Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

How to treat C-F stretching vibrations? A vibrational CD study on chiral fluorinated molecules

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Conformational analysis of TFAE

Table S1. Conformational distribution of (S)-TFAE obtained for two different functionals at DFT level with the 6-31+G(2d,p) basis set and using the IEFPCM of chloroform.

		ΔE_{ZPC}[a]	ΔG_{298K}[a]	pop-ΔE[b]	pop-ΔG[b]
B3LYP	TFAE-c1	0.00	0.00	60.1	56.7
	TFAE-c2	0.24	0.16	39.9	43.3
M06-2X	TFAE-c1	0.00	0.00	53.0	50.7
	TFAE-c2	0.07	0.02	47.0	49.3

[a] Zero-point corrected electronic energies (ΔE_{ZPC}) and the Gibbs free energies at 298 K (ΔG_{298K}) are given in kcal/mol. [b] Conformer populations were calculated by using either ΔE_{ZPC} or ΔG_{298K} are given in percentage.

Comparison of calculated spectra of TFAE-c1

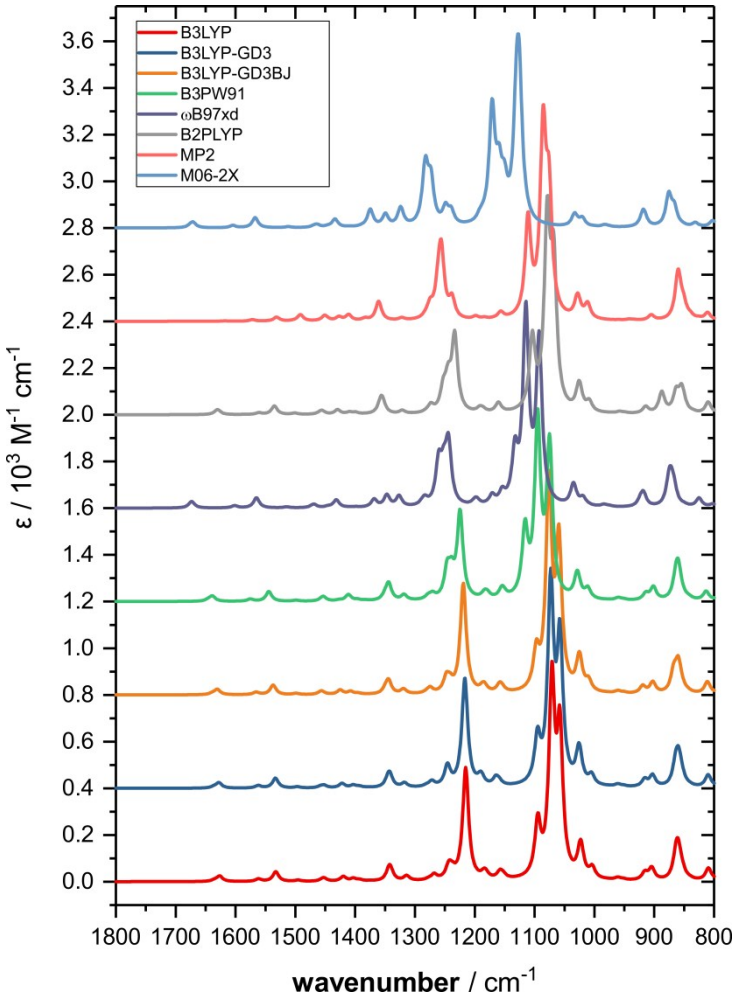

Figure S1. Comparison of the IR spectra of conformer c1 of TFAE obtained with different methods and using the 6-31+g(2d,p) basis set and the IEFPCM of chloroform. The frequency axis was uniformly scaled by a scaling factor of 0.98.

Conformational analysis FTUP

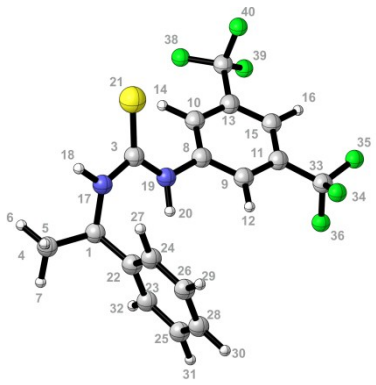

Figure S2. Atom numbering for conformational analysis (Table S2 and S3) and vibrational energy distribution analysis (Tables S5 and S6).

