

Electronic Supplementary Information

Structural implications on the excitation dynamics of fluorescent 3*H*-indolium cations

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Synthesis

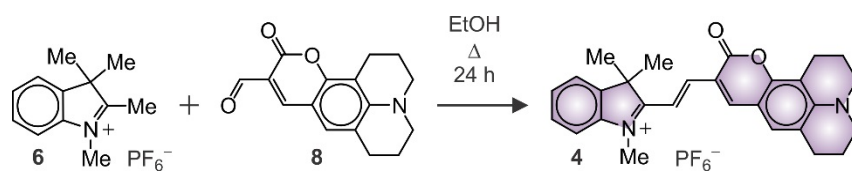


Fig. S1. Synthesis of the hexafluorophosphate salt of **4**.

Crystallographic data

Table S1. Crystallographic data.

	3•PF₆	3•I
<i>Empirical Formula</i>	[C ₂₆ H ₂₉ N ₂ O ₂][PF ₆]•CH ₂ Cl ₂	[C ₂₆ H ₂₉ N ₂ O ₂][I]
<i>Formula Weight</i>	631.41	528.41
<i>Crystal System</i>	Monoclinic	Monoclinic
<i>Lattice Parameters:</i>		
<i>a</i> (Å)	8.4113(6)	19.3336(15)
<i>b</i> (Å)	15.7520(12)	23.1519(18)
<i>c</i> (Å)	21.6939(16)	14.0857(12)
<i>α</i> (°)	90	90
<i>β</i> (°)	95.386(1)	130.241(1)
<i>γ</i> (°)	90	90
<i>V</i> (Å ³)	2861.6(4)	4812.7(7)
<i>Space Group</i>	<i>P2₁/c</i> (# 14)	<i>C2/c</i> (# 14)
<i>Z</i> Value	4	8
<i>ρ_{calc}</i> (g cm ⁻³)	1.466	1.459
<i>μ</i> (Mo Kα) (mm ⁻¹)	0.351	1.355
<i>T</i> (K)	100	296
<i>2θ_{max}</i> (°)	50.0	54.0
<i>No. Obs.</i> (<i>I</i> > 2σ(<i>I</i>))	4014	3451
<i>No. Parameters</i>	366	286
<i>Goodness of Fit</i>	1.034	1.010
<i>Max. Shift in Cycle</i>	0.000	0.001
<i>Residuals*:</i> R1; wR2	0.0802; 0.2262	0.0390; 0.0765
<i>Absorption Correction,</i> <i>Max/min</i>	Multi-Scan, 0.7457/0.6534	Multi-Scan, 0.7457/0.6125
<i>Largest Peak in Final Diff. Map</i> (e ⁻ Å ⁻³)	3.776	0.594

$$* R1 = \sum_{hkl} (| |F_{obs}| - |F_{calc}| |) / \sum_{hkl} |F_{obs}|; wR2 = [\sum_{hkl} w(|F_{obs}| - |F_{calc}|)^2 / \sum_{hkl} wF_{obs}^2]^{1/2}$$

$$w = 1/\sigma^2(F_{obs}); GOF = [\sum_{hkl} w(|F_{obs}| - |F_{calc}|)^2 / (n_{data} - n_{var})]^{1/2}.$$

Computational data

Table S2. Calculated free-energy barriers for the conformational and configurational interconversions of **3** [a].

<i>Process</i>	ΔG^\ddagger (kcal mol ⁻¹)
<i>ttc</i> → <i>ttt</i>	12.50
<i>ttt</i> → <i>ctt</i>	10.07
<i>ctt</i> → <i>ctc</i>	12.08
<i>ctc</i> → <i>ctt</i>	11.78
<i>ctt</i> → <i>ttt</i>	7.51
<i>ttt</i> → <i>ttc</i>	13.60
<i>ttc</i> → <i>tcc</i>	25.38
<i>tcc</i> → <i>ttc</i>	17.81
<i>ttt</i> → <i>tct</i>	30.71
<i>tct</i> → <i>ttt</i>	21.18
<i>ctt</i> → <i>cct</i>	28.72
<i>cct</i> → <i>ctt</i>	21.76
<i>ctc</i> → <i>ccc</i>	25.38
<i>ccc</i> → <i>ctc</i>	18.02

[a] The free-energy barriers were computed with the restricted B3LYP functional, the 6-311+G(d,p) basis set and the IEFPCM solvation model for MeCN at 298 K.

Table S3. Calculated vertical energy (ΔE), wavelength (λ), oscillator strength (f) and main orbital pair with its contribution for electronic transitions from the ground state of the four conformational isomers of **3** with a *trans* configuration for their central [C=C] bond to the corresponding first singlet excited state [a].

<i>Isomer</i>	ΔE (eV)	λ_{Ab} (nm)	f	<i>Main Orbital Pair</i>	<i>Contribution</i> (%)
<i>ctt</i>	2.42	512	1.7673	[HOMO] → [LUMO]	99
<i>ttt</i>	2.40	516	1.8522	[HOMO] → [LUMO]	99
<i>ctc</i>	2.31	536	1.6971	[HOMO] → [LUMO]	99
<i>ttc</i>	2.31	536	1.6969	[HOMO] → [LUMO]	99

[a] The photophysical parameters were computed with the restricted B3LYP functional, the 6-311+G(d,p) basis set and the IEFPCM solvation model for MeCN.

Coordinates of the optimized geometry of ctt

N	4.176876000	-1.044568000	-0.272775000
C	5.579615000	-0.930525000	-0.058250000
C	6.534949000	-1.938746000	-0.058470000
H	6.282100000	-2.978478000	-0.218829000
C	7.858505000	-1.555821000	0.173070000
H	8.633277000	-2.312932000	0.183444000
C	8.193815000	-0.218137000	0.394288000
H	9.227966000	0.051834000	0.571804000
C	7.209820000	0.777003000	0.393657000
H	7.480107000	1.811812000	0.568332000
C	5.892329000	0.408203000	0.168251000
C	4.619932000	1.225010000	0.111727000
C	3.573939000	0.138659000	-0.147396000
C	3.562680000	-2.313850000	-0.662600000
H	2.711779000	-2.118569000	-1.311556000
H	3.242814000	-2.876460000	0.216250000
C	4.647361000	2.242391000	-1.056036000
H	5.452080000	2.960148000	-0.884188000
H	3.708105000	2.795519000	-1.115125000
H	4.824699000	1.746416000	-2.012160000
C	4.334985000	1.945765000	1.449982000
H	5.128139000	2.669938000	1.646156000
H	4.299074000	1.238559000	2.280886000
H	3.385505000	2.482550000	1.405647000
C	2.192797000	0.443305000	-0.233895000
C	1.142833000	-0.417462000	-0.033906000
H	1.352046000	-1.445142000	0.237455000
C	-5.338867000	-0.307636000	0.130414000
C	-4.366897000	0.681763000	-0.183386000
C	-3.029143000	0.370603000	-0.131994000
C	-2.550385000	-0.913734000	0.226148000
C	-3.527212000	-1.895503000	0.541680000
C	-4.863808000	-1.613649000	0.499465000
H	-4.644284000	1.690485000	-0.447841000
C	-1.170157000	-1.124686000	0.243046000
H	-3.196490000	-2.891065000	0.815149000
H	-5.566410000	-2.399112000	0.732205000
C	-0.255087000	-0.121513000	-0.070674000
C	-0.762832000	1.201399000	-0.429246000
H	-0.794314000	-2.107025000	0.511642000
H	1.964941000	1.487694000	-0.392941000
O	-2.141161000	1.364628000	-0.438161000
O	-0.110489000	2.179610000	-0.724220000
N	-6.664073000	-0.032335000	0.081362000
C	-7.689801000	-1.008210000	0.486341000
H	-8.539189000	-0.433731000	0.860121000
H	-7.323219000	-1.589100000	1.332714000
C	-8.141259000	-1.923993000	-0.654147000
H	-8.543405000	-1.342942000	-1.487574000
H	-7.315374000	-2.532374000	-1.029078000
H	-8.927107000	-2.595237000	-0.298432000
C	-7.176762000	1.266338000	-0.384203000
H	-6.542851000	1.635241000	-1.191263000

