

## SUPPLEMENTARY MATERIAL (SI)

for

### Chiral bis(benzo[1,2-*b*:4,3-*b'*]dithiophene) atropisomers: experimental and theoretical investigations of the stereochemical and chiroptical properties

Valentina Pelliccioli,<sup>a</sup> Roberta Franzini,<sup>b</sup> Giuseppe Mazzeo,<sup>c</sup> Claudio Villani,<sup>b,\*</sup> Sergio Abbate,<sup>c,d</sup>

Giovanna Longhi,<sup>c,d,\*</sup> Emanuela Licandro,<sup>a</sup> Silvia Cauteruccio<sup>a,\*</sup>

<sup>a</sup>*Dipartimento di Chimica, Università degli Studi di Milano, via Golgi 19, I-20133 Milan, Italy*

<sup>b</sup>*Dipartimento di Chimica e Tecnologie del Farmaco, Sapienza Università di Roma, P.le A. Moro 5, 00185 Roma, Italy*

<sup>c</sup>*Dipartimento di Medicina Molecolare e Traslazionale, Università di Brescia, Viale Europa 11, 25123 Brescia, Italy*

<sup>d</sup>*Istituto Nazionale di Ottica (INO), CNR, Research Unit of Brescia, c/o CSMT, via Branze 45, 25123 Brescia, Italy*