Table S2. Conformational distribution and conformer geometries obtained at the M06-2X/6-311++G(2dp)/ IEFPCM($CHCl_3$) level of theory. The atom numbers are given in Figure S2. Relative zero-point corrected and Gibbs free energy (298 K), ΔE and ΔG, are given in kcal/mol and populations (pop-ΔE and pop-ΔG) in percentage.

conf	ΔE[a]	ΔG[a]	pop-ΔE	pop-ΔG	(8-19-3-17)	(19-3-17-1)	(9-8-19-3)	(3-17-1-22)	(17-1-22-24)	(9-11-33-35)	(10-13-37-39)
anti-C^{α}_c1	0.0	0.03	46.4	38.2	-175.1	-1.0	129.4	63.7	36.3	-172.4	-127.0
anti-C^{α}_c2	0.7	0.00	15.3	40.3	-179.7	-2.4	-132.2	65.1	33.3	131.7	176.7
anti-C^{α}_c3	2.5	3.0	0.6	0.2	158.2	-10.6	-120.7	-47.1	134.8	130.7	177.2
anti-C^{α}_c4	3.6	3.5	0.1	0.1	179.6	-4.3	132.4	165.7	60.4	-171.5	-132.9
anti-C^{α}_c5	3.7	4.7	0.1	0.0	-179.6	12.4	132.1	-62.3	135.9	-173.0	-125.8
anti-C^{α}_c6	3.8	4.3	0.1	0.0	179.6	1.0	-129.7	156.2	60.9	137.5	172.9
anti-C^{Ar}_c1	1.0	2.0	9.2	1.4	28.6	-164.2	-144.9	84.1	63.9	167.8	-111.8
anti-C^{Ar}_c2	1.0	1.3	7.9	4.5	24.7	-168.8	-143.4	80.2	59.5	173.9	137.9
anti-C^{Ar}_c3	1.4	1.1	4.7	6.5	14.4	-173.8	-143.4	146.1	73.5	-178.6	10.1
anti-C^{Ar}_c4	1.4	1.6	4.6	2.8	-6.2	-177.8	137.7	74.3	32.8	117.2	-173.0
anti-C^{Ar}_c5	1.5	2.3	3.8	0.8	15.8	-169.2	-143.7	138.8	68.3	177.0	131.8
anti-C^{Ar}_c6	1.7	2.2	2.7	1.0	-7.9	178.2	137.8	157.9	60.1	-172.7	-141.2
anti-C^{Ar}_c7	5.1	5.3	0.0	0.0	-8.2	-178.5	137.1	-60.8	134.3	70.5	-176.6
anti-C^{Ar}_c8	5.1	5.3	0.0	0.0	-8.6	-178.8	137.1	-60.8	134.2	170.8	-172.2
anti-C^{Ar}_c9	5.3	6.2	0.0	0.0	9.1	-178.9	-137.7	-62.0	139.0	175.8	-120.4
anti-C^{Ar}_c10	5.4	6.5	0.0	0.0	9.4	-178.9	-137.2	-62.0	139.1	166.3	156.2
syn-syn_c1	1.9	2.0	1.8	1.5	178.6	-178.9	133.9	73.3	34.7	-172.3	-126.4
syn-syn_c2	2.0	1.8	1.6	1.9	-179.0	-177.2	-133.1	72.6	34.3	176.6	129.4
syn-syn_c3	2.7	2.8	0.5	0.4	-178.7	-177.3	-133.0	152.5	67.0	131.8	174.1
syn-syn_c4	2.7	2.6	0.5	0.5	179.2	178.8	132.5	153.3	66.2	-135.7	69.1
syn-syn_c5	5.9	6.0	0.0	0.0	177.8	177.2	134.6	-60.1	136.8	-171.0	-125.1
syn-syn_c6	5.9	6.0	0.0	0.0	179.0	-178.7	-131.3	-61.5	137.0	173.6	135.0

[a] References to E(anti-C^{α}_c1)=-1762.68294 hartree and G(anti-C^{α}_c2)=-1762.74196 hartree

