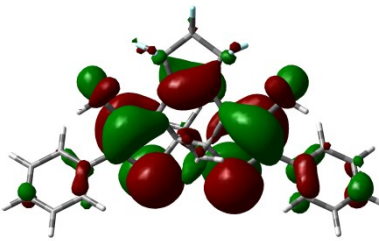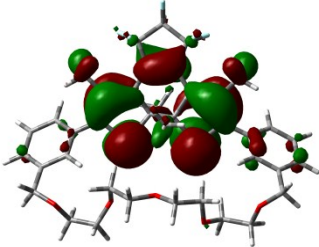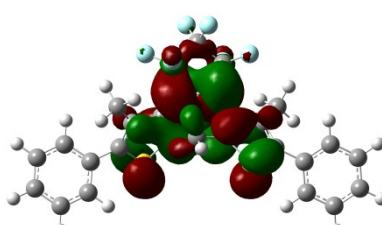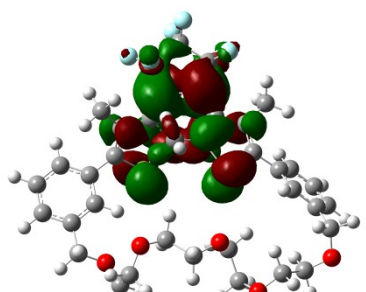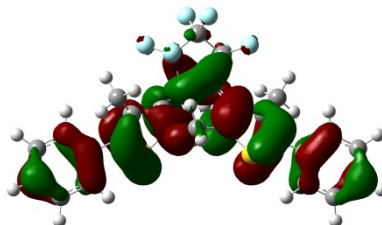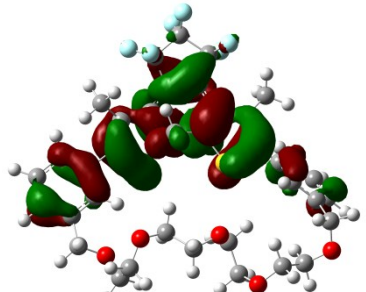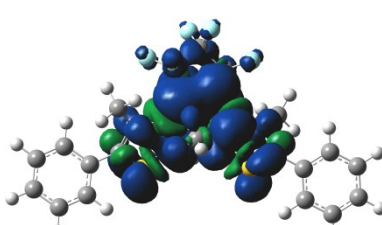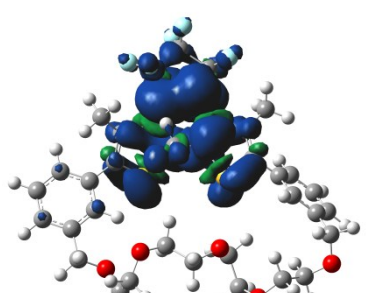
	DTE	DTE-m5
LUMO+2		
LUMO+1		
LUMO		
HOMO		
HOMO-1		

Figure S.24. Open Form ³AP conformer of DTE and DTE-m5: Top: Representation of the SOMOs (Singly Occupied Molecular Orbitals) contour plot (isovalue : 0.02 a.u.) computed at the PCM(chloroform)-uCAM-B3LYP/6-311+G(2d,p) level. Bottom : Orbitals Spin Density : Blue (green) surfaces indicate excess of alpha (beta) over beta (alpha) spin electrons.
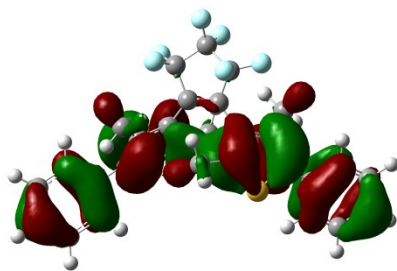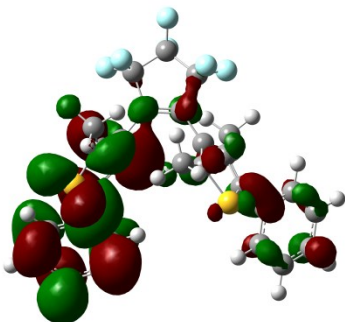
	DTE	DTE-m5
SOMO (highest energy)		
SOMO (lowest energy)		
Spin Density		

S.25. GEOMETRIES : DTE

AP	
```
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C  1.42295900   0.38781900   0.71126000
C  1.00066500  -0.50417200   1.66310200
S  2.11232000  -1.81455500   1.79425400
C  3.14666700  -1.16956000   0.55312400
C  0.62754800   1.56974300   0.34295700
C -0.61124800   1.58175800  -0.18481900
C -1.08434700   2.99737200  -0.41619700
C  0.20519500   3.84034500  -0.29117400
C  1.09527300   2.97645700   0.62185300
C -1.41592400   0.41361700  -0.58343300
C -0.99175000  -0.46166100  -1.55036100
S -2.12752200  -1.74417300  -1.74326300
C -3.18031900  -1.10686000  -0.51463900
C -2.68149300   0.05662900   0.01083900
C  0.24971300  -0.41079100  -2.38528800
F  0.86545900   3.30549900   1.92155600
F  2.40617600   3.19130400   0.38764500
F -0.01346700   5.07195900   0.18935100
F  0.79145300   3.94016400  -1.50364200
F -1.66346500   3.14903600  -1.62566600
F -1.97703000   3.42399200   0.51526400
C -0.22988600  -0.44950100   2.51406800
H -0.06689500  -0.92481400   3.48499400
H -0.51569400   0.59101700   2.69132000
H -1.07076300  -0.95449400   2.02482500
H  1.07267900  -0.95127800  -1.90422200
H  0.08507000  -0.85223000  -3.37186100
H  0.56464700   0.62654700  -2.52789500
C  4.34780100  -1.91763800   0.13837600
C  4.28415000  -3.29864700  -0.09079900
C  5.57483600  -1.26479100  -0.03313400
C  5.41517900  -4.00541900  -0.48406800
H  3.33690000  -3.81808000   0.02541600
C  6.70338200  -1.97185200  -0.43562900
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H  5.34535900  -5.07461600  -0.65988700
H  7.64695300  -1.44997100  -0.56332900
H  7.51039900  -3.89507300  -0.97240700
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C -5.63480600  -1.14535500  -0.04520600
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H -5.66816300  -0.07586800  -0.22911500
C -6.77284400  -3.20565600   0.49107200
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H  2.55743000   1.40002800  -1.57878000
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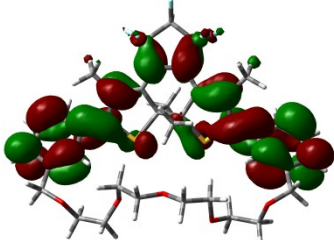| ```
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C 3.483104 -1.056404   0.478672
C 0.740648   1.350958 -0.065617
C -0.740571   1.350921   0.065846
C -1.125267   2.705126   0.553904
C -0.000294   3.649489 -0.000358
C 1.125416   2.705244 -0.553475
C -1.593461   0.335525 -0.411757
C -1.198306 -0.590722 -1.399146
S -2.422086 -1.766917 -1.673406
C -3.483158 -1.056219 -0.478813
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C 0.02036   -0.592386 -2.273392
F 2.330733   3.141637 -0.124943
F 1.12919   2.806893 -1.92286
F 0.49399   4.437795   0.970259
F -0.495276   4.435947 -0.97214
F -2.331078   3.141256   0.126561
F -1.127641   2.806843   1.923315
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C 4.886229 -3.078938   0.033847
C 5.948825 -0.916565   0.133984
C 6.119362 -3.672184 -0.21306
H 3.990977 -3.693233   0.078707
C 7.180484 -1.511413 -0.118252
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H 8.232037 -3.354786 -0.484214
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C -5.948796 -0.916511 -0.133448
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C -3.571727   0.774977   1.25111
H -2.81807   1.081394   1.980686
H -4.095153   1.67875   0.928087
H -4.293496   0.129684   1.757462
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H 2.818804   1.081979 -1.980178
H 4.094995   1.679607 -0.926668
H 4.294588   0.130896 -1.756383
```
|

| P | |
|---|---|
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C -0.47773800 -1.04577600   1.94864400
S -2.17028800 -0.90431600   2.24701700
C -2.57953200 -1.39111600   0.62736800
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| ```
³P
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C -0.1092883986  -1.3161715453   0.7336465615
C -0.2830364631  -0.6397790785   1.9123364941
S -1.9306057049  -0.1704699415   2.098008224
C -2.3872437916  -0.8741620723   0.5735079656
```
|

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C 0.88642200 1.63719900 -0.44353300	C 1.0518702125 1.3278386352 -0.8466282379