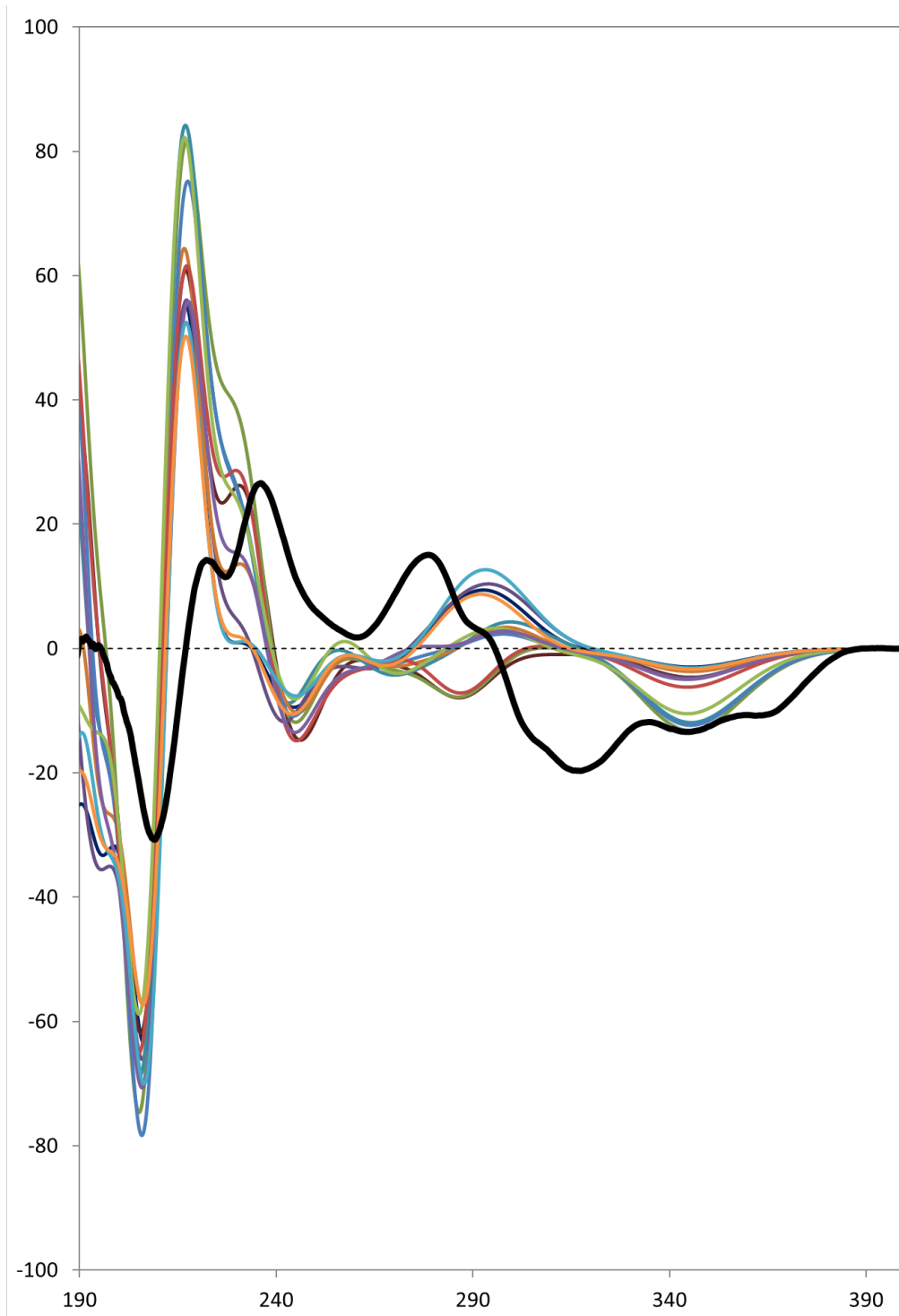


Figure 1-SI. ECD spectra of calculated conformers of compound **3** compared with experimental spectrum. Calculations are performed at CAM-B3LYP/TZVP level of theory.