H	-8.15527000	1.07792500	-0.82952800
C	-7.30370200	2.30602500	0.73260200
H	-7.72033700	3.23164700	0.32746700
H	-7.96952700	1.95193800	1.52330100
H	-6.33379100	2.53480000	1.17945500
H	4.29662900	-2.89791300	-1.21336500

Coordinates of the optimized geometry of ttt

N	4.52259200	1.20011800	-0.09979600
C	5.82127400	0.63175400	-0.06709400
C	7.05457200	1.26807700	-0.14259700
H	7.15084800	2.34068600	-0.24399600
C	8.19148400	0.45904100	-0.08429000
H	9.17031900	0.91983500	-0.14073500
C	8.08465800	-0.92769300	0.04408800
H	8.98235800	-1.53270300	0.08689000
C	6.83058300	-1.54405300	0.11654800
H	6.75746100	-2.62105000	0.21412600
C	5.69528400	-0.75034000	0.05893900
C	4.22410700	-1.11831500	0.10889500
C	3.56999500	0.26354500	-0.01472200
C	4.27440800	2.63877400	-0.22646300
H	5.21825200	3.16933400	-0.15459000
H	3.62112900	2.97564900	0.57783100
C	3.88569600	-1.79005000	1.46342000
H	4.47859700	-2.70076000	1.56647200
H	2.83245500	-2.06393200	1.52888700
H	4.12427400	-1.12951500	2.29922400
C	3.85878900	-2.03380400	-1.08556300
H	4.44539400	-2.95243800	-1.02376300
H	4.08368100	-1.54717500	-2.03663400
H	2.80353900	-2.30691300	-1.07859500
C	2.20158800	0.61456800	-0.05248700
C	1.16141600	-0.27770200	0.04260800
H	1.38823800	-1.33030000	0.15925800
C	-5.32085800	-0.29208100	0.03634900
C	-4.36017600	0.75005700	-0.08309700
C	-3.01889400	0.45380000	-0.04976500
C	-2.52506000	-0.86577600	0.10266900
C	-3.49093800	-1.90107700	0.22205400
C	-4.83064400	-1.63527200	0.19185600
H	-4.65002200	1.78482100	-0.18225600
C	-1.14336900	-1.05748100	0.12627600
H	-3.14741800	-2.92323200	0.33289700
H	-5.52455700	-2.45809500	0.27046300
C	-0.23800500	-0.00234800	0.00960400
C	-0.76218900	1.35474900	-0.14223400
H	-0.75756500	-2.06553500	0.24076400
H	1.95785700	1.65982500	-0.16741100
O	-2.14253200	1.49735600	-0.16254200
O	-0.12179400	2.37769700	-0.25364300
N	-6.64887600	-0.03217300	0.00270400
C	-7.66367800	-1.07686900	0.22088700
H	-8.53211100	-0.58315400	0.66028200
H	-7.30359300	-1.77934700	0.97282000

C	-8.073168000	-1.806168000	-1.061329000
H	-8.470661000	-1.106859000	-1.800811000
H	-7.228428000	-2.333641000	-1.509736000
H	-8.852114000	-2.538447000	-0.834230000
C	-7.175411000	1.319857000	-0.244761000
H	-6.533477000	1.828941000	-0.964420000
H	-8.142874000	1.197144000	-0.734719000
C	-7.339396000	2.151942000	1.029944000
H	-7.759424000	3.129155000	0.778724000
H	-8.017626000	1.662317000	1.732921000
H	-6.382772000	2.310201000	1.532384000
H	3.814442000	2.856332000	-1.191346000

*Coordinates of the optimized geometry of **ctc***

N	-4.289072000	0.915088000	-0.223517000
C	-5.655748000	0.543931000	-0.080331000
C	-6.776024000	1.365292000	-0.070501000
H	-6.708787000	2.441044000	-0.163906000
C	-8.017384000	0.742108000	0.080092000
H	-8.914351000	1.349430000	0.095364000
C	-8.116651000	-0.644429000	0.215344000
H	-9.091533000	-1.102459000	0.332166000
C	-6.971156000	-1.448307000	0.206687000
H	-7.057558000	-2.523333000	0.314847000
C	-5.733856000	-0.839988000	0.060700000
C	-4.336551000	-1.417820000	0.017009000
C	-3.489509000	-0.150923000	-0.131806000
C	-3.889848000	2.294443000	-0.499362000
H	-3.046501000	2.296296000	-1.187521000
H	-3.621220000	2.812727000	0.422902000
C	-4.146705000	-2.341690000	-1.212209000
H	-4.826530000	-3.191638000	-1.127318000
H	-3.126891000	-2.728516000	-1.260134000
H	-4.367111000	-1.814995000	-2.142665000
C	-3.982296000	-2.168247000	1.321452000
H	-4.644592000	-3.028946000	1.433349000
H	-4.103661000	-1.523860000	2.194231000
H	-2.953220000	-2.531790000	1.295409000
C	-2.077013000	-0.206291000	-0.159166000
C	-1.185796000	0.820156000	0.037632000
H	-1.549579000	1.814315000	0.255754000
C	5.205129000	-0.365394000	-0.077455000
C	4.421012000	0.792778000	0.185397000
C	3.050949000	0.722863000	0.125220000
C	2.353514000	-0.470483000	-0.193534000
C	3.144523000	-1.621093000	-0.459742000
C	4.508750000	-1.579915000	-0.406956000
H	4.870865000	1.745512000	0.418639000
C	0.958685000	-0.441997000	-0.223042000
H	2.644014000	-2.551371000	-0.702726000
H	5.062937000	-2.485136000	-0.601629000
C	0.238303000	0.718876000	0.044814000
C	0.970232000	1.947638000	0.358103000
H	0.433561000	-1.359068000	-0.465935000
H	-1.689535000	-1.210733000	-0.279134000

O	2.353505000	1.871647000	0.381162000
O	0.485644000	3.031905000	0.600567000
N	6.556166000	-0.327798000	-0.016998000
C	7.395528000	-1.490442000	-0.354367000
H	8.340873000	-1.095733000	-0.730567000
H	6.944003000	-2.034864000	-1.183700000
C	7.654291000	-2.417415000	0.836121000
H	8.136887000	-1.878714000	1.655183000
H	6.726485000	-2.852870000	1.213624000
H	8.315208000	-3.232257000	0.530077000
C	7.287304000	0.880350000	0.399319000
H	6.728790000	1.384638000	1.188605000
H	8.219404000	0.542986000	0.855444000
C	7.590147000	1.836596000	-0.757358000
H	8.157025000	2.693557000	-0.384994000
H	8.188095000	1.343394000	-1.527549000
H	6.674356000	2.208624000	-1.221649000
H	-4.723259000	2.810732000	-0.968770000