C 3.60938400 0.96494000 2.14707500	C 3.794513612 1.1479799811 1.7646240448
F 2.13588000 -3.59391500 0.81942900	F 2.1784259012 -3.555944748 1.2592857833
F 0.83554500 -3.75846500 -0.91914300	F 0.8033232199 -3.955203672 -0.3830175054
F 3.88941200 -3.44300200 -1.12360100	F 3.8766326698 -3.8458307468 -0.7081513856
F 2.46211300 -2.44447000 -2.45089600	F 2.4453203636 -3.0742491359 -2.1744251971
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H 1.45846400 -1.26445900 2.82147100	H 1.6452946347 -0.8732956064 2.8004098099
H 0.73190700 0.33181900 3.07233500	H 1.0244623929 0.7865644476 2.8428582562
H 4.60899200 1.15288800 1.74158100	H 4.7831950782 1.552343923 1.5117767593
H 3.54619800 1.44455300 3.12778700	H 3.520520307 1.5543159096 2.7463183543
H 3.50833700 -0.11293900 2.28803500	H 3.8874522689 0.0646067555 1.8552035462
C -3.99385200 -1.44434700 0.21410200	C -3.7680272623 -0.719393085 0.0824637252
C -4.87670000 -0.40758700 0.54470900	C -4.4212647796 0.5162751927 0.1928868969
C -4.48414700 -2.53922100 -0.50867400	C -4.4501207337 -1.7883014332 -0.5113866051
C -6.21227600 -0.46457500 0.16153700	C -5.7156948565 0.6802243493 -0.2871290337
H -4.50969800 0.45549500 1.09354100	H -3.901055157 1.3581685693 0.642173185
C -5.81814300 -2.58988800 -0.89979500	C -5.7422944546 -1.6196205427 -0.9993192801
H -3.81910600 -3.36270200 -0.74865500	H -3.9709909474 -2.7601072252 -0.5765485245
C -6.68696900 -1.55450400 -0.56443200	C -6.379334852 -0.3860201992 -0.8902501314
H -6.88254400 0.34765700 0.42620800	H -6.2038135247 1.6461333217 -0.195795061
H -6.18144100 -3.44750600 -1.45790100	H -6.2558538837 -2.45855091 -1.4592410651
H -7.72943900 -1.59814700 -0.86474000	H -7.3880239742 -0.2577574757 -1.2708445493
C 0.04931800 4.06147800 -0.40514700	C -0.2966891165 3.500465726 -0.3448137332
C 0.61118000 5.32752700 -0.61396600	C -0.2860375506 4.8646448253 0.0735469777
C -1.32762500 3.89536600 -0.60288300	C -1.5598158625 2.9484887626 -0.7179295028
C -0.18204000 6.39700100 -1.01575800	C -1.4437488242 5.618969934 0.0880979803
H 1.67911900 5.47072600 -0.47438100	H 0.6509871737 5.3243160115 0.3740974795
C -2.11745100 4.96357900 -1.01542000	C -2.7078836557 3.7184910814 -0.6979219083
H -1.78200600 2.92725200 -0.41503000	H -1.63407553 1.9029853754 -0.9890685054
C -1.54781200 6.21759600 -1.22215600	C -2.665031918 5.0597932018 -0.3038694021
H 0.27065200 7.37089400 -1.17556100	H -1.4007178824 6.6571699804 0.4035555107
H -3.18271000 4.81667900 -1.16581200	H -3.6529645764 3.2663237616 -0.9860304099
H -2.16589900 7.05172000 -1.54022700	H -3.5697763681 5.6591351652 -0.2958545319
C 0.05945400 1.14285200 -1.59569100	C 0.3820472398 0.7721179097 -2.0630207012
H 0.62370700 0.41677600 -2.18950400	H 0.969898001 -0.0485611095 -2.4842677935
H -0.85578700 0.64967000 -1.25073900	H -0.6224327091 0.3843447454 -1.8590930641
H -0.23196200 1.96672200 -2.25189000	H 0.2789087922 1.5496985096 -2.8269143816
C -1.46553800 -2.07299000 -1.55674400	C -1.3625887759 -2.1630837708 -1.3747805052
H -0.54379000 -1.76189000 -2.05577500	H -0.394751095 -2.1050743917 -1.8802228808
H -1.54600800 -3.15730500 -1.67714000	H -1.6070711716 -3.2249068789 -1.2708338266
H -2.30998700 -1.61508300 -2.07937700	H -2.1156477188 -1.7095834185 -2.0255036082

¹p
C -0.22024700 0.55671200 -0.34556400
C -0.60165700 -0.16811800 0.85869700
C -0.02167400 -1.47072500 0.89320500
S 0.82873700 -1.81287200 -0.55261500
C 0.52199100 -0.20722500 -1.20006800
C -1.55931800 0.25584600 1.81383900
C -2.39257700 -0.63817100 2.57378500
C -2.62637800 -0.06670400 3.91941600
C -2.23840700 1.44159700 3.78465400
C -1.81153300 1.63493000 2.29738100
C -2.90255800 -1.85651200 2.05323400
C -3.14541700 -3.03083500 2.80208400
S -3.43482300 -4.35556600 1.77650400
C -3.35268600 -3.39388900 0.32438700
C -3.10550100 -2.08320100 0.61616100

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C  -2.99933200  -3.25298100   4.27051800
F  -0.75246400   2.47803900   2.21944200
F  -2.85175300   2.26495600   1.64606200
F  -1.19666700   1.74099600   4.58651900
F  -3.26750600   2.23847000   4.12667800
F  -3.90673000  -0.18972200   4.36595400
F  -1.84197200  -0.61749800   4.91251800
C   0.14074100  -2.40506000   2.04954500
H   1.20574900  -2.58209200   2.24126800
H  -0.29616000  -1.98383500   2.95520300
H  -0.32065800  -3.38230900   1.85485500
H  -3.65511700  -2.58765300   4.83823600
H  -3.24084900  -4.28452400   4.53837000
H  -1.97205400  -3.04626900   4.59266700
C   1.03009300   0.11628000  -2.54062500
C   0.91330400  -0.80514700  -3.59095800
C   1.65973400   1.34440600  -2.78597000
C   1.40327400  -0.50121600  -4.85545100
H   0.42219400  -1.75913300  -3.41885800
C   2.14533600   1.64680700  -4.05325100
H   1.78466900   2.05383200  -1.97400900
C   2.01835700   0.72647100  -5.09104000
H   1.30127400  -1.22394200  -5.65904500
H   2.63299200   2.60102000  -4.22678200
H   2.40228100   0.96241800  -6.07870500
C  -3.57914200  -4.01780200  -0.98884100
C  -4.59557600  -4.96147200  -1.18617900
C  -2.75544100  -3.67835500  -2.07077500