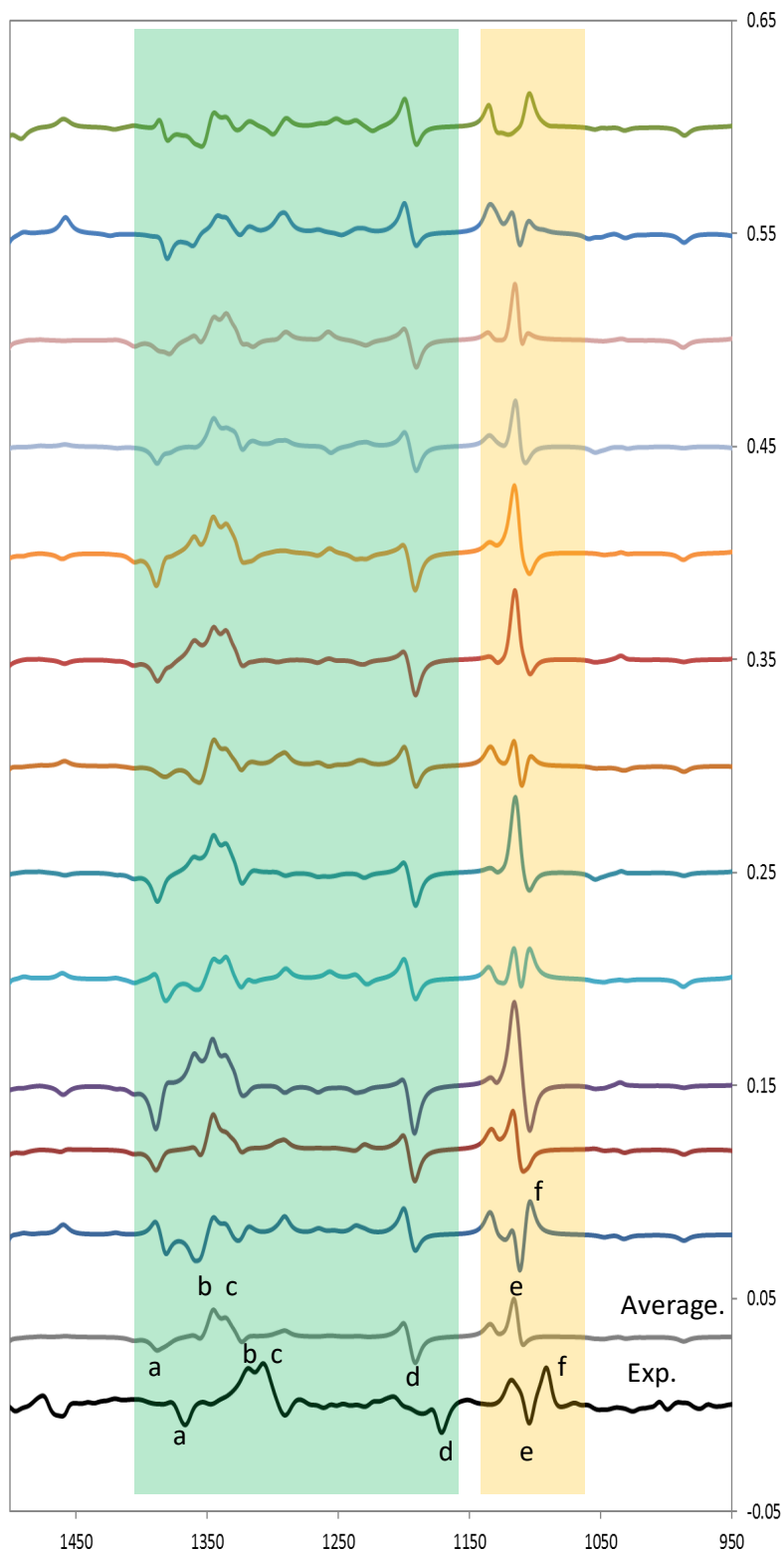


Figure 2-SI. VCD spectra of calculated conformers of compound **3** compared with Boltzmann average and with experimental spectrum. Evidenced in green the region bearing features (a-d) present in all conformers, evidenced in yellow features highly dependent on propyl groups' conformations (e,f).

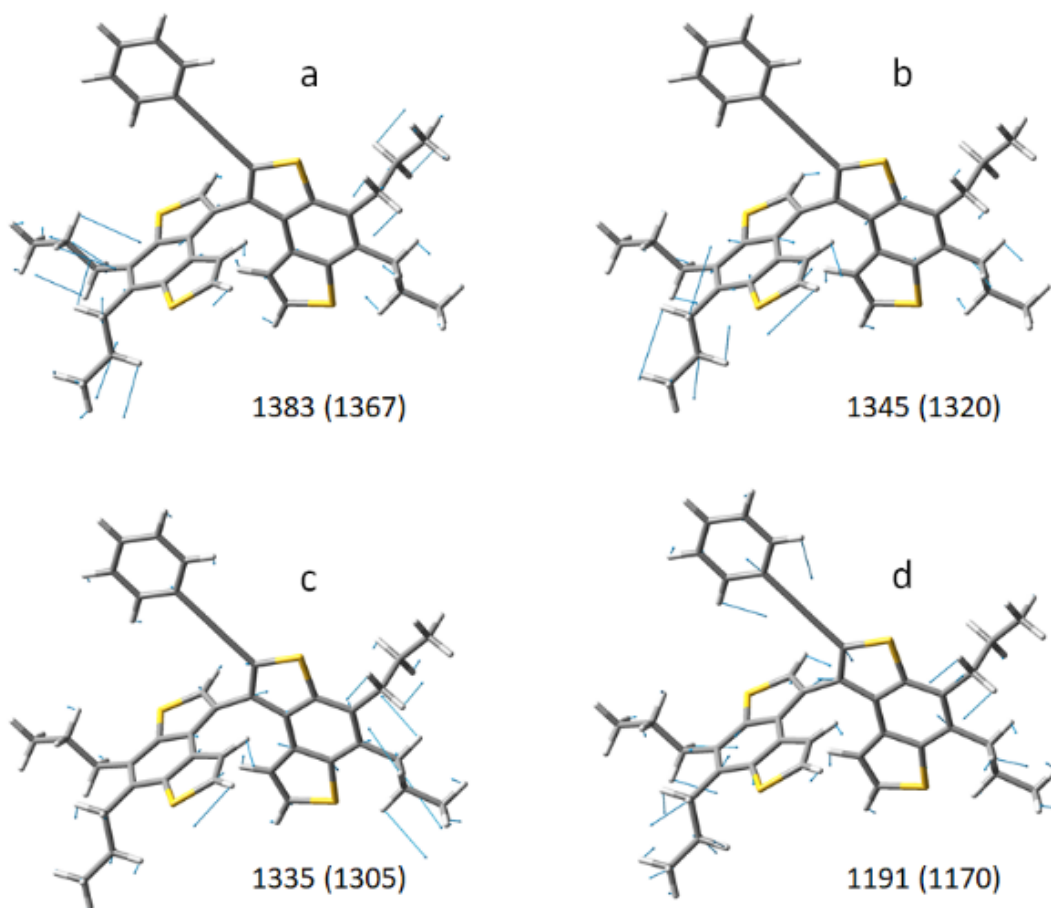


Figure 3a-SI. Examples of modes responsible of bands not much influenced by propyl conformations. Calculated and experimental (in brackets) wavenumbers are reported.