Coordinates of the optimized geometry of ttc

N	4.266975000	1.381746000	-0.184218000
C	5.640106000	1.036121000	-0.110069000
C	6.753519000	1.864597000	-0.186872000
H	6.674654000	2.935694000	-0.316420000
C	8.006435000	1.256012000	-0.084747000
H	8.897220000	1.870107000	-0.139647000
C	8.126033000	-0.124905000	0.087752000
H	9.109789000	-0.572192000	0.164572000
C	6.988899000	-0.936611000	0.163793000
H	7.091293000	-2.007154000	0.298620000
C	5.740021000	-0.342806000	0.064449000
C	4.348927000	-0.946763000	0.110579000
C	3.478858000	0.306577000	-0.051973000
C	3.791606000	2.754748000	-0.371459000
H	4.638268000	3.394628000	-0.597696000
H	3.306091000	3.113462000	0.537270000
C	4.107684000	-1.640623000	1.473344000
H	4.834425000	-2.445739000	1.597465000
H	3.109902000	-2.075252000	1.534834000
H	4.231102000	-0.937486000	2.299216000
C	4.154906000	-1.931904000	-1.069581000
H	4.890996000	-2.733811000	-0.987423000
H	4.300709000	-1.429833000	-2.027960000
H	3.162199000	-2.382326000	-1.062337000
C	2.072343000	0.420649000	-0.064163000
C	1.198966000	-0.634573000	0.038390000
H	1.589687000	-1.638782000	0.128639000
C	-5.217244000	0.394714000	-0.030830000
C	-4.405641000	-0.771269000	0.058048000
C	-3.037482000	-0.658050000	0.049462000
C	-2.367971000	0.589094000	-0.049057000
C	-3.186307000	1.748337000	-0.137707000
C	-4.549303000	1.664968000	-0.129492000
H	-4.832530000	-1.760681000	0.116783000
C	-0.973277000	0.600650000	-0.052823000

H	-2.707641000	2.718393000	-0.207056000
H	-5.124670000	2.576361000	-0.182085000
C	-0.224982000	-0.571135000	0.036158000
C	-0.928091000	-1.852025000	0.137685000
H	-0.469854000	1.558311000	-0.126820000
H	1.673468000	1.422076000	-0.160076000
O	-2.312955000	-1.815186000	0.135110000
O	-0.417972000	-2.947978000	0.223348000
N	-6.567234000	0.313278000	-0.020164000
C	-7.432638000	1.492795000	-0.194085000
H	-8.349206000	1.141557000	-0.671160000
H	-6.969420000	2.180992000	-0.900987000
C	-7.766543000	2.198168000	1.122514000
H	-8.267260000	1.518020000	1.815702000
H	-6.867737000	2.582042000	1.609860000
H	-8.437091000	3.039160000	0.928781000
C	-7.273900000	-0.964933000	0.167286000
H	-6.717629000	-1.583788000	0.871851000
H	-8.223259000	-0.731605000	0.652285000
C	-7.527313000	-1.715264000	-1.142865000
H	-8.081440000	-2.634616000	-0.937755000
H	-8.119049000	-1.109301000	-1.833113000
H	-6.591893000	-1.983200000	-1.638697000
H	3.092446000	2.795694000	-1.206068000

Coordinates of the optimized geometry of cct

N	3.122654000	-0.062172000	-0.973045000
C	4.063059000	0.994291000	-0.805690000
C	4.123949000	2.203427000	-1.484299000
H	3.406169000	2.476283000	-2.246766000
C	5.159703000	3.071157000	-1.129679000
H	5.243521000	4.027907000	-1.630809000
C	6.083065000	2.724003000	-0.140058000
H	6.876307000	3.416286000	0.115771000
C	5.996956000	1.496600000	0.526647000
H	6.719435000	1.238668000	1.292102000
C	4.969843000	0.628893000	0.186260000
C	4.602530000	-0.745950000	0.702282000
C	3.349170000	-1.044147000	-0.118507000
C	2.118217000	-0.036081000	-2.034301000
H	1.734983000	-1.040027000	-2.189858000
H	2.592772000	0.318122000	-2.948679000
C	4.270393000	-0.739559000	2.212277000
H	5.163424000	-0.462613000	2.775880000
H	3.951736000	-1.732241000	2.536472000
H	3.475995000	-0.027176000	2.436879000
C	5.713324000	-1.782205000	0.395906000
H	6.623785000	-1.491256000	0.922967000
H	5.933078000	-1.829053000	-0.672314000
H	5.425786000	-2.776394000	0.743416000
C	2.622606000	-2.273376000	-0.015079000
C	1.287318000	-2.551413000	-0.045863000
H	1.061445000	-3.614342000	-0.080010000
C	-4.679513000	0.016870000	0.023710000
C	-3.408146000	0.531468000	0.394238000

C	-2.287658000	-0.259208000	0.280878000
C	-2.329888000	-1.591422000	-0.192579000
C	-3.604088000	-2.101570000	-0.552359000
C	-4.734363000	-1.337378000	-0.453446000
H	-3.288336000	1.529175000	0.787783000
C	-1.126690000	-2.301208000	-0.281435000
H	-3.673352000	-3.117667000	-0.923709000
H	-5.676916000	-1.765428000	-0.758751000
C	0.101577000	-1.735162000	0.041749000
C	0.120871000	-0.384192000	0.586754000
H	-1.152737000	-3.328047000	-0.632907000
H	3.269718000	-3.131334000	0.141699000
O	-1.093552000	0.283483000	0.667083000
O	1.086930000	0.217313000	1.008991000
N	-5.801241000	0.774044000	0.115583000
C	-7.140365000	0.239233000	-0.179750000
H	-7.846130000	0.799674000	0.435980000
H	-7.201260000	-0.795152000	0.159464000
C	-7.530661000	0.355772000	-1.655549000
H	-7.509252000	1.397380000	-1.985231000
H	-6.855920000	-0.218515000	-2.294298000
H	-8.545137000	-0.024709000	-1.800097000
C	-5.757619000	2.189436000	0.513403000
H	-4.856518000	2.650429000	0.106855000
H	-6.597947000	2.682778000	0.021517000
C	-5.844768000	2.399959000	2.027544000
H	-5.832212000	3.469588000	2.252315000
H	-6.770699000	1.980260000	2.428360000
H	-5.005267000	1.931894000	2.546218000
H	1.303700000	0.636602000	-1.764932000

Coordinates of the optimized geometry of tct

N	-3.127002000	0.030017000	-0.936864000
C	-4.077718000	1.050167000	-0.646647000
C	-4.152957000	2.329137000	-1.180449000
H	-3.438792000	2.697131000	-1.905489000
C	-5.198295000	3.138190000	-0.728453000
H	-5.292923000	4.145781000	-1.114803000
C	-6.117333000	2.667716000	0.212949000
H	-6.918627000	3.316206000	0.546649000
C	-6.016616000	1.372434000	0.732920000
H	-6.736815000	1.018946000	1.461549000
C	-4.979584000	0.561946000	0.295725000
C	-4.598211000	-0.860481000	0.646800000
C	-3.342549000	-1.047544000	-0.202971000
C	-2.128843000	0.187803000	-1.992667000
H	-1.318561000	0.832583000	-1.652219000
H	-2.612286000	0.640681000	-2.857468000
C	-5.699132000	-1.862993000	0.217148000
H	-6.610891000	-1.648916000	0.777731000
H	-5.400758000	-2.889380000	0.438547000
H	-5.921654000	-1.780377000	-0.848419000
C	-4.265862000	-1.029671000	2.147136000
H	-5.159457000	-0.825113000	2.740239000
H	-3.474901000	-0.344223000	2.453188000