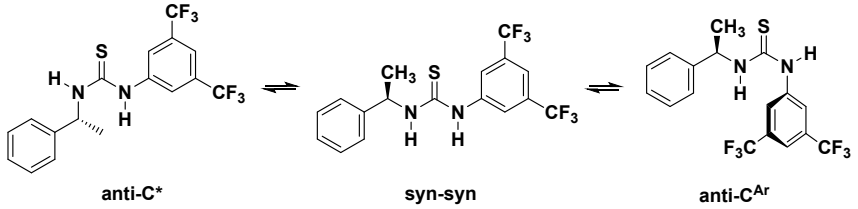

Table S3. Conformational distribution and conformer geometries obtained at the B3LYP/6-311++G(2dp)/ IEFPCM($CHCl_3$) level of theory. The atom numbers are given in Figure S2. Relative zero-point corrected and Gibbs free energy (298 K), ΔE and ΔG, are given in kcal/mol and populations (pop-ΔE and pop-ΔG) in percentage.

conf	ΔE[a]	ΔG[a]	pop-ΔE	pop-ΔG
anti-C^{α}_c1	0.0	1.1	31.5	9.5
anti-C^{α}_c2	0.8	2.1	8.6	1.6
anti-C^{α}_c3	3.3	4.4	0.1	0.0
anti-C^{α}_c4	2.4	3.1	0.6	0.3
anti-C^{α}_c5	4.3	5.8	0.0	0.0
anti-C^{α}_c6	2.3	3.5	0.6	0.1
anti-C^{Ar}_c1	0.9	2.3	6.7	1.1
anti-C^{Ar}_c2	1.0	2.4	5.8	1.0
anti-C^{Ar}_c3	5.8	7.7	0.0	0.0
anti-C^{Ar}_c4	1.0	2.3	6.0	1.2
anti-C^{Ar}_c5	0.6	1.2	11.9	7.3
anti-C^{Ar}_c6	0.7	0.6	9.8	19.2
anti-C^{Ar}_c7	0.6	0.0	10.9	56.3
anti-C^{Ar}_c8	5.8	7.4	0.0	0.0
anti-C^{Ar}_c9	5.8	7.8	0.0	0.0
anti-C^{Ar}_c10	5.8	7.3	0.0	0.0
syn-syn_c1	1.8	2.9	1.6	0.4
syn-syn_c2	1.6	2.8	2.0	0.5
syn-syn_c3	1.6	2.6	2.1	0.7
syn-syn_c4	1.7	2.7	1.7	0.6
syn-syn_c5	6.6	7.9	0.0	0.0
syn-syn_c6	6.6	7.6	0.0	0.0

[a] References to E(anti-C^{α}_c1)= -1763.206526 hartree and G(anti-C^{Ar}_c7)= -1763.268247 hartree

Table S4. Overall conformer distributions of (R)-FTUP obtained for three different functionals at DFT level with the 6-311++G(2d,p) basis set and using the IEFPCM of chloroform.

	population[a]	anti-C*	anti-C^{Ar}	syn-syn
B3LYP	pop-ΔE / %	41.5	51.0	7.5
	pop-ΔG / %	11.6	86.1	2.3
M06-2X	pop-ΔE / %	62.6	33.0	4.4
	pop-ΔG / %	78.9	16.9	4.2

[a] Conformer populations were calculated by using either the zero-point corrected electronic energy (ΔE_{ZPC}) or the Gibbs free energy (ΔG_{298K}).

Vibrational energy distribution analysis for FTUP

Table S5. Vibrational energy distribution analysis for anti-C^{α}_c1 (***B3LYP***/6-311++G(2d,p)/IEFPCM($CHCl_3$)). For better comparison, only the range from 1800-1000 cm^{-1} is shown. Modes highlighted in bold/blue contain >10% contributions by C-F modes. Atom numbers are given in Figure S2. Dipole strength D and rotational strength R are given in units of 10^{-40} esu^2 cm^2 and 10^{-44} esu^2 cm^2.