C  -4.78484500  -5.54568200  -2.43397500
H  -5.25178600  -5.22851500  -0.36215900
C  -2.95359300  -4.25570700  -3.31981600
H  -1.94500100  -2.97069100  -1.92201800
C  -3.96753800  -5.19279300  -3.50549400
H  -5.57795700  -6.27451000  -2.57057900
H  -2.30618400  -3.98046300  -4.14710100
H  -4.11837200  -5.64837100  -4.47932100
C  -3.27844100  -0.98129100  -0.39750200
H  -3.58467700  -0.05601000   0.09656300
H  -2.36604300  -0.76731300  -0.96110200
H  -4.05027600  -1.26313900  -1.11921800
C  -0.74963000   1.91655400  -0.69932600
H  -1.79854800   2.00412700  -0.40622800
H  -0.20251100   2.71202500  -0.18551900
H  -0.67842600   2.09364100  -1.77444500
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CF
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C  -1.24609500   2.97854000  -0.15009600
C  -0.73077900   1.56957500  -0.10699300
C   0.73783600   1.58939900  -0.05734000
C   1.20863400   3.00362400  -0.21351900
C  -0.01832900   3.84834000   0.20706600
C   1.45925700   0.45833300   0.14646500
C   0.64911100  -0.75574800   0.61057000
C  -0.60201800  -0.87240900  -0.27513800
C  -1.42807500   0.41072000  -0.17429900
S   1.78117800  -2.19818700   0.45490700
C   3.15878200  -1.14662100   0.14625900
C   2.87572100   0.17826200   0.01107000
C  -2.85630200   0.13973500  -0.24854500
C  -3.14261500  -1.17058600  -0.02191800
S  -1.74523600  -2.20999900   0.26765700
C   0.34211100  -0.56485300   2.11257100
C  -0.27895500  -1.08581500  -1.77174000
F   2.26807700   3.33847300   0.55802300
F   1.53251100   3.32163600  -1.50070100
F   0.01871700   4.01712700   1.54617500
F  -0.04637400   5.05375700  -0.37957600
F  -1.67399300   3.33955100  -1.39403900
F  -2.26004400   3.23587700   0.70957900
H   0.33123800  -0.26089800  -2.15177500
H   0.25694500  -2.02337300  -1.92922400
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³CF
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C  -1.235093   3.015623  -0.225412
C  -0.675037   1.622014  -0.226809
C   0.688987   1.651949  -0.052119
C   1.201302   3.057555  -0.079138
C  -0.049792   3.909246   0.216996
C   1.45904    0.452826   0.200129
C   0.618233  -0.713567   0.676208
C  -0.54862   -0.86265   -0.356708
C  -1.409896   0.386758  -0.3033
S   1.764315  -2.147091   0.692827
C   3.133002  -1.175696   0.198196
C   2.796395   0.175007  -0.035719
C  -2.786875   0.13547   -0.320128
C  -3.097135  -1.2189    -0.129577
S  -1.689451  -2.244398   0.04318
C   0.104829  -0.496014   2.110722
C  -0.035814  -1.071373  -1.795649
F   2.180794   3.302304   0.819986
F   1.68623    3.417328  -1.304924
F  -0.126414   4.128827   1.545141
F  -0.038015   5.094724  -0.411972
F  -1.673287   3.414253  -1.44998
F  -2.266385   3.181197   0.638861
H   0.588095  -0.22963   -2.108994
H   0.552302  -1.990178  -1.868419
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H -1.21338500 -1.11462200 -2.33785200
H -0.28385400   0.31816400   2.26750000
H -0.16947500 -1.43567900   2.52675900
H   1.28275800 -0.42264700   2.65051400
C   3.89151000   1.20101400 -0.41686700
H   3.47581000   1.84620000 -1.19509300
H   4.20202300   1.84430600   0.41065600
H   4.78043800   0.71472800 -0.82287500
C -3.89014700   1.17643800 -0.59215800
H -4.17127300   1.77701200   0.27779700
H -3.50791200   1.86182000 -1.35126200
H -4.79358900   0.70275000 -0.98230600
C -4.47494300 -1.80418200   0.01616300
C -4.70930200 -3.01480400 -0.64907000
C -5.51975800 -1.21482200   0.73896600
C -5.96523500 -3.60941200 -0.60794700
H -3.90590900 -3.48368600 -1.20958400
C -6.77403600 -1.81398200   0.78118700
H -5.34158700 -0.29306100   1.28352900
C -7.00084800 -3.01080400   0.10632600
H -6.13446200 -4.54385400 -1.13396400
H -7.57374900 -1.34717300   1.34781400
H -7.97966200 -3.47904500   0.14143200
C   4.48183100 -1.79051900   0.03642900
C   4.64929600 -2.94002700 -0.74619100
C   5.58436200 -1.27294000   0.72749200
C   5.89660600 -3.54490900 -0.85113900
H   3.80218500 -3.35092300 -1.28812700
C   6.83012400 -1.88215400   0.62315600
H   5.45795400 -0.39884900   1.35881100
C   6.98999900 -3.01703000 -0.16823200
H   6.01451000 -4.42991600 -1.46857000
H   7.67624900 -1.47116800   1.16495200
H   7.96315800 -3.49108200 -0.25046400

H -0.886351 -1.143364 -2.478174
H -0.576967   0.358289   2.150314
H -0.429228 -1.378028   2.473183
H   0.94893   -0.298377   2.776084
C   3.788893   1.163746 -0.585901
H   3.305598   1.852101 -1.279614
H   4.239491   1.762813   0.211509
H   4.592627   0.652533 -1.119493
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H -4.17315   1.668533   0.335979
H -3.502273   1.925153 -1.274111
H -4.736226   0.687469 -1.022298
C -4.42214   -1.841721 -0.034035
C -4.668655 -3.087437 -0.633176
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C -5.914816 -3.69281   -0.52439
H -3.881162 -3.574042 -1.201326
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H -5.278112 -0.288953   1.196359
C -6.937909 -3.070261   0.187177
H -6.087555 -4.652896 -1.000879