H	-3.941961000	-2.051785000	2.353507000
C	-2.605224000	-2.273565000	-0.243442000
C	-1.268198000	-2.536674000	-0.313508000
H	-1.036403000	-3.587378000	-0.469181000
C	4.682248000	0.052756000	-0.024723000
C	3.412996000	0.511531000	0.419046000
C	2.296367000	-0.270838000	0.233427000
C	2.340458000	-1.539272000	-0.391406000
C	3.612056000	-1.993269000	-0.827419000
C	4.738674000	-1.236321000	-0.657396000
H	3.286841000	1.472514000	0.893581000
C	1.141246000	-2.244793000	-0.542701000
H	3.684089000	-2.964652000	-1.303281000
H	5.684387000	-1.633404000	-0.993512000
C	-0.086571000	-1.727825000	-0.144266000
C	-0.108365000	-0.445365000	0.546615000
H	1.169291000	-3.225972000	-1.006470000
H	-3.244446000	-3.149236000	-0.181249000
O	1.102867000	0.218802000	0.686452000
O	-1.072881000	0.098220000	1.044067000
N	5.801531000	0.799748000	0.146578000
C	7.112100000	0.390690000	-0.383954000
H	7.665793000	1.307410000	-0.595408000
H	6.974564000	-0.106160000	-1.344658000
C	7.912720000	-0.489727000	0.579043000
H	8.088175000	0.025080000	1.526768000
H	7.392511000	-1.426369000	0.790869000
H	8.884047000	-0.729446000	0.138775000
C	5.783682000	2.075669000	0.878367000
H	5.084366000	2.001755000	1.712275000
H	6.772815000	2.199276000	1.322977000
C	5.456902000	3.282314000	-0.005700000
H	5.487281000	4.196557000	0.592585000
H	6.184442000	3.382502000	-0.814850000
H	4.462665000	3.197296000	-0.449482000
H	-1.738328000	-0.787926000	-2.265761000

Coordinates of the optimized geometry of ccc

N	-2.940695000	0.097531000	-0.882344000
C	-3.702538000	-1.106304000	-0.854406000
C	-3.599850000	-2.205414000	-1.696215000
H	-2.874002000	-2.256045000	-2.497228000
C	-4.479643000	-3.263692000	-1.457911000
H	-4.432645000	-4.143031000	-2.088750000
C	-5.413550000	-3.204277000	-0.420179000
H	-6.084107000	-4.039514000	-0.257303000
C	-5.494050000	-2.082740000	0.412570000
H	-6.223986000	-2.048025000	1.212871000
C	-4.622249000	-1.027577000	0.188685000
C	-4.457241000	0.303578000	0.889962000
C	-3.288669000	0.908515000	0.110528000
C	-2.010967000	0.398116000	-1.968643000
H	-1.890794000	1.475110000	-2.048197000
H	-2.428563000	0.008233000	-2.895214000
C	-4.094710000	0.143895000	2.384016000

H	-4.928490000	-0.325418000	2.909779000
H	-3.905776000	1.118057000	2.839085000
H	-3.210284000	-0.482008000	2.515043000
C	-5.723702000	1.183951000	0.732470000
H	-6.565456000	0.679327000	1.209929000
H	-5.969210000	1.346937000	-0.318512000
H	-5.589745000	2.151496000	1.219858000
C	-2.762961000	2.203477000	0.393312000
C	-1.501235000	2.727525000	0.303513000
H	-1.448564000	3.803952000	0.437377000
C	4.107397000	-0.579424000	0.201575000
C	3.744743000	0.759183000	-0.110957000
C	2.434191000	1.159842000	-0.000954000
C	1.395954000	0.292166000	0.414325000
C	1.767470000	-1.038627000	0.737708000
C	3.063185000	-1.465239000	0.636519000
H	4.469562000	1.482801000	-0.451034000
C	0.090319000	0.795573000	0.482553000
H	1.000240000	-1.727356000	1.073057000
H	3.295176000	-2.483995000	0.907089000
C	-0.211307000	2.110743000	0.159561000
C	0.878023000	3.005765000	-0.235225000
H	-0.691771000	0.135958000	0.841226000
H	-3.513120000	2.881881000	0.787709000
O	2.149433000	2.462919000	-0.309656000
O	0.774015000	4.180827000	-0.515804000
N	5.390766000	-1.003811000	0.099095000
C	5.778976000	-2.405138000	0.328358000
H	6.649245000	-2.597235000	-0.301921000
H	4.990649000	-3.063435000	-0.037330000
C	6.115920000	-2.713510000	1.789474000
H	6.934912000	-2.083499000	2.144889000
H	5.254230000	-2.552978000	2.441157000
H	6.426274000	-3.757369000	1.883213000
C	6.489110000	-0.091958000	-0.257385000
H	6.311250000	0.882254000	0.199733000
H	7.392154000	-0.486063000	0.212038000
C	6.703817000	0.042323000	-1.767577000
H	7.547821000	0.709193000	-1.961264000
H	6.927443000	-0.927527000	-2.218634000
H	5.822168000	0.454573000	-2.263024000
H	-1.041287000	-0.066808000	-1.783273000

Coordinates of the optimized geometry of tcc

N	-2.953039000	-0.032604000	-0.877865000
C	-3.722216000	1.156872000	-0.721860000
C	-3.633772000	2.336933000	-1.447527000
H	-2.916670000	2.473736000	-2.246200000
C	-4.515367000	3.360565000	-1.092921000
H	-4.478459000	4.300234000	-1.630536000
C	-5.437711000	3.190426000	-0.057159000
H	-6.109625000	4.001171000	0.197789000
C	-5.504372000	1.988809000	0.656679000
H	-6.224558000	1.868115000	1.457335000
C	-4.630539000	0.966985000	0.316787000

C	-4.450664000	-0.426694000	0.879212000
C	-3.284858000	-0.941182000	0.032992000
C	-2.033393000	-0.216523000	-1.998404000
H	-1.063885000	0.233509000	-1.778361000
H	-2.462793000	0.262011000	-2.876780000
C	-5.712361000	-1.296338000	0.642551000
H	-6.552919000	-0.852266000	1.178806000
H	-5.566929000	-2.309012000	1.023053000
H	-5.967933000	-1.349608000	-0.417246000
C	-4.078180000	-0.412410000	2.379271000
H	-4.912271000	-0.004247000	2.953464000
H	-3.198617000	0.206478000	2.565607000
H	-3.878246000	-1.424394000	2.736812000
C	-2.744584000	-2.251975000	0.181901000
C	-1.478886000	-2.752697000	0.030922000
H	-1.416251000	-3.836467000	0.059563000
C	4.106767000	0.587265000	0.232985000
C	3.752348000	-0.718086000	-0.204981000
C	2.443138000	-1.132893000	-0.141633000
C	1.399009000	-0.313761000	0.350319000
C	1.761900000	0.983218000	0.797001000
C	3.055435000	1.424429000	0.741397000
H	4.487737000	-1.417220000	-0.572418000
C	0.097228000	-0.830288000	0.373723000
H	0.987209000	1.638412000	1.179051000
H	3.274704000	2.427523000	1.073841000
C	-0.194952000	-2.114863000	-0.061853000
C	0.901157000	-2.963712000	-0.533406000
H	-0.688340000	-0.210399000	0.790661000
H	-3.483999000	-2.973798000	0.514761000
O	2.168380000	-2.406789000	-0.561138000
O	0.805866000	-4.110728000	-0.914888000
N	5.387658000	1.026741000	0.174543000
C	5.796423000	2.338371000	0.703379000
H	6.836296000	2.239634000	1.019807000
H	5.226779000	2.559386000	1.606414000
C	5.668184000	3.472350000	-0.316933000
H	6.271715000	3.270637000	-1.205221000
H	4.631779000	3.610943000	-0.632429000
H	6.019066000	4.407913000	0.126137000
C	6.464896000	0.220028000	-0.420478000
H	6.069920000	-0.336632000	-1.271059000
H	7.195563000	0.920092000	-0.829941000
C	7.145559000	-0.718054000	0.580004000
H	7.949939000	-1.266020000	0.082668000
H	7.580802000	-0.156054000	1.409817000
H	6.440935000	-1.443897000	0.991667000
H	-1.908394000	-1.279264000	-2.187418000