ν_{scaled}			**Contributing internal coordination and contribution in percentage**				
1632	41.0	14.8	$\sigma(C_{15}=C_{11})$ 28	$\delta(C_{10}-C_{13}-C_{15})$ 15			
1621	118.1	24.8	$\sigma(C_{10}=C_{13})$ 23	$\sigma(C_9=C_8)$ -14	$\sigma(C_{11}=C_9)$ 14	$\delta(H_{12}-C_9=C_8)$ 14	
1614	7.6	-0.5	$\sigma(C_{24}=C_{26})$ 30	$\sigma(C_{28}=C_{25})$ -10			
1597	1.9	1.1	$\sigma(C_{28}=C_{25})$ -24	$\sigma(C_{22}=C_{23})$ 19			
1566	1086.3	157.5	$\delta(H_{20}-N_{19}-C_8)$ 63				
1506	60.7	2.0	$\delta(H_{27}-C_{24}=C_{26})$ 15	$\delta(H_{31}-C_{25}=C_{23})$ -17	$\delta(H_{29}-C_{26}=C_{28})$ 18	$\delta(H_{32}-C_{23}=C_{25})$ 17	
1492	941.5	11.1	$\delta(N_{18}-N_{17}-C_3)$ 55				
1473	255.7	75.9	$\delta(H_5-C_4-H_7)$ 10	$\delta(H_6-C_4-H_5)$ -12			
1471	63.6	-27.1	$\delta(H_5-C_4-H_7)$ 18	$\delta(H_6-C_4-H_5)$ -18			
1468	30.2	4.1	$\delta(H_5-C_4-H_7)$ -17	$\delta(H_7-C_4-H_6)$ 46	$\tau(H_7-C_4-C_1-N_{17})$ 15		
1464	95.4	-68.4	$\delta(H_{30}-C_{28}=C_{25})$ 19	$\delta(H_6-C_4-H_5)$ -15			
1445	128.0	-36.9	$\sigma(C_9=C_8)$ 10	$\delta(N_{18}-N_{17}-C_3)$ 15			
1390	25.9	3.0	$\delta(H_5-C_4-H_7)$ 32	$\delta(H_6-C_4-H_5)$ 26	$\delta(H_7-C_4-H_6)$ 31		
1376	51.8	3.0	$\delta(H_2-C_1=C_{22})$ 36				
1362	78.9	-40.3	$\sigma(N_{17}-C_3)$ 15	**$\sigma(C_{33}-C_{11})$ -12**	**$\sigma(C_{37}-C_{13})$ -11**		
1346	1593.4	113.8					
1336	7.7	35.8	$\sigma(C_9=C_8)$ 11	$\delta(H_{12}-C_9=C_8)$ -13	$\delta(H_{14}-C_{10}=C_8)$ 10	$\delta(H_{16}-C_{15}=C_{13})$ 19	
1329	887.1	-111.2	$\tau(H_2-C_1-C_{22}=C_{23})$ -15				
1322	112.1	-28.7	$\delta(H_2-C_1=C_{22})$ -11	$\tau(H_2-C_1-C_{22}=C_{23})$ -43			
1285	88.9	18.9	$\delta(H_{14}-C_{10}=C_8)$ 12				
1282	82.0	-5.1	$\sigma(C_{22}=C_{23})$ 15				
1245	931.1	-572.3	**$\sigma(C_{33}-C_{11})$ 21**	$\delta(H_{16}-C_{15}=C_{13})$ 13			
1239	2058.1	545.0	$\sigma(N_{19}-C_8)$ -16	**$\sigma(C_{37}-C_{13})$ 15**	$\delta(H_{14}-C_{10}=C_8)$ 15		
1214	463.2	-40.4	$\sigma(C_1-C_{22})$ 16				
1185	415.1	-42.5	$\sigma(N_{19}-C_3)$ 10	$\sigma(C_1-C_{22})$ -13			
1183	32.8	1.6	$\delta(H_{27}-C_{24}=C_{26})$ 21	$\delta(H_{31}-C_{25}=C_{23})$ 12	$\delta(H_{29}-C_{26}=C_{28})$ -12	$\delta(H_{32}-C_{23}=C_{25})$ 24	
1164	0.6	0.1	$\sigma(C_{26}=C_{28})$ -10	$\delta(H_{31}-C_{25}=C_{23})$ -18	$\delta(H_{29}-C_{26}=C_{28})$ -18	$\delta(H_{30}-C_{28}=C_{25})$ 36	
1132	614.4	-17.0	**$\sigma(F_{35}-C_{33})$ -14**				
1122	869.3	-14.1	$\sigma(C_{13}=C_{15})$ 11	**$\sigma(F_{35}-C_{33})$ -10**	**$\sigma(F_{34}-C_{33})$ 10**	$\delta(H_{16}-C_{15}=C_{13})$ 11	
1116	1056.1	215.6					
1095	39.2	-119.7	**$\sigma(C_{10}=C_{13})$ 10**	**$\sigma(F_{35}-C_{33})$ 18**	**$\sigma(F_{39}-C_{37})$ -17**		
1087	84.6	-37.4	$\sigma(C_{23}=C_{25})$ 11	$\tau(H_5-C_4-C_1-N_{17})$ 13			
1079	161.4	62.0	**σ ($F_{38}-C_{37}$) 12**	**σ ($F_{34}-C_{33}$) 13**			
1077	116.4	-16.2	**$\sigma(F_{34}-C_{33})$ 12**	σ (C_4-C_1) 10			
1064	1803.4	10.3	**σ ($F_{39}-C_{37}$) -19**	**$\sigma(F_{40}-C_{37})$ 46**	**o($F_{39}-C_{13}-F_{38}-C_{37}$) -11**		
1059	596.0	-90.9	**σ ($F_{34}-C_{33}$) -17**	**$\sigma(F_{36}-C_{33})$ 48**	**o($F_{36}-C_{11}-F_{35}-C_{33}$) 13**		
1032	32.5	0.8	$\sigma(C_{26}=C_{28})$ 19	$\sigma(C_{28}=C_{25})$ 18	$\delta(C_{24}=C_{26}=C_{28})$ -15	$\delta(H_{29}-C_{26}=C_{28})$ 11	$\delta(C_{23}=C_{25}=C_{28})$ -11
1006	19.6	5.9	$\delta(C_{24}=C_{26}=C_{28})$ 23	$\delta(C_{26}=C_{28}=C_{25})$ -13	$\delta(C_{22}=C_{23}=C_{25})$ -10		