H -7.491006 -1.352901   1.363465
H -7.910507 -3.544827   0.272787
C   4.438819 -1.818948   0.057067
C   4.545753 -3.110603 -0.486057
C   5.612641 -1.177589   0.487132
C   5.783722 -3.727922 -0.613268
H   3.651626 -3.622525 -0.830917
C   6.848968 -1.79841   0.356829
H   5.549915 -0.198711   0.950831
C   6.941355 -3.073803 -0.196299
H   5.845616 -4.721543 -1.046499
H   7.743358 -1.287272   0.699869
H   7.908264 -3.55674   -0.297662

¹CF(relax)
C -1.23017   3.028411 -0.144245
C -0.683647   1.636091 -0.18121
C   0.711057   1.658654   0.003094
C   1.215551   3.061311 -0.044994
C -0.030534   3.909531   0.283163
C   1.454862   0.477908   0.247101
C   0.613819 -0.701797   0.670628
C -0.543823 -0.818294 -0.403708
C -1.400713   0.423176 -0.309533
S   1.746866 -2.129598   0.672828
C   3.123885 -1.163072   0.217929
C   2.814611   0.184009   0.026523
C -2.790398   0.155223 -0.319079
C -3.086908 -1.197319 -0.173077
S -1.673095 -2.216841 -0.078681
C   0.050477 -0.53046   2.093633
C   0.018929 -0.974677 -1.830822
F   2.217268   3.325658   0.827919
F   1.671061   3.42913   -1.284303
F -0.078526   4.117799   1.616221
F -0.027253   5.104837 -0.330576
F -1.694668   3.45799   -1.353326
F -2.247828   3.199016   0.741356
H   0.638275 -0.112046 -2.091475
H   0.622844 -1.883758 -1.909218
H -0.806425 -1.037429 -2.544201
H -0.609054   0.340902   2.132498
H -0.519752 -1.413684   2.394583
H   0.869967 -0.381532   2.800828
C   3.808522   1.180483 -0.503507
H   3.328299   1.858526 -1.210861
H   4.231939   1.791991   0.299113
H   4.630102   0.678989 -1.018388
C -3.857398   1.19628   -0.528984
H -4.139208   1.691211   0.404481

H -3.507179 1.967213 -1.216411
H -4.753861 0.742833 -0.957174
C -4.400842 -1.832639 -0.063708
C -4.640504 -3.085627 -0.65447
C -5.438934 -1.231975 0.669189
C -5.87797 -3.704459 -0.530597
H -3.856725 -3.564942 -1.234044
C -6.675477 -1.853562 0.788193
H -5.264262 -0.288481 1.174479
C -6.901819 -3.090321 0.187498
H -6.0445 -4.667929 -1.002512
H -7.462215 -1.374548 1.362993
H -7.868421 -3.574969 0.283708
C 4.416906 -1.822943 0.055902
C 4.503359 -3.101703 -0.522631
C 5.601696 -1.210394 0.500745
C 5.731725 -3.732085 -0.670872
H 3.602095 -3.590269 -0.882574
C 6.827622 -1.845953 0.350578
H 5.553763 -0.245296 0.993973
C 6.899813 -3.106617 -0.238648
H 5.778371 -4.713618 -1.132533
H 7.730019 -1.358352 0.70654
H 7.859389 -3.600386 -0.356111

TS(AP-CF)				TS(³AP-³CF)		
C	-2.71446900	0.15465200 -0.25988800		C	2.77527200	0.15649700 0.14803900
C	-1.34354000	0.43464900 -0.49748600		C	1.42124500	0.50687900 0.50098100
C	-0.52667100	-0.74600100 -0.73159400		C	0.71363700	-0.57920300 1.09053100
S	-1.59810900	-2.15998100 -0.72423300		S	1.73851200	-1.97881600 1.21553000
C	-3.00331400	-1.19873800 -0.34275000		C	3.07554000	-1.14594600 0.45852800
C	-0.62793300	1.66607000 -0.20957300		C	0.69843100	1.68290900 0.11271000
C	0.65412700	1.69050300 0.28219700		C	-0.67546700	1.64431200 -0.26203200
C	1.05448200	3.10416800 0.59857600		C	-1.23990900	3.02890400 -0.21574300
C	0.11134200	3.94284000 -0.28306600		C	0.00320600	3.94010100 -0.29910800
C	-1.15751900	3.06759000 -0.35191000		C	1.13753300	3.09789000 0.31669600
C	1.40585200	0.47423700 0.58284500		C	-1.36733700	0.45542000 -0.56804300
C	0.60871800	-0.68013300 0.95332700		C	-0.60923300	-0.73181200 -0.94582700
S	1.68667900	-2.08120400 1.03266600		S	-1.62527200	-2.15577500 -0.85746500
C	3.03985200	-1.18225700 0.39486200		C	-3.02531900	-1.18781500 -0.42071800
C	2.72927100	0.15969700 0.19613500		C	-2.76250300	0.15558300 -0.34416900
C	-0.40069800	-0.62267900 2.08288600		C	0.46884000	-0.74291000 -1.99181300
F	-1.84462300	3.26334900 -1.49889800		F	1.23800800	3.39456800 1.64784400
F	-1.96824700	3.44722600 0.67523100		F	2.32515700	3.46274200 -0.23062700
F	0.64779700	4.06547800 -1.51573300		F	-0.17009200	5.11814500 0.32114700
F	-0.12226400	5.16826900 0.20817400		F	0.28459200	4.17754000 -1.59898400
F	0.81706700	3.39257600 1.90918800		F	-2.09917600	3.32469300 -1.22243600
F	2.34501900	3.42655700 0.36681500		F	-1.88926600	3.30929500 0.95621300
C	0.46960300	-0.76777800 -1.87784700		C	-0.42405800	-0.47881500 2.06989600
H	1.18719500	-1.58738600 -1.77592700		H	-0.04291100	-0.60964200 3.08785300
H	-0.06712000	-0.89984000 -2.82164600		H	-0.90001900	0.50057000 2.01379700
H	1.01982500	0.17250800 -1.93862600		H	-1.18189500	-1.25081000 1.89381900
H	-0.95819500	0.31535400 2.06295200		H	1.21986000	-1.51519200 -1.78813300
H	-1.11359700	-1.45074600 2.02227200		H	0.02925000	-0.95363800 -2.97376000
H	0.11652500	-0.68387000 3.04459300		H	0.97046500	0.22359300 -2.05276500
C	-4.28817600	-1.88003600 -0.11532500		C	4.31139000	-1.89445400 0.17560800
C	-4.37280900	-2.97459600 0.75608400		C	4.25985100	-3.17643200 -0.38830400
C	-5.44531000	-1.46343300 -0.78800100		C	5.56195100	-1.34004900 0.47890300
C	-5.58614900	-3.62179600 0.96221200		C	5.43012700	-3.87817000 -0.65470600
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C	-6.65835500	-2.10985000 -0.57638900		C	6.73100000	-2.04297200 0.20823000