*Coordinates of the transition state for **ttc** → **ttt***

N	-4.307727000	0.836248000	-0.968939000
C	-5.673006000	0.478171000	-0.784040000
C	-6.787285000	0.965827000	-1.454880000
H	-6.716294000	1.710540000	-2.236272000
C	-8.023242000	0.441893000	-1.074640000

H	-8.921041000	0.790440000	-1.570078000
C	-8.117844000	-0.523474000	-0.067313000
H	-9.090841000	-0.912414000	0.207777000
C	-6.977382000	-0.995832000	0.589304000
H	-7.065411000	-1.744288000	1.367752000
C	-5.742964000	-0.483617000	0.217470000
C	-4.345668000	-0.778705000	0.721200000
C	-3.512328000	0.155013000	-0.161004000
C	-3.938281000	1.845904000	-1.968636000
H	-4.566587000	2.722638000	-1.818675000
H	-4.107620000	1.437799000	-2.965386000
C	-3.983156000	-2.265311000	0.474012000
H	-4.686437000	-2.894000000	1.022459000
H	-2.977201000	-2.498543000	0.821769000
H	-4.052790000	-2.516785000	-0.585754000
C	-4.225576000	-0.403046000	2.221263000
H	-4.940936000	-1.000590000	2.788804000
H	-4.454791000	0.651632000	2.383509000
H	-3.229013000	-0.607001000	2.611223000
C	-2.080540000	0.309639000	-0.188815000
C	-1.212696000	-0.313040000	0.630099000
H	-1.560858000	-0.988446000	1.403352000
C	5.269441000	-0.241657000	-0.258521000
C	4.372499000	0.593162000	0.453224000
C	3.020478000	0.310502000	0.455478000
C	2.465077000	-0.787117000	-0.228745000
C	3.362574000	-1.613756000	-0.938408000
C	4.712687000	-1.359669000	-0.957687000
H	4.707959000	1.467922000	0.989637000
C	1.061126000	-0.979763000	-0.160583000
H	2.972726000	-2.472569000	-1.473626000
H	5.356311000	-2.034355000	-1.501593000
C	0.255174000	-0.120829000	0.533468000
C	0.831830000	1.003443000	1.245519000
H	0.625546000	-1.827457000	-0.679907000
H	-1.671390000	0.973557000	-0.939102000
O	2.204772000	1.159857000	1.160819000
O	0.226451000	1.820816000	1.913957000
N	6.611284000	0.007570000	-0.276230000
C	7.544556000	-0.781925000	-1.090506000
H	8.369122000	-0.119159000	-1.361910000
H	7.062913000	-1.059196000	-2.029444000
C	8.091885000	-2.020134000	-0.374092000
H	8.610886000	-1.741098000	0.546434000
H	7.292932000	-2.718832000	-0.115512000
H	8.804343000	-2.539705000	-1.020578000
C	7.210938000	1.083338000	0.522556000
H	6.687385000	1.158434000	1.477553000
H	8.230208000	0.773396000	0.762556000
C	7.237723000	2.439022000	-0.190184000
H	7.716694000	3.185763000	0.448870000
H	7.803913000	2.378490000	-1.123138000
H	6.229877000	2.787835000	-0.425848000
H	-2.900403000	2.135651000	-1.860121000

Coordinates of the transition state for ttt → ctt

N	4.359347000	-0.710167000	-0.883042000
C	5.712576000	-0.268342000	-0.728276000
C	6.793701000	-0.513273000	-1.560990000
H	6.708482000	-1.100352000	-2.465827000
C	8.015783000	0.039977000	-1.172867000
H	8.891077000	-0.123328000	-1.789476000
C	8.123049000	0.798660000	-0.003875000
H	9.084040000	1.215406000	0.273070000
C	7.012271000	1.030167000	0.814262000
H	7.111616000	1.621736000	1.716573000
C	5.792631000	0.484298000	0.440207000
C	4.421969000	0.539539000	1.079267000
C	3.603869000	-0.283331000	0.094554000
C	3.936503000	-1.549175000	-2.010112000
H	4.142133000	-1.019945000	-2.940253000
H	2.873200000	-1.749400000	-1.922564000
C	3.869477000	1.983264000	1.165682000
H	4.502686000	2.560173000	1.841825000
H	2.853440000	1.982135000	1.562887000
H	3.871836000	2.474023000	0.190489000
C	4.387881000	-0.134973000	2.473666000
H	5.015281000	0.437541000	3.158848000
H	4.764912000	-1.158420000	2.432273000
H	3.369145000	-0.147189000	2.865152000
C	2.187360000	-0.622146000	0.251325000
C	1.191281000	0.159931000	-0.204819000
H	1.453578000	1.066706000	-0.744027000
C	-5.320116000	0.295651000	-0.198681000
C	-4.375778000	-0.625912000	0.321321000
C	-3.025661000	-0.390765000	0.164484000
C	-2.514768000	0.740170000	-0.505616000
C	-3.462144000	1.655103000	-1.023172000
C	-4.810502000	1.450325000	-0.879092000
H	-4.677660000	-1.528618000	0.830445000
C	-1.116175000	0.877383000	-0.605921000
H	-3.107052000	2.541452000	-1.536996000
H	-5.490574000	2.189426000	-1.274717000
C	-0.240827000	-0.048397000	-0.075775000
C	-0.781396000	-1.213962000	0.607777000
H	-0.715147000	1.746787000	-1.118133000
H	1.975008000	-1.535824000	0.797717000
O	-2.162517000	-1.317372000	0.686171000
O	-0.149689000	-2.116512000	1.122685000
N	-6.659651000	0.096124000	-0.055916000
C	-7.655753000	0.987875000	-0.666860000
H	-8.542411000	0.383006000	-0.866903000
H	-7.295194000	1.321831000	-1.640836000
C	-8.032355000	2.182542000	0.214071000
H	-8.435340000	1.849225000	1.173716000
H	-7.169179000	2.822294000	0.410750000
H	-8.797379000	2.784087000	-0.284041000
C	-7.200279000	-1.028646000	0.719089000
H	-6.558949000	-1.212862000	1.582544000

H	-8.162265000	-0.705626000	1.122118000
C	-7.386918000	-2.306879000	-0.103946000
H	-7.813074000	-3.093666000	0.524155000
H	-8.068118000	-2.135921000	-0.941341000
H	-6.437387000	-2.667570000	-0.505588000
H	4.499012000	-2.482221000	-1.984223000