Table S6. Vibrational energy distribution analysis for anti-C^{α}_c1 (***M06-2X***/6-311++G(2d,p)/ IEFPCM($CHCl_3$)). For better comparison, only the range from 1800-1000 cm^{-1} is shown. Modes highlighted in bold/blue contain >10% contributions by C-F modes. Atom numbers are given in Figure S2. Dipole strength D and rotational strength R are given in units of 10^{-40} esu^2 cm^2 and 10^{-44} esu^2 cm^2.

ν_{scaled}	D	R	Contributing internal coordination and contribution in percentage				
1656	35.5	-1.1	σ(C_{15}=C_{11}) 32	δ(C_{10}-C_{13}-C_{15}) 15			
1644	95.8	17.2	σ(C_{10}=C_{13}) 27	σ(C_9=C_8) -16	σ(C_{11}=C_9) 14	δ(H_{12}-C_9=C_8) 10	
1630	9.5	-0.3	σ(C_{23}=C_{25}) 30	σ(C_{24}=C_{26}) -10			
1613	1.4	-0.1	σ(C_{24}=C_{26}) -25	σ(C_{28}=C_{25}) 21	δ(C_{26}=C_{28}=C_{25}) -10		
1564	1287.1	109.8	δ(H_{20}-N_{19}-C_8) 58				
1503	333.5	14.9	δ(N_{18}-N_{17}-C_3) 12	δ(H_{27}-C_{24}=C_{26}) -11	δ(H_{31}-C_{25}=C_{23}) 13	δ(H_{29}-C_{26}=C_{28}) -15	δ(H_{32}-C_{23}=C_25) -12
1499	894.5	48.4	δ(N_{18}-N_{17}-C_3) 37				
1483	236.4	46.6	σ(C_{13}=C_{15}) 13	δ(H_{12}-C_9=C_8) 10	δ(H_{14}-C_{10}=C_8) 10		
1465	43.8	29.3	δ(H_{30}-C_{28}=C_{25}) 12	δ(H_6-C_4-H_5) 17			
1459	91.6	-27.4	δ(H_6-C4-H_5) -11	δ(H_7-C_4-H_6) 34			
1456	39.4	-41.1	δ(H_5-C_4-H_7) -29	δ(H_7-C_4-H_6) 13	τ(H_7-C_4-C_1-N1$_7$) 10		
1452	155.2	-102.3	δ(N_{18}-N_{17}-C_3) -13	δ(H_6-C_4-H_5) -24			
1396	315.5	5.2	σ(C_{26}=C_{28}) -10	**σ(F_{40}-C_{37}) 17**	**σ(C_{37}-C_{13}) 14**		
1376	25.8	3.3	δ(H_5-C_4-H_7) 32	δ(H_6-C_4-H_5) 25	δ(H_7-C_4-H_6) 27		
1367	836.1	-11.3	σ(C_{26}=C_{28}) -13	δ(H_{20}-N_{19}-C_8) -13	δ(H_2-C_1=C_{22}) -22		
1349	1013.1	27.8	σ(C_{26}=C_{28}) -14	δ(H_2-C_1=C_{22}) 27			
1321	297.1	-81.5	τ(H_2-C_1-C_{22}=C_{23}) -61				
1317	10.6	1.5	σ(C_9=C_8) 17	σ(C_{13}=C_{15}) -11	δ(H_{12}-C_9=C_8) -15	δ(H_{14}-C_{10}=C_8) 11	δ(H_{16}-C_{15}=C_{13}) 18