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C	-6.73324100	-3.18970100 0.30031800		C	6.66886300	-3.31280500 -0.36057600
H	-5.63586200	-4.46271000 1.64730100		H	5.37328200	-4.86687800 -1.09953000
H	-7.54494400	-1.77463000 -1.10592800		H	7.69201800	-1.59903700 0.44891100
H	-7.68037000	-3.69473900 0.46315400		H	7.58234500	-3.86066300 -0.57052300
C	4.28278600	-1.88918800 0.06565400		C	-4.28444100	-1.89460000 -0.12033000
C	4.25148700	-3.15844900 -0.53226400		C	-4.81166300	-2.81956800 -1.02997200
C	5.53070500	-1.31690900 0.35562400		C	-4.95127900	-1.67847600 1.09216600
C	5.43054800	-3.82543000 -0.84307500		C	-5.99102800	-3.49764300 -0.74121200
H	3.29546400	-3.61683900 -0.76919600		H	-4.30351500	-2.99434400 -1.97413200

C 6.70819300 -1.98484000 0.03890900
H 5.57564900 -0.35262100 0.85183700
C 6.66339600 -3.24021600 -0.56300200
H 5.38499400 -4.80341300 -1.31242100
H 7.66398600 -1.52534200 0.27158100
H 7.58386300 -3.76127000 -0.80770300
C 3.65457300 1.09945700 -0.52996400
H 3.09016800 1.75739800 -1.19460700
H 4.22034400 1.73455000 0.15736400
H 4.36948100 0.53707000 -1.13442000
C -3.72983500 1.17543900 0.17306200
H -3.40854000 1.66739100 1.09416900
H -3.86218400 1.95254100 -0.58479500
H -4.69853200 0.71105200 0.35954200

C -6.12974800 -2.35909400 1.37881700
H -4.53420800 -0.98478400 1.81612600
C -6.65346300 -3.26803900 0.46236400
H -6.39309500 -4.20565900 -1.45930000
H -6.63484500 -2.18430500 2.32371000
H -7.57406900 -3.79792800 0.68678600
C -3.81304500 1.16821500 0.01469500
H -3.61685700 1.61310200 0.99489700
H -3.83390600 1.98082300 -0.71250000
H -4.80137700 0.70715300 0.03821400
C 3.69003600 1.03452300 -0.65821800
H 3.12780700 1.55414300 -1.43846200
H 4.17273800 1.79859700 -0.04290500
H 4.47182500 0.44026700 -1.13554100

TS(AP-P)
C 2.47807 -0.22674 -0.26461
C 1.84384 0.58886 0.73907
C 2.4781 0.58796 1.94745
S 3.84684 -0.46733 1.90128
C 3.57839 -0.87368 0.2278
C 0.71106 1.46432 0.38555
C -0.61799 1.27709 0.15646
C -1.1514 2.56747 -0.46778
C 0.08041 3.41564 -0.84296
C 1.15241 2.87921 0.09349
C -1.5144 0.10176 0.35682
C -1.10227 -1.12646 0.87258
S -2.35736 -2.29593 0.81547
C -3.49816 -1.17749 0.1803
C -2.95016 0.06727 0.01633
C 0.14475 -1.64674 1.53219
F 1.19731 3.63278 1.22733
F 2.37775 2.94353 -0.47066
F -0.14471 4.73216 -0.72076
F 0.43567 3.15435 -2.11803
F -1.86539 2.35241 -1.59397
F -1.91057 3.29277 0.39598
C 2.0931 1.31018 3.20193
H 2.00816 0.61922 4.04719
H 2.83022 2.07501 3.46652
H 1.12896 1.8056 3.06713
H 0.47801 -0.97482 2.32335
H -0.0638 -2.61695 1.99155
H 0.96997 -1.78735 0.83205
C 4.48703 -1.81734 -0.45182
C 4.77595 -3.06319 0.11842
C 5.08058 -1.48044 -1.6744
C 5.63201 -3.95304 -0.52162
H 4.31445 -3.33906 1.06259
C 5.92966 -2.37555 -2.31782
H 4.88503 -0.50578 -2.11161
C 6.20831 -3.61348 -1.74336
H 5.84258 -4.91666 -0.06777
H 6.3827 -2.1003 -3.2654
H 6.87411 -4.30924 -2.24478
C -4.88233 -1.63251 -0.06979
C -5.59869 -2.31126 0.92343
C -5.49087 -1.41854 -1.3125
C -6.89296 -2.76036 0.6815
H -5.14254 -2.47522 1.89584
C -6.78702 -1.86246 -1.55155
H -4.9373 -0.90784 -2.09484
C -7.49121 -2.53602 -0.55577
H -7.43625 -3.28135 1.46408
H -7.24508 -1.6891 -2.52058
H -8.50192 -2.8853 -0.74379
C -3.89823 1.19693 -0.32118
H -3.6569 2.10994 0.21692
H -3.92189 1.43061 -1.38683
H -4.90836 0.90434 -0.02737

```
C  1.90517 -0.36777 -1.64561
H  0.85926 -0.69292 -1.59412
H  1.91964  0.59225 -2.17332
H  2.45991 -1.09664 -2.2393
```

S.26. GEOMETRIES : DTE-m5

AP	³AP
C -2.2989 -2.15363 0.21995	C 0.0389 -3.21585 -0.11082
C -0.98532 -2.30368 0.79163	C -1.04008 -2.32421 -0.53944
C -0.70665 -1.4089 1.79241	C -0.53087 -1.12259 -1.09152
S -2.05531 -0.37653 2.06833	S 1.17899 -1.03457 -0.94277
C -2.99705 -1.12771 0.81248	C 1.26168 -2.62235 -0.20389
C -0.0087 -3.31032 0.34691	C -2.41434 -2.4979 -0.28252
C 1.1885 -3.10239 -0.23164	C -3.34223 -1.36107 -0.09924
C 1.88454 -4.41384 -0.51247	C -4.6404 -1.76309 -0.69576
C 0.76617 -5.46784 -0.35023	C -4.69336 -3.30166 -0.44236
C -0.21704 -4.78085 0.61551	C -3.20713 -3.75615 -0.22083
C 1.77112 -1.81628 -0.64962	C -3.00373 -0.18864 0.59767
C 1.16894 -1.02012 -1.58976	C -1.96378 -0.16444 1.56093
S 2.09724 0.4067 -1.85645	S -1.54038 1.44877 1.98368
C 3.30107 -0.0584 -0.68814	C -2.76938 2.11937 0.92875
C 3.00247 -1.27288 -0.12775	C -3.49493 1.15604 0.29694
C -0.0965 -1.25402 -2.35405	C -1.36828 -1.29276 2.34673
F 0.11944 -5.08284 1.89825	F -2.86601 -4.66622 -1.17009
F -1.48194 -5.21073 0.42882	F -3.1332 -4.41003 0.98177
F 1.21463 -6.64914 0.09554	F -5.25977 -3.96549 -1.46378
F 0.15208 -5.65195 -1.53923	F -5.42117 -3.53225 0.66809
F 2.42763 -4.4482 -1.74707	F -5.73239 -1.16881 -0.16554
F 2.87643 -4.69307 0.37344	F -4.69541 -1.55786 -2.05515
C 0.55886 -1.25999 2.57876	C -1.23033 -0.07635 -1.90579
H 0.37418 -0.81673 3.56059	H -0.67855 0.10475 -2.83398
H 1.02727 -2.23689 2.72939	H -2.23596 -0.40108 -2.17489
H 1.27273 -0.61988 2.04703	H -1.30623 0.87972 -1.37442
H -0.96428 -0.862 -1.81124	H -0.31423 -1.45651 2.09223