*Coordinates of the transition state for **ctt** → **ctc***

N	4.305895000	0.805551000	-0.534056000
C	5.668347000	0.380411000	-0.452914000
C	6.773759000	0.917533000	-1.097442000
H	6.701374000	1.759254000	-1.773118000
C	8.003336000	0.308131000	-0.841025000
H	8.894200000	0.690781000	-1.323677000
C	8.099109000	-0.785823000	0.023836000
H	9.066534000	-1.238944000	0.204018000
C	6.966322000	-1.306472000	0.657774000
H	7.053522000	-2.155863000	1.324769000
C	5.738933000	-0.710499000	0.408915000
C	4.350056000	-1.021376000	0.919466000
C	3.526637000	0.032632000	0.191895000
C	3.923782000	1.997507000	-1.300032000
H	2.986297000	2.389130000	-0.916056000
H	3.821578000	1.743913000	-2.355532000
C	4.244482000	-0.819986000	2.453350000
H	4.912985000	-1.528259000	2.945557000
H	3.229307000	-1.013024000	2.804118000
H	4.535863000	0.190577000	2.744679000
C	3.882168000	-2.442713000	0.522463000
H	4.529657000	-3.177432000	1.004091000
H	3.934326000	-2.591035000	-0.557696000
H	2.857255000	-2.619326000	0.853435000
C	2.090076000	0.122331000	0.325466000
C	1.222740000	0.472851000	-0.639208000
H	1.578758000	0.734981000	-1.631438000
C	-5.250903000	-0.337073000	-0.116468000
C	-4.371258000	0.730062000	0.191256000
C	-3.016871000	0.598773000	-0.045410000
C	-2.441901000	-0.565451000	-0.588713000
C	-3.322593000	-1.626028000	-0.892613000
C	-4.674803000	-1.525089000	-0.669614000
H	-4.721062000	1.652334000	0.629533000
C	-1.036330000	-0.591869000	-0.782078000
H	-2.917710000	-2.537595000	-1.318132000
H	-5.305165000	-2.360108000	-0.936307000
C	-0.247633000	0.470483000	-0.438337000
C	-0.845327000	1.672532000	0.111245000
H	-0.585008000	-1.483320000	-1.205977000
H	1.701706000	-0.218076000	1.279575000
O	-2.219137000	1.666926000	0.281339000
O	-0.257247000	2.688649000	0.432636000
N	-6.594356000	-0.237379000	0.103635000
C	-7.508835000	-1.367939000	-0.103060000
H	-8.334640000	-1.241760000	0.600363000
H	-7.010854000	-2.295226000	0.184324000

C	-8.056760000	-1.464358000	-1.530065000
H	-8.595120000	-0.553418000	-1.803806000
H	-7.255566000	-1.617550000	-2.256560000
H	-8.752260000	-2.304619000	-1.605937000
C	-7.214295000	1.008705000	0.570623000
H	-6.702589000	1.859042000	0.116298000
H	-8.232891000	1.026530000	0.177009000
C	-7.248415000	1.146895000	2.095978000
H	-7.743172000	2.081519000	2.373665000
H	-7.803589000	0.322249000	2.550163000
H	-6.242237000	1.154334000	2.520991000
H	4.705877000	2.744078000	-1.178943000

*Coordinates of the transition state for **ttc** → **tcc***

N	3.525109000	0.371569000	-0.868837000
C	4.551427000	-0.578352000	-0.945732000
C	5.039674000	-1.241322000	-2.069518000
H	4.622253000	-1.079926000	-3.055454000
C	6.096034000	-2.142691000	-1.887092000
H	6.491415000	-2.670361000	-2.747892000
C	6.639876000	-2.374402000	-0.624586000
H	7.455960000	-3.077481000	-0.506364000
C	6.128455000	-1.700745000	0.495439000
H	6.551017000	-1.882698000	1.477961000
C	5.083850000	-0.807970000	0.328671000
C	4.348802000	0.056008000	1.340960000
C	3.286149000	0.735627000	0.448845000
C	2.799545000	0.846835000	-2.033651000
H	1.927769000	0.224040000	-2.259587000
H	3.465249000	0.845676000	-2.897177000
C	5.293908000	1.112409000	1.955577000
H	6.090110000	0.620674000	2.520625000
H	4.746398000	1.768807000	2.636990000
H	5.754008000	1.728026000	1.179290000
C	3.702613000	-0.793329000	2.452544000
H	4.474979000	-1.319082000	3.019833000
H	3.018866000	-1.535423000	2.034673000
H	3.144391000	-0.163259000	3.149616000
C	2.313343000	1.532409000	0.939496000
C	1.229323000	2.248034000	0.253032000
H	1.410086000	3.262598000	-0.100195000
C	-4.509120000	-0.641506000	0.122330000
C	-4.039121000	0.641567000	-0.314759000
C	-2.727326000	0.972513000	-0.170806000
C	-1.762623000	0.079002000	0.409837000
C	-2.244362000	-1.207621000	0.831169000
C	-3.545493000	-1.557822000	0.699067000
H	-4.705733000	1.372918000	-0.743952000
C	-0.465159000	0.488243000	0.540152000
H	-1.534811000	-1.904215000	1.261143000
H	-3.858316000	-2.539412000	1.018459000
C	-0.048176000	1.788228000	0.110579000
C	-1.051147000	2.689158000	-0.512102000
H	0.278443000	-0.166930000	0.979227000
H	2.334939000	1.717958000	2.011538000

O	-2.347155000	2.212197000	-0.601463000
O	-0.844711000	3.791475000	-0.942948000
N	-5.793710000	-0.981408000	0.001120000
C	-6.334216000	-2.266172000	0.499720000
H	-7.372343000	-2.075480000	0.773213000
H	-5.819436000	-2.540659000	1.418426000
C	-6.257141000	-3.384175000	-0.540879000
H	-6.794040000	-3.113378000	-1.452554000
H	-5.223150000	-3.614007000	-0.805488000
H	-6.715993000	-4.286872000	-0.131585000
C	-6.793739000	-0.095688000	-0.634987000
H	-6.331216000	0.422835000	-1.473232000
H	-7.557036000	-0.748454000	-1.058898000
C	-7.425001000	0.886955000	0.352835000
H	-8.178997000	1.482538000	-0.166430000
H	-7.914287000	0.359751000	1.174537000
H	-6.680946000	1.566198000	0.773508000
H	2.473320000	1.873958000	-1.877778000

Coordinates of the transition state for $ttt \rightarrow tct$

N	4.606298000	1.131144000	0.457015000
C	5.522999000	0.345075000	-0.245368000
C	6.831348000	0.645094000	-0.621119000
H	7.296898000	1.589414000	-0.368723000
C	7.543583000	-0.321709000	-1.340810000
H	8.563338000	-0.107471000	-1.640946000
C	6.968368000	-1.547498000	-1.673019000
H	7.538663000	-2.282057000	-2.229263000
C	5.650386000	-1.831714000	-1.283284000
H	5.203297000	-2.786122000	-1.540985000
C	4.936343000	-0.885822000	-0.568283000
C	3.509589000	-0.923423000	-0.036219000
C	3.427145000	0.430916000	0.698028000
C	4.883762000	2.438682000	1.014386000
H	5.790491000	2.841902000	0.568912000
H	5.017921000	2.391147000	2.101444000
C	3.296638000	-2.107870000	0.926536000
H	3.457181000	-3.051418000	0.398840000
H	2.276458000	-2.121594000	1.318832000
H	3.990354000	-2.062746000	1.768683000
C	2.504356000	-0.997832000	-1.208009000
H	2.681763000	-1.907819000	-1.786936000
H	2.610676000	-0.140195000	-1.875010000
H	1.476192000	-1.028655000	-0.843208000
C	2.435576000	0.911061000	1.476159000
C	1.175776000	0.261232000	1.843317000
H	1.183448000	-0.324311000	2.764734000
C	-4.964554000	-0.165289000	0.012079000
C	-3.832863000	0.520519000	-0.540170000
C	-2.623740000	0.450170000	0.081350000
C	-2.415521000	-0.304637000	1.284983000
C	-3.556101000	-0.990505000	1.826186000
C	-4.769935000	-0.927408000	1.229690000
H	-3.914083000	1.121385000	-1.432210000
C	-1.167474000	-0.338307000	1.838807000