1312	67.7	-85.3	σ(C_{23}=C_{25}) 10	δ(H_{27}-C_{24}=C_{26}) -21	δ(H_2-C_1=C_{22}) 13	δ(H_{32}-C_{23}=C_{25}) 17	
1277	1822.8	-213.7	**σ(F_{40}-C_{37}) -15**	**σ(C_{37}-C_{13}) 16**	δ(H_{16}-C_{15}=C_{13}) -14		
1272	429.6	104.3	σ(C_{28}=C_{25}) -17	σ(N_{17}-C_3) 12	σ(C_{22}=C_{23}) 10		
1264	92.3	66.0	δ(H_{14}-C_{10}=C_8) 22	δ(H_{16}-C_{15}=C_{13}) 13			
1257	920.9	163.5	σ(C_{26}=C_{28}) -10	σ(N_{19}-C_3) -10	σ(N_{19}-C_8) 20		
1225	264.0	-111.4	σ(N_{17}-C_1) -13				
1192	471.5	-239.2	σ(N_{19}-C_3) -11	σ(N_{17}-C_1) 15			
1184	1472.7	35.7	**σ(F_{35}-C_{33}) 26**	**σ(F_{38}-C_{37}) -15**	**σ(F_{34}-C_{33}) -11**		
1176	518.3	178.0	**σ(F_{35}-C_{33}) 16**	**σ(F_{38}-C_{37}) 23**			
1171	14.0	-4.8	δ(H_{27}-C_{24}=C_{26}) 23	δ(H_{31}-C_{25}=C_{23}) 17	δ(H_{29}-C_{26}=C_{28}) -18	δ(H_{32}-C_{23}=C_{25}) 21	
1146	6.1	-1.3	σ(C_{24}=C_{26}) 10	σ(C_{22}=C_{23}) -11	δ(H_{31}-C_{25}=C_{23}) -17	δ(H_{29}-C_{26}=C_{28}) -15	δ(H_{30}-C_{28}=C_{25}) 38
1142	1966.6	73.0	σ(C_{33}-C_{11}) -30	**σ(F_{36}-C_{33}) 36**			
1140	243.0	-28.4	**σ(F_{34}-C_{33}) -29**	**σ(F_{39}-C_{37}) 36**			
1129	116.1	51.4	σ(C_1-C_{22}) 19	τ(H_6-C_4-C_1-N_{17}) 10			
1109	101.8	-9.0	σ(C_{10}=C_{13}) 13	σ(C_{11}=C_9) -10	σ(C_{13}=C_{15}) 13	δ(H_{14}-C_{10}=C_8) -10	δ(H_{16}-C_{15}=C_{13}) 24
1103	49.0	24.3	δ(H_{12}-C_9=C_8) 16	δ(H_{14}-C_{10}=C_8) 12			
1094	130.0	-63.4	σ(C_4-C_1) 31	τ(H_7-C_4-C_1-N_{17}) -11			
1080	20.2	-30.5	σ(C_{23}=C_{25}) -12	σ(N_{17}-C_3) 20	δ(H_{27}-C_{24}=C_{26}) -14	δ(H_{30}-C_{28}=C_{25}) 11	
1033	14.2	0.0	σ(C_{24}=C26) 21	σ(C_{22}=C_{23}) 22	δ(H_{29}-C_{26}=C_{28}) 10		
1010	74.2	15.8	σ(C_1-C_{22}) -12	τ(H_5-C_4-C_1-N_{17}) -20	τ(H_7-C_4-C_1-N_{17}) 11		
1006	0.3	-0.2	τ(H_{31}-C_{25}=C_{28}=C_{26}) -15	τ(H_{29}-C_{26}=C_{28}=C_{25}) 25	τ(H_{30}-C_{28}=C_{26}=C_{24}) 32	τ(C_{24}=C_{26}=C_{28}=C_{25}) -14	