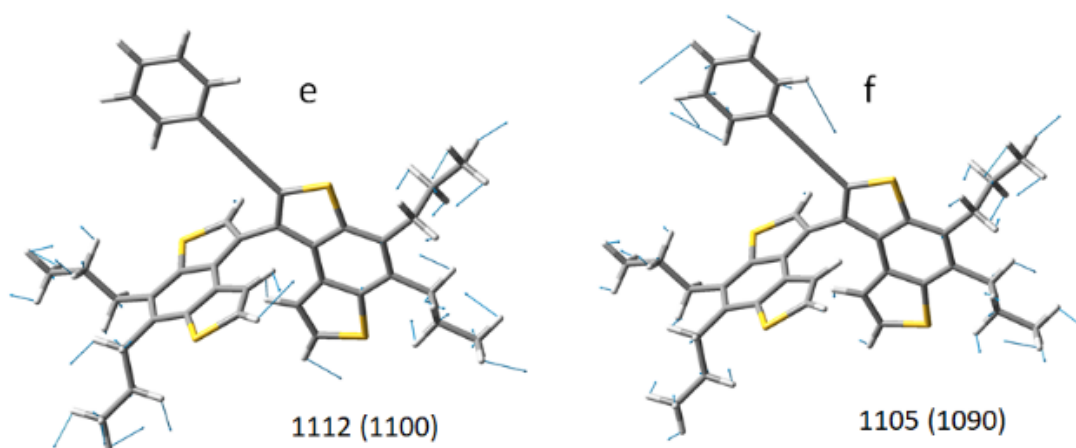


Figure 3b-SI. Examples of modes responsible of bands not much influenced by propyl conformations. Calculated and experimental (in brackets) wavenumbers are reported.

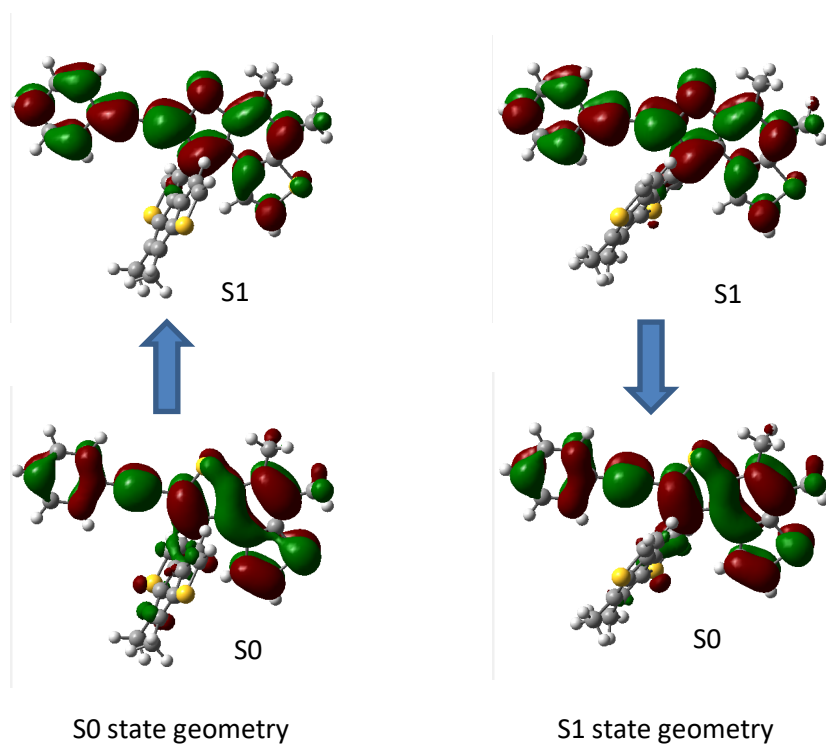


Figure 4-SI. Kohn-Sham HOMO-LUMO orbitals of methyl model for compound **3** for the ground (left) and first excited state structure (right).