H -0.06369 -0.77081 -3.33424	H -1.41952 -1.07159 3.41805
H -0.25152 -2.32452 -2.51227	H -1.91251 -2.22143 2.17243
C 3.81409 -1.92915 0.95423	C -4.53716 1.4551 -0.74176
H 3.17338 -2.48812 1.64074	H -4.42276 0.79959 -1.60909
H 4.53862 -2.6391 0.54206	H -5.54813 1.30511 -0.35265
H 4.36646 -1.18238 1.53039	H -4.45432 2.48911 -1.0841
C -2.78285 -2.97949 -0.94209	C -0.18321 -4.58925 0.45272
H -1.9428 -3.42805 -1.47745	H -0.82492 -5.17946 -0.20365
H -3.42488 -3.80361 -0.61715	H 0.76425 -5.11954 0.56335
H -3.35225 -2.36838 -1.64847	H -0.6706 -4.54665 1.43235
C 4.40877 0.86948 -0.39822	C -2.81338 3.58432 0.77122
C 4.13583 2.23619 -0.30425	C -1.62393 4.27912 0.53133
C 5.72695 0.43467 -0.21923	C -4.01228 4.29855 0.86929
H 3.12506 2.59364 -0.44146	H -0.68639 3.74152 0.43712
C 6.73 1.36004 0.0582	C -4.0074 5.6829 0.72822
H 5.97101 -0.61802 -0.32056	H -4.93939 3.77273 1.07571
C 6.43979 2.71921 0.14946	C -2.81469 6.36491 0.50207
H 7.75197 1.01738 0.1902	H -4.93854 6.23463 0.81326
H 7.23437 3.43103 0.35978	H -2.81997 7.44802 0.40774
C 5.13072 3.16576 -0.03296	C -1.61326 5.66369 0.39966
C 4.75852 4.62408 0.11892	C -0.31555 6.3718 0.09385
H 5.55484 5.27171 -0.27583	H -0.32985 7.39763 0.49252
H 4.65869 4.8481 1.18821	H -0.20793 6.44752 -0.99645
O 3.54963 4.86679 -0.56818	O 0.75057 5.63936 0.65642
C 2.66074 5.79938 -0.00035	C 2.01685 5.86812 0.08444
H 1.81335 5.82512 -0.69237	H 2.71193 5.29759 0.70776
H 3.0918 6.81225 0.02737	H 2.30861 6.92801 0.15144
C 2.18774 5.44254 1.41679	C 2.12165 5.42647 -1.38048
H 2.92862 5.74349 2.16219	H 1.6657 6.16425 -2.04608
H 1.27468 6.02056 1.62555	H 3.18813 5.37797 -1.64677
O 2.00384 4.06142 1.63787	O 1.44499 4.22136 -1.66478
C 1.03279 3.41572 0.84275	C 1.88741 3.07238 -0.9704
H 1.11765 2.35137 1.08536	H 1.19047 2.27597 -1.24779
H 1.25929 3.53477 -0.22616	H 1.81028 3.21724 0.11587
C -0.39607 3.87056 1.15118	C 3.29724 2.63977 -1.38927
H -0.4823 4.03441 2.22906	H 3.36195 2.69746 -2.47983
H -0.64214 4.81046 0.63887	H 4.06503 3.30778 -0.9762
O -1.35798 2.88012 0.84405	O 3.55914 1.29466 -1.05181
C -1.43704 2.46697 -0.50349	C 3.88077 1.03554 0.29776
H -2.29579 1.79053 -0.53567	H 3.85152 -0.05512 0.39103

H -0.55727 1.87198 -0.79705	H 3.12506 1.43328 0.99107
C -1.59641 3.58865 -1.53274	C 5.24923 1.5701 0.7223
H -0.63419 4.08137 -1.70826	H 5.22241 2.65771 0.83825
H -1.89183 3.11414 -2.48162	H 5.47508 1.14968 1.71457
O -2.47425 4.64016 -1.18585	O 6.29164 1.333 -0.20072
C -4.3308 -0.59784 0.4773	C 2.57259 -3.0694 0.30483
C -4.61254 0.77098 0.60694	C 3.73634 -2.86585 -0.45085
C -5.3476 -1.43795 0.00597	C 2.69323 -3.62243 1.58385
C -5.84469 1.30063 0.23108	C 4.98855 -3.21828 0.04217
H -3.85023 1.44106 1.0012	H 3.65938 -2.42472 -1.44258
C -6.57859 -0.91591 -0.37932	C 3.94253 -3.98649 2.07938
H -5.18627 -2.50809 -0.04518	H 1.80991 -3.74251 2.20308
C -6.82371 0.44793 -0.28296	C 5.08528 -3.78599 1.31539
H -7.3514 -1.58436 -0.7464	H 4.02216 -4.4153 3.07356
H -7.78254 0.85593 -0.59136	H 6.06287 -4.04916 1.70932
C -3.69329 4.29974 -0.55481	C 6.42552 0.00826 -0.67615
H -3.48894 3.77817 0.3867	H 5.50669 -0.30927 -1.18541
H -4.17264 5.25355 -0.31568	H 7.22546 0.04078 -1.42142
C -4.64976 3.49839 -1.44131	C 6.82032 -0.97641 0.42631
H -4.73549 3.99305 -2.41298	H 7.68386 -0.57562 0.96417
H -4.27452 2.4787 -1.61294	H 6.00079 -1.10313 1.14841
O -5.96073 3.46874 -0.90988	O 7.23161 -2.23447 -0.07504
C -6.11162 2.78541 0.32819	C 6.23971 -2.96981 -0.77213
H -5.47994 3.23059 1.10757	H 5.97639 -2.48258 -1.72078
H -7.15321 2.95924 0.61066	H 6.72368 -3.91989 -1.01744

P	**³P**
C -1.4929 -2.00021 0.13408	C -1.33688 -2.20419 0.26271
C -2.63049 -1.38067 -0.50329	C -2.41702 -1.38844 -0.2916
C -2.51632 -1.27598 -1.86552	C -2.23749 -1.14104 -1.66235
S -1.01615 -1.93287 -2.39597	S -0.80694 -1.89138 -2.24791
C -0.52195 -2.34363 -0.77602	C -0.40225 -2.53933 -0.67581
C -3.80201 -0.85454 0.21868	C -3.46911 -0.8186 0.46565
C -4.20203 0.4294 0.28036	C -4.22384 0.41478 0.10762
C -5.44953 0.57348 1.11288	C -5.67376 0.12578 0.28665
C -5.58562 -0.7951 1.8215	C -5.7115 -1.11427 1.25059
C -4.80443 -1.75192 0.89883	C -4.22052 -1.43906 1.59095
C -3.49368 1.58157 -0.30332	C -3.61417 1.64249 -0.19811
C -3.97896 2.36087 -1.32136	C -4.17728 2.66061 -0.99914
S -2.77587 3.49258 -1.83783	S -2.98767 3.82669 -1.44305
C -1.62436 2.91979 -0.6706	C -1.74295 3.02739 -0.50969
C -2.15321 1.91862 0.09694	C -2.21893 1.92562 0.13199
C -5.31361 2.31076 -2.0012	C -5.55274 2.75833 -1.57507
F -5.6533 -2.29245 -0.01635	F -4.06416 -2.77252 1.73143
F -4.26509 -2.77778 1.58937	F -3.93222 -0.86781 2.80592
F -6.85929 -1.16488 2.01255	F -6.25476 -2.17665 0.62596
F -4.96039 -0.73879 3.01707	F -6.43599 -0.85288 2.35103
F -5.34909 1.58322 2.00346	F -6.37209 1.15096 0.83117
F -6.56187 0.8036 0.36708	F -6.32544 -0.21155 -0.87474
C -3.49012 -0.70051 -2.84586	C -3.12837 -0.42941 -2.63639
H -3.50967 -1.27694 -3.775	H -3.03275 -0.86776 -3.63395
H -4.49686 -0.70751 -2.42005	H -4.17491 -0.50274 -2.3355