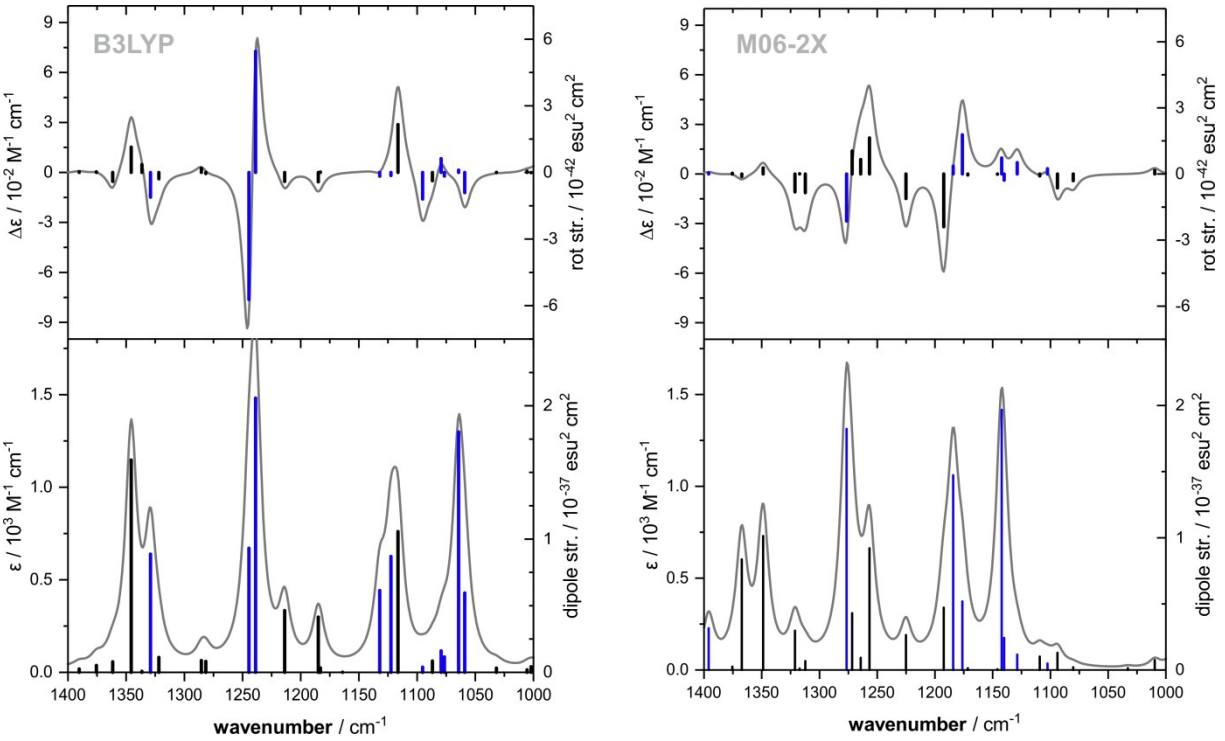

Figure S3. Strick spectra of the lowest energy conformer of FTUP (anti-C^{α}_c1) calculated with the B3LYP and M06-2X functional combined with the 6-311++G(2d,p) basis set and the IEFPCM of chloroform.