T (°C)	T (K)	1/T (K <sup>-1</sup> )	k <sub>1,2</sub> (min <sup>-1</sup> )	k <sub>2,1</sub> (min <sup>-1</sup> )	k <sub>av</sub> (min <sup>-1</sup> )	k <sub>av</sub> (s <sup>-1</sup> )	ln k (s <sup>-1</sup> )/T (K)
40	313.15	0.003194	0.0234	0.0216	0.0225	0.000375	-13.6352
50	323.15	0.003094	0.0565	0.052	0.0542	0.000904	-12.78661
55	328.15	0.003047	0.0953	0.0885	0.0919	0.001532	-12.27486

Table 1-SI. Kinetic rate constants (k) of the on-column enantiomerization of **4**.

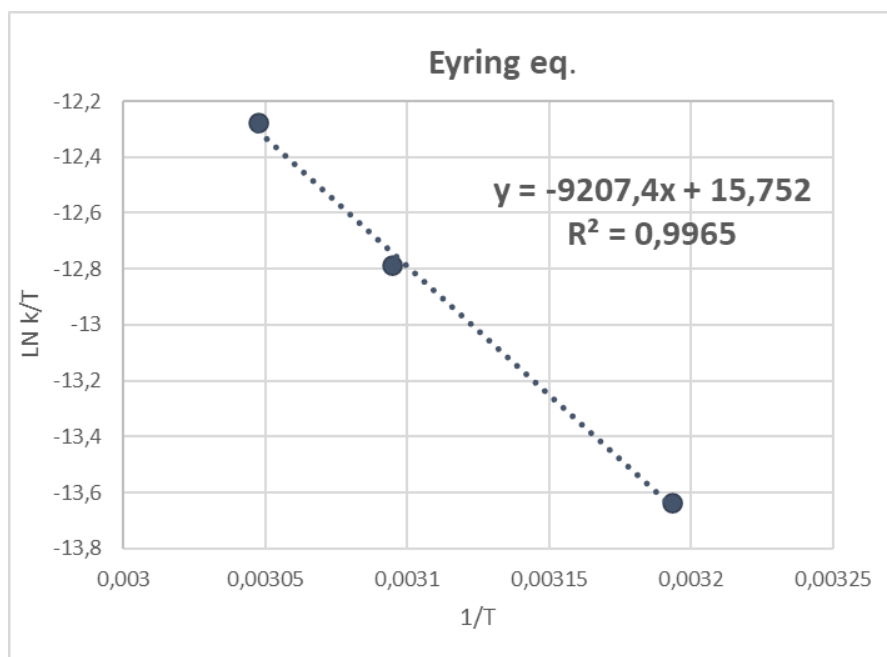


Figure 5-SI. Eyring plot enantiomerization of compound **4**.

$\Delta H^\ddagger$ (kJ/mol)	$\Delta S^\ddagger$ (J/mol*K)	$\Delta G^\ddagger$ (kJ/mol) 25 °C
76.60	- 66.94	96.56
$\Delta H^\ddagger$ (kJ/mol)	$\Delta S^\ddagger$ (J/mol*K)	$\Delta G^\ddagger$ (kJ/mol) 25 °C
18.30	- 15.99	23.06

Table 2-SI. Energetic barrier of the on-column enantiomerization ( $\Delta G^\ddagger$ ) of **4**.