H	-3.424073000	-1.573608000	2.729583000
H	-5.594918000	-1.470501000	1.662976000
C	-0.055816000	0.357621000	1.256241000
C	-0.303021000	1.183962000	0.045753000
H	-0.993119000	-0.910738000	2.743470000
H	2.578325000	1.865908000	1.979706000
O	-1.591344000	1.145188000	-0.476379000
O	0.482077000	1.887624000	-0.524083000
N	-6.161671000	-0.104220000	-0.575191000
C	-7.372422000	-0.726890000	0.005296000
H	-8.214920000	-0.114742000	-0.317781000
H	-7.332813000	-0.646322000	1.089984000
C	-7.569016000	-2.176021000	-0.442540000
H	-7.640529000	-2.247628000	-1.529954000
H	-6.748104000	-2.813913000	-0.109006000
H	-8.497967000	-2.560363000	-0.015414000
C	-6.384234000	0.600604000	-1.856378000
H	-5.506456000	0.479399000	-2.488888000
H	-7.199813000	0.077967000	-2.356700000
C	-6.738676000	2.076802000	-1.667357000
H	-6.930144000	2.527123000	-2.643807000
H	-7.637865000	2.191739000	-1.058376000
H	-5.926039000	2.627169000	-1.189124000
H	4.062614000	3.125201000	0.792578000

*Coordinates of the transition state for **ctt** → **cct***

N	-3.562405000	0.908823000	0.351507000
C	-4.761882000	1.136571000	-0.332003000
C	-5.235781000	2.323805000	-0.887304000
H	-4.662145000	3.241307000	-0.851366000
C	-6.489206000	2.298829000	-1.511348000
H	-6.875895000	3.211874000	-1.950318000
C	-7.239811000	1.126167000	-1.581459000
H	-8.206499000	1.128999000	-2.071152000
C	-6.741242000	-0.060778000	-1.022136000
H	-7.324623000	-0.973840000	-1.078817000
C	-5.503120000	-0.049799000	-0.403164000
C	-4.729301000	-1.166187000	0.279847000
C	-3.433325000	-0.433524000	0.693061000
C	-2.576655000	1.945893000	0.594469000
H	-2.077648000	1.773265000	1.547470000
H	-3.077297000	2.911688000	0.662042000
C	-4.440831000	-2.329117000	-0.690185000
H	-5.378271000	-2.790058000	-1.012142000
H	-3.835274000	-3.099315000	-0.205988000
H	-3.907564000	-1.979853000	-1.576781000
C	-5.484454000	-1.682926000	1.524189000
H	-6.437675000	-2.128302000	1.227404000
H	-5.689220000	-0.871088000	2.225966000
H	-4.898367000	-2.446459000	2.042500000
C	-2.391661000	-1.052713000	1.281284000
C	-1.118322000	-0.520990000	1.776668000
H	-1.102495000	-0.178699000	2.813436000
C	5.029707000	0.137556000	0.041041000
C	3.874795000	-0.358822000	-0.648578000

C	2.666301000	-0.386429000	-0.022280000
C	2.484681000	0.068197000	1.327559000
C	3.649828000	0.560545000	2.008765000
C	4.861933000	0.594634000	1.406324000
H	3.935535000	-0.735082000	-1.657576000
C	1.238297000	0.011541000	1.883615000
H	3.538888000	0.914861000	3.026438000
H	5.706061000	0.986782000	1.951315000
C	0.103048000	-0.486980000	1.161939000
C	0.310028000	-0.962799000	-0.229739000
H	1.084820000	0.351630000	2.902116000
H	-2.513736000	-2.114140000	1.491590000
O	1.606469000	-0.876038000	-0.726804000
O	-0.513753000	-1.422104000	-0.969082000
N	6.222955000	0.180854000	-0.555736000
C	7.453273000	0.616786000	0.142000000
H	8.277442000	0.076669000	-0.324810000
H	7.416656000	0.284876000	1.177876000
C	7.687073000	2.125068000	0.044470000
H	7.754542000	2.447459000	-0.996796000
H	6.885361000	2.686876000	0.527849000
H	8.628382000	2.374875000	0.538976000
C	6.417597000	-0.200421000	-1.971555000
H	5.546043000	0.106416000	-2.547702000
H	7.254173000	0.395180000	-2.337590000
C	6.711079000	-1.690986000	-2.150477000
H	6.881168000	-1.897994000	-3.209315000
H	7.606173000	-1.985655000	-1.598621000
H	5.877765000	-2.308481000	-1.809598000
H	-1.824157000	1.994864000	-0.199731000

*Coordinates of the transition state for **ctc** → **ccc***

N	3.525199000	0.371776000	-0.868899000
C	4.551309000	-0.578377000	-0.945723000
C	5.039437000	-1.241513000	-2.069463000
H	4.622066000	-1.080090000	-3.055416000
C	6.095607000	-2.143093000	-1.886971000
H	6.490889000	-2.670894000	-2.747736000
C	6.639385000	-2.374848000	-0.624445000
H	7.455316000	-3.078095000	-0.506171000
C	6.128083000	-1.701022000	0.495534000
H	6.550578000	-1.883015000	1.478079000
C	5.083666000	-0.808041000	0.328699000
C	4.348792000	0.056158000	1.340921000
C	3.286156000	0.735788000	0.448794000
C	2.799433000	0.846673000	-2.033738000
H	1.927856000	0.223561000	-2.259580000
H	3.465119000	0.845652000	-2.897280000
C	5.294081000	1.112551000	1.955275000
H	6.090239000	0.620819000	2.520391000
H	4.746683000	1.769167000	2.636565000
H	5.754231000	1.727935000	1.178833000
C	3.702612000	-0.792924000	2.452699000
H	4.474961000	-1.318696000	3.019992000
H	3.018723000	-1.534997000	2.035016000