H -3.2337 0.33574 -3.0923	H -2.86807 0.63218 -2.71288
H -6.00103 3.05373 -1.58274	H -6.2834 3.03329 -0.80799
H -5.21945 2.50491 -3.07339	H -5.59642 3.50675 -2.36991
H -5.77249 1.32855 -1.87238	H -5.8655 1.79677 -1.99134
C -1.45645 1.28466 1.26783	C -1.45044 1.20995 1.2137
H -2.18139 1.00486 2.03842	H -2.13534 0.84948 1.9861
H -0.91251 0.38107 0.97735	H -0.88483 0.35038 0.84472
H -0.73545 1.9757 1.71135	H -0.73849 1.89705 1.67879
C -1.39041 -2.17836 1.6258	C -1.18433 -2.48391 1.73307
H -2.02865 -1.46152 2.14857	H -1.58455 -1.65563 2.32401
H -1.71257 -3.17677 1.93765	H -1.71613 -3.38792 2.04238
H -0.36324 -2.03279 1.97324	H -0.13015 -2.60806 1.9942
C 0.77639 -3.01839 -0.58267	C 0.82102 -3.35229 -0.54256
C 1.84273 -2.78726 -1.46266	C 1.96983 -3.05994 -1.2907
C 0.95083 -3.96592 0.43793	C 0.827 -4.48207 0.2877
C 3.03635 -3.50199 -1.36261	C 3.09934 -3.87435 -1.22286
H 1.74828 -2.03881 -2.24553	H 1.99538 -2.18141 -1.93083
C 2.15793 -4.63781 0.57974	C 1.96269 -5.27586 0.38571
H 0.13052 -4.20518 1.10404	H -0.06845 -4.75273 0.8366

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C  3.196   -4.41315 -0.32007          C  3.09521 -4.97293 -0.36363
H  2.27829 -5.36255  1.37924          H  1.9591  -6.14255  1.03973
H  4.13085 -4.95873 -0.21973          H  3.97824 -5.60291 -0.28963
C -0.23294  3.39972 -0.6215           C -0.35456  3.51127 -0.47643
C  0.11859  4.74989 -0.55801          C -0.00461  4.8553  -0.31669
C  0.77704  2.43191 -0.60327          C  0.6587   2.55295 -0.57354
C  1.46067  5.10824 -0.4446           C  1.33854  5.21043 -0.21919
H -0.65275  5.5147  -0.56926          H -0.77661  5.6158  -0.23899
C  2.11265  2.77924 -0.45595          C  1.99785  2.89397 -0.4387
H  0.51576  1.38313 -0.69815          H  0.40094  1.51222 -0.73714
C  2.45047  4.13198 -0.37364          C  2.33408  4.23641 -0.25801
H  1.73223  6.15794 -0.3837           H  1.60822  6.25306 -0.08096
H  3.4916   4.42297 -0.25211          H  3.37698  4.52225 -0.14056
O  6.06602  0.36529 -0.26311          O  5.9043   0.43779 -0.41167
C  6.79706  1.56271 -0.28619          C  6.6424   1.61513 -0.61621
H  7.84418  1.37131 -0.56989          H  7.66782  1.37488 -0.93928
H  6.37355  2.2674  -1.02217          H  6.1792   2.2322  -1.40508
C  6.73997  2.20029  1.08873          C  6.68431  2.42303  0.66685
H  5.69952  2.41173  1.35391          H  5.66757  2.68032  0.97926
H  7.28493  3.15403  1.05203          H  7.22371  3.35836  0.46186
O  7.34294  1.3628   2.05488          O  7.36099  1.72201  1.69073
C  6.52943  0.98193  3.14295          C  6.61983  1.46384  2.86383
H  6.0272   1.85418  3.58718          H  6.1292   2.37692  3.23238
H  7.22159  0.57907  3.88898          H  7.36081  1.15786  3.60855
C  5.49175 -0.08701  2.83369          C  5.58705  0.35488  2.73879
H  5.92926 -0.8247   2.14615          H  6.00152 -0.44706  2.11177
H  5.22499 -0.60096  3.77262          H  5.38417 -0.05815  3.74137
O  4.33589  0.48739  2.26221          O  4.38889  0.84616  2.17668
C  3.35755 -0.48157  1.96387          C  3.44277 -0.18088  1.98942
H  3.8037  -1.33002  1.4252           H  3.90309 -1.03496  1.47312
H  2.91659 -0.87902  2.8947           H  3.07678 -0.54409  2.96561
C  2.25154  0.11969  1.11841          C  2.25486  0.3132   1.18508
H  1.84583  1.01445  1.60994          H  1.84121  1.22064  1.64592
H  1.44609 -0.61924  1.03895          H  1.48122 -0.4622   1.21233
O  2.64994  0.40826 -0.20845          O  2.53831  0.52873 -0.18544
C  3.17853  1.70319 -0.40125          C  3.05501  1.80933 -0.49036
H  3.70901  1.66446 -1.35816          H  3.45758  1.72512 -1.50558
H  3.91511  1.93495  0.37278          H  3.88515  2.05268  0.1763
C  5.90257 -0.23474 -1.52345          C  5.70789 -0.31038 -1.58535
H  5.30047  0.40177 -2.1905           H  5.11625  0.25805 -2.32064
H  6.87424 -0.40807 -2.01109          H  6.66846 -0.57065 -2.05655
C  5.16546 -1.53591 -1.27337          C  4.95205 -1.56139 -1.18154
H  4.36283 -1.33118 -0.55923          H  4.05908 -1.26417 -0.62414
H  5.84656 -2.28223 -0.83434          H  5.58643 -2.18232 -0.53049
O  4.63311 -2.00217 -2.49401          O  4.59615 -2.26787 -2.35325
C  4.136   -3.31779 -2.39239          C  4.30464 -3.62222 -2.11093
H  4.95778 -4.01519 -2.16385          H  5.18233 -4.12732 -1.67699
H  3.75611 -3.56242 -3.389            H  4.12591 -4.0637  -3.09725
```

¹P
```
C -1.31634 -2.08739  0.20041
C -2.37694 -1.22682 -0.30762
C -2.09915 -0.79044 -1.63492
S -0.60312 -1.40065 -2.19428
C -0.31074 -2.28673 -0.70695
C -3.51967 -0.8085   0.4259
C -4.25064  0.41598  0.21192
C -5.69482  0.17784  0.43575
C -5.76154 -1.1931   1.1805
C -4.28014 -1.61807  1.40991
C -3.62524  1.64331 -0.12075
C -4.17113  2.67614 -0.9185
S -2.949    3.74538 -1.43869
C -1.70545  2.94307 -0.51481
C -2.21581  1.88992  0.18537
C -5.55143  2.80429 -1.47067
F -4.1542  -2.96152  1.27283
F -3.96597 -1.33571  2.72342
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H  -4.00036  -0.02761  -2.26471
H  -2.61529   0.95777  -2.78458