Cartesian coordinates of selected structures

TFAE-c1 (M06-2X)

```
0 1
 C                  2.19860200    3.45743800   -0.19935700
 C                  0.84050700    3.46053700   -0.26512300
 C                  0.09159200    2.25582800   -0.07937100
 C                  0.77125700    1.02011700    0.19950600
 C                  2.20664500    1.06897800    0.25212000
 C                  2.88442000    2.23558200    0.05661000
 C                 -1.29617000    2.27686600   -0.17483500
 C                  0.00974500   -0.15436500    0.38916200
 C                 -1.39563400   -0.12905600    0.24171000
 C                 -2.05279000    1.11846500   -0.03371700
 C                 -3.47630600    1.16720300   -0.16328600
 H                 -3.93641600    2.12997500   -0.36288100
 C                 -4.23087200    0.04174000   -0.04652700
 C                 -3.59092400   -1.20586000    0.20087800
 C                 -2.23682500   -1.29016500    0.33746200
 H                 -1.80011400    3.21846900   -0.37610900
 H                  2.76157900    4.37240700   -0.34497100
 H                  0.29201100    4.37523000   -0.46712700
 H                  2.76229200    0.16521900    0.44596900
 H                  3.96829100    2.23354700    0.09569900
 H                 -5.30912700    0.08423000   -0.14837000
 H                 -4.19052500   -2.10646200    0.27408600
 H                 -1.80872500   -2.27101600    0.49291600
 C                  0.66612000   -1.47089300    0.76756200
 H                 -0.08631100   -2.13017100    1.20395900
 C                  1.18349600   -2.22970100   -0.45394000
 F                  0.18475000   -2.51599900   -1.29808300
 F                  2.11520300   -1.56561500   -1.14073400
 F                  1.73323800   -3.39736100   -0.07477400
 O                  1.71426000   -1.29457000    1.69023200
 H                  1.89706200   -2.14037500    2.11417800
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FTUP: anti-C$^{\alpha}$_c1 (M06-2X)

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0 1
 C                  3.57252400   -1.49882700   -0.77167200
 H                  3.12514900   -1.53306400   -1.77085400
 C                  1.39189400   -1.98266400    0.37583000
 C                  4.91289100   -2.22608100   -0.81377200
 H                  5.37705900   -2.21326400    0.17448300
 H                  4.77925800   -3.25968800   -1.13512300
 H                  5.58057000   -1.72361300   -1.51177300
 C                 -0.43917300   -0.42091300   -0.20318900
 C                 -0.59103600    0.94461900   -0.02571100
 C                 -1.56362600   -1.23727800   -0.32485800
 C                 -1.86652300    1.49497700    0.03911200
 H                  0.28448000    1.57747000    0.07241700
 C                 -2.81913600   -0.66893100   -0.24123700
 H                 -1.44542100   -2.29814500   -0.48605400
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C	-2.99034600	0.70014600	-0.05803500
H	-3.98111800	1.13110000	0.00048100
N	2.69443900	-2.21881500	0.14725900
H	3.07999200	-2.98835400	0.67478200
N	0.86710600	-0.93870600	-0.32692200
H	1.52978500	-0.28626800	-0.72743000
S	0.52198800	-2.92583600	1.46555100
C	3.75683400	-0.04024100	-0.38083100
C	3.87299200	0.92668800	-1.37550800
C	3.82421400	0.34475600	0.95583200
C	4.06165200	2.26276300	-1.04101400
C	4.01113700	1.67896900	1.29075000
H	3.71465900	-0.40030600	1.73592800
C	4.13020100	2.64072500	0.29339100
H	4.05761600	1.96979800	2.33259700
H	4.26977500	3.68140300	0.55672700
H	4.14743200	3.00695100	-1.82265200
H	3.81102900	0.63286000	-2.41829200
C	-1.98711200	2.98079700	0.20694500
F	-1.25399900	3.42357400	1.23757900
F	-3.24687300	3.36823600	0.41749100
F	-1.54808900	3.63583000	-0.87954600
C	-4.04900700	-1.52256600	-0.34863600
F	-3.76640900	-2.78946400	-0.65818400
F	-4.88747400	-1.05993300	-1.28803900
F	-4.73973000	-1.53851800	0.80061000