H	3.144543000	-0.162680000	3.149738000
C	2.313369000	1.532575000	0.939457000
C	1.229339000	2.248204000	0.252989000
H	1.410089000	3.262774000	-0.100237000
C	-4.508989000	-0.641535000	0.122362000
C	-4.039024000	0.641528000	-0.314799000
C	-2.727242000	0.972522000	-0.170865000
C	-1.762514000	0.079071000	0.409840000
C	-2.244216000	-1.207551000	0.831226000
C	-3.545332000	-1.557803000	0.699128000
H	-4.705659000	1.372828000	-0.744040000
C	-0.465075000	0.488371000	0.540165000
H	-1.534642000	-1.904102000	1.261233000
H	-3.858121000	-2.539392000	1.018557000
C	-0.048135000	1.788352000	0.110520000
C	-1.051126000	2.689211000	-0.512231000
H	0.278558000	-0.166725000	0.979305000
H	2.334970000	1.718159000	2.011498000
O	-2.347112000	2.212190000	-0.601600000
O	-0.844723000	3.791511000	-0.943131000
N	-5.793574000	-0.981457000	0.001184000
C	-6.334056000	-2.266226000	0.499800000
H	-7.372165000	-2.075534000	0.773361000
H	-5.819220000	-2.540737000	1.418465000
C	-6.257046000	-3.384201000	-0.540834000
H	-6.793991000	-3.113377000	-1.452474000
H	-5.223070000	-3.614029000	-0.805505000
H	-6.715881000	-4.286907000	-0.131542000
C	-6.793638000	-0.095742000	-0.634879000
H	-6.331164000	0.422778000	-1.473154000
H	-7.556961000	-0.748510000	-1.058740000
C	-7.424843000	0.886909000	0.352974000
H	-8.178911000	1.482445000	-0.166240000
H	-7.914030000	0.359711000	1.174738000
H	-6.680773000	1.566194000	0.773554000
H	2.472878000	1.873705000	-1.877973000

Spectroscopic data

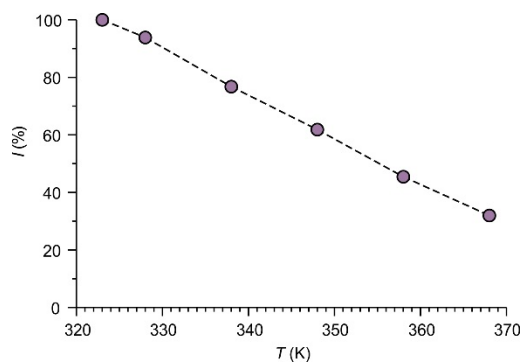


Fig. S2. Dependence of the relative emission intensity ($\lambda_{\text{Ex}} = 550$ nm) of the hexafluorophosphate salt of **3** on the solution temperature in glycerol/MeCN (94:6, v/v).

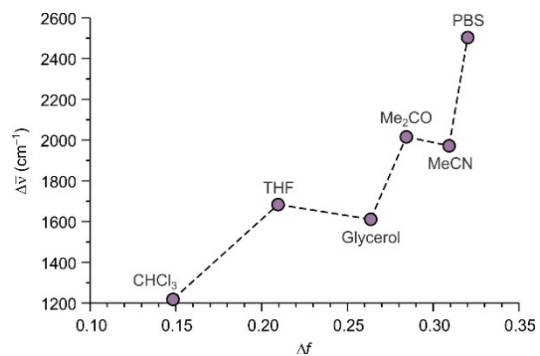


Fig. S3. Dependence of the Stokes' shift of the hexafluorophosphate salt of **3** on the orientation polarizability of the solvent at 298 K.

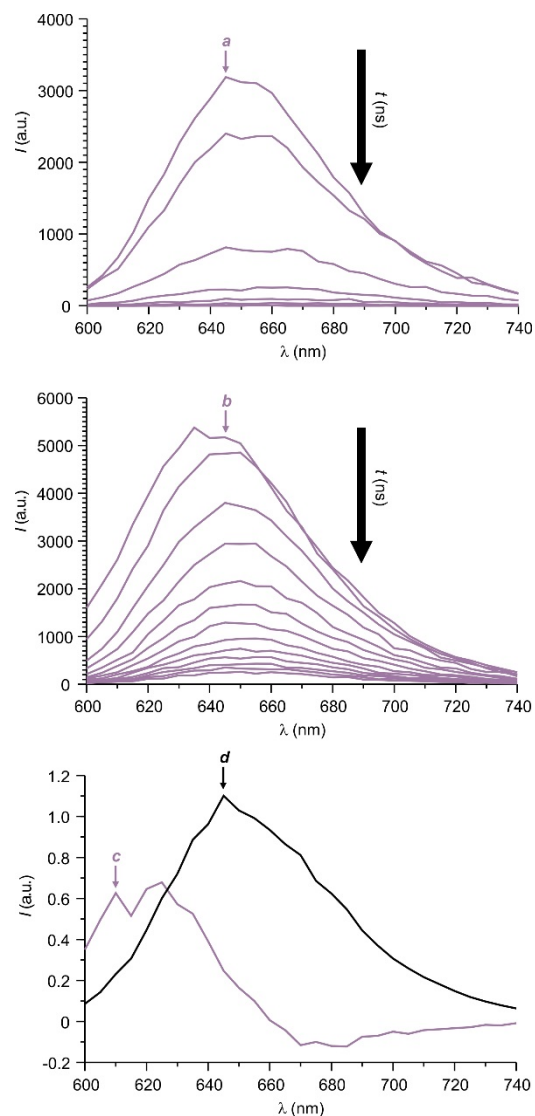


Fig. S4. Time-resolved emission spectra of the hexafluorophosphate salt of **3** ($7 \mu\text{M}$) recorded in either MeCN (**a**) or glycerol (**b**) at 298 K over the course of 6 ns after the led pulse (502 nm, 900 ps pulse width, ~ 1 pJ per pulse). Emission spectra of the two components with τ of 0.51 (37%, **c**) and 1.84 ns (63%, **d**), observed in glycerol, recovered from global analysis of the fluorescence decays.

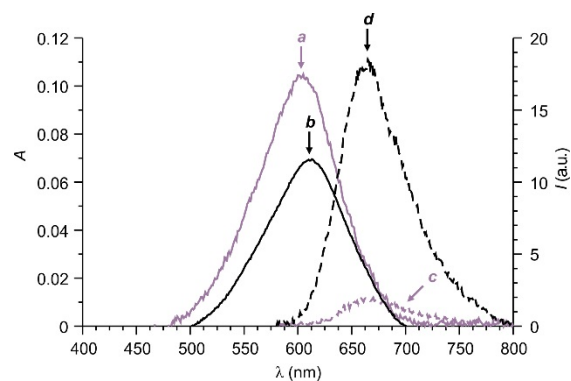


Fig. S5. Absorption (**a** and **b**) and emission ($\lambda_{\text{Ex}} = 550$ nm, **c** and **d**) spectra of the hexafluorophosphate salt of **4** (1 μM) in either MeCN (**a** and **c**) or glycerol/MeCN (94:6, v/v, **b** and **d**) at 298 K.

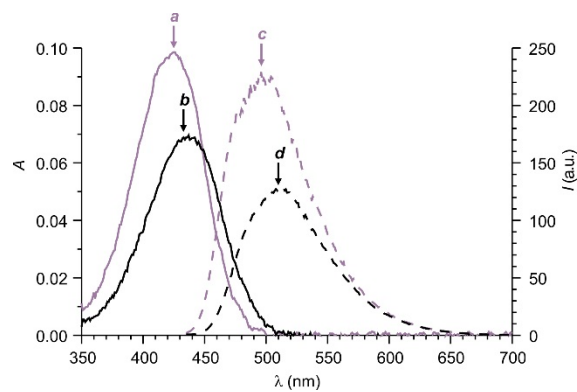


Fig. S6. Absorption (**a** and **b**) and emission ($\lambda_{\text{Ex}} = 420$ nm, **c** and **d**) spectra of **5** (2 μM) in either MeCN (**a** and **c**) or glycerol/MeCN (98:2, v/v, **b** and **d**) at 298 K.