H  -6.29725   2.76253  -0.67261
H  -5.6755    3.74791  -2.00768
H  -5.77328   1.98363  -2.16352
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H  -2.19101   0.86922   2.07123
H  -0.87743   0.36592   1.00823
H  -0.80331   1.94162   1.79159
C  -1.25577  -2.55391   1.6286
H  -1.67964  -1.79333   2.28893
H  -1.82322  -3.47418   1.79279
H  -0.22176  -2.73254   1.934
C   0.87504  -3.15355  -0.63328
C   2.05614  -2.84284  -1.32601
C   0.79891  -4.37341   0.05751
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H   2.14959  -1.89343  -1.84609
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H  -0.12258  -4.65825   0.55221
C   3.04573  -4.91859  -0.61768
H   1.8153   -6.17628   0.62016
H   3.88642  -5.608    -0.61101
C  -0.29973   3.36639  -0.53454
C   0.12077   4.69603  -0.43132
C   0.6619    2.35578  -0.62012
C   1.48184   4.98536  -0.37802
H  -0.61069   5.49646  -0.36218
C   2.01873   2.63279  -0.52864
H   0.34615   1.32491  -0.74243
C   2.42695   3.96145  -0.40395
H   1.80741   6.01697  -0.28384
H   3.4856    4.19765  -0.32216
O   6.02679   0.44563  -0.23559
C   6.68377   1.68105  -0.36478
H   7.7502    1.52808  -0.59278
H   6.24502   2.27009  -1.18801
C   6.53411   2.46538   0.92471
H   5.47277   2.63486   1.13411
H   7.01563   3.44411   0.78902
O   7.15763   1.79303   2.00004
C   6.33216   1.47859   3.10043
H   5.75539   2.3564    3.42784
H   7.02177   1.2106    3.90667
C   5.38331   0.31021   2.88242
H   5.89835  -0.46616   2.29906
H   5.11585  -0.11473   3.86466
O   4.21229   0.73009   2.21502
C   3.31725  -0.33937   2.01206
H   3.82852  -1.1867    1.53262
H   2.92793  -0.69592   2.98154
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H   1.70304   1.01176   1.56679
H   1.38207  -0.69461   1.19778
O   2.44696   0.24836  -0.2187
C   3.01512   1.49413  -0.578
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H   4.26961  -1.26699  -0.51463
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O   4.73118  -2.12521  -2.33853
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C	1.32339	2.09127	-0.00784
S	-1.77717	-0.48986	-1.11881
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C	2.76748	1.9215	-0.09297
C	3.10897	0.72814	-0.63968
S	1.76788	-0.31943	-1.09509
C	-0.50837	1.57912	-2.38878
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F	-1.74434	4.33483	2.14556
F	-0.3956	5.9735	-0.59383
F	-0.27504	6.38182	1.55165
F	1.52232	4.59194	1.92001
F	1.93954	5.10161	-0.16374
H	-0.3164	0.77263	1.80137
H	-0.0326	-0.86308	1.14582
H	1.32773	0.10869	1.72875
H	0.04398	2.52213	-2.34628
H	0.04435	0.87552	-3.01387
H	-1.48165	1.76752	-2.84887
C	-4.05898	2.52621	0.44239
H	-3.70644	2.95684	1.3833
H	-4.36055	3.35392	-0.20454
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C	4.4737	0.20627	-0.86803
C	4.87534	-0.96119	-0.21705
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H	4.19762	-1.45128	0.47292
C	6.62501	0.30422	-1.95584
H	5.05388	1.7513	-2.25197
C	7.00688	-0.87215	-1.31581
H	7.30993	0.79452	-2.64072
H	7.98957	-1.29703	-1.50563
C	-4.52251	-0.23051	-0.81478
C	-4.73119	-1.52708	-0.3341
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C	-5.96326	-2.15568	-0.48363
H	-3.92309	-2.06052	0.1533
C	-6.79735	-0.19534	-1.62759
H	-5.40718	1.43134	-1.86309
C	-6.99528	-1.48289	-1.14009
H	-7.60276	0.31933	-2.14252
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C	1.36518	-4.00811	2.35448
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C	1.286191	2.179619	0.126445
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C	-3.216114	0.47415	-0.567503
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C	-0.260259	1.432568	-2.29893
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F	-0.280648	6.229728	-0.949092
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C	-4.021709	2.692992	0.380064
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C	3.709741	3.086809	0.227694
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C	4.390969	0.204945	-0.619846
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C	6.519119	0.381981	-1.759736
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S -0.16297 1.53109 0.83427
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C -5.00968 -0.42455 0.33203
C -1.71394 -1.99027 -0.48701
C -0.93152 -0.83656 -0.85328
S 0.74558 -1.34954 -1.03213
C 0.40124 -2.93372 -0.51243
C -0.96815 -3.13631 -0.22579
C -1.39352 0.12977 -1.92735
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F -5.43046 0.3 -0.74639
F -5.63214 -2.49357 1.29709
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F -4.50114 -2.40238 -2.00526
F -4.24161 -3.85935 -0.42382
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H 0.21825 -1.3389 1.78026

TS(³AP-³CF)
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C -3.32437 -0.04298 -1.2787
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C 0.12614 4.36009 0.97155
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TS(AP-P)

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