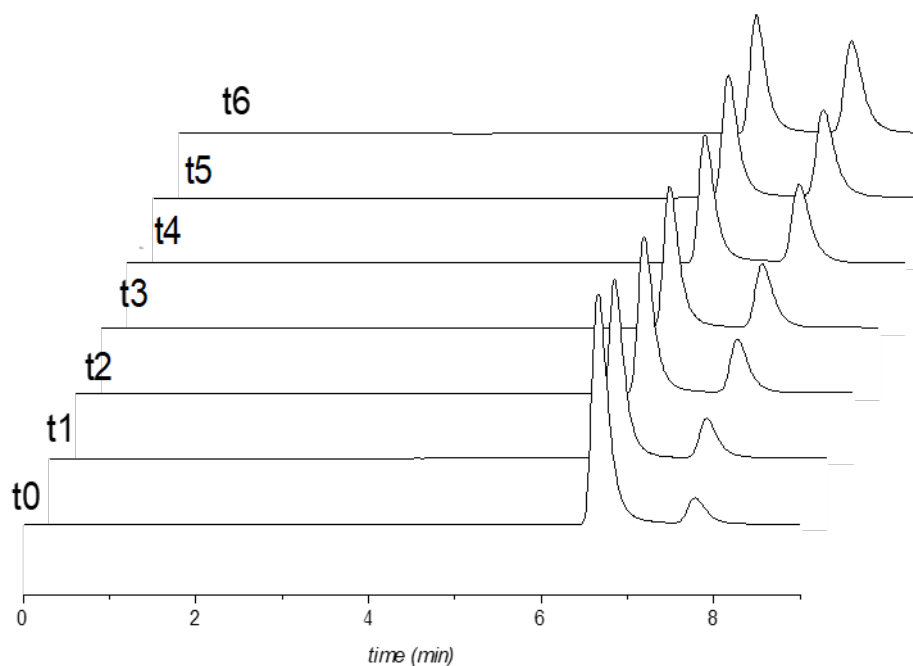


Figure 6-SI. Thermal racemization of compound **4** in Hexane at 35.5 °C starting from a solution enriched in the 1<sup>st</sup> eluted enantiomer, monitored over time by CSP-HPLC ( $t_0=0$  min,  $t_1=10$  min,  $t_2=20$  min,  $t_3=30$  min,  $t_4=50$  min,  $t_5=70$  min,  $t_6=90$  min). Column: Chiralpak IB 250 mm (L)  $\times$  4.6 mm (I.D.). Eluent: hexane/isopropyl alcohol 100/0.025 (v/v), flow rate: 1 ml/min, detector: UV @300 nm.

Table 3-SI. Energetic Characteristics of the lowest energy transition: wavelength (nm), dipole (D) and rotational strengths (R), orbital involved in the transition. D and R given as  $10^{-40}$  esu<sup>2</sup>cm<sup>2</sup>.

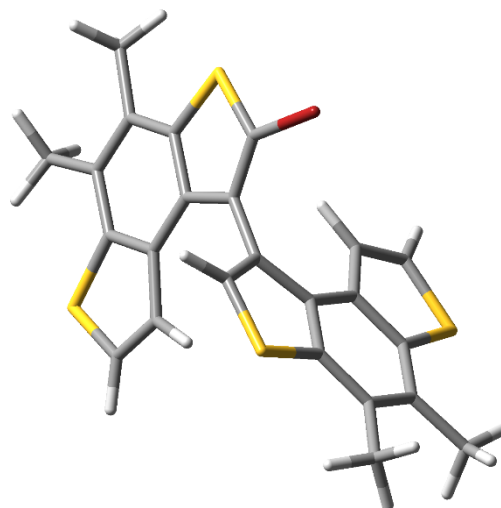
Compound 1 (methyl)				Compound 1 (propyl)				
#	$\lambda$	D	R	MOs	$\lambda$	D	R	MOs
1	281	235790	3.08	HO-1→LU;HO→LU	281	234520	-7.34	HO-1→LU;HO→LU
2	277	151298	-20.1	HO→LU+1	277	123269	-68.3	HO→LU+1
3	275	47435	50.25	HO-3→LU	275	68474	78.42	HO-3→LU
4	273	25282	-2.75	HO-2→LU+1	274	38536	-13.4	HO-2→LU+1
Compound 2 (methyl)				Compound 2 (propyl)				
#	$\lambda$	D	R	MOs	$\lambda$	D	R	MOs
1	293	310060	-106	HO→LU+1;HO→LU	296	388335	-80.8	HO→LU+1;HO→LU
2	290	189754	74.48	HO-1→LU;HO-1→LU+1	282	37200	-5.84	HO-2→LU
3	273	17580	-1.97	HO-2→LU;HO-2→LU+1	278	138651	47.36	HO-1→LU+1
4	271	14419	-6.67	HO-3→LU;HO-3→LU+1	274	45878	-4.14	HO-3→LU+1
Compound 3 (methyl)				Compound 3 (propyl)				
#	$\lambda$	D	R	MOs	$\lambda$	D	R	MOs
1	330	761396	-34.2	HO→LU	336	775737	-13.2	HO→LU
2	298	44462	-12.6	HO-1→LU	296	52745	-16.3	HO-2→LU
3	290	7955	27.05	HO-1→LU+1	291	6874	31.77	HO-1→LU
4	283	172286	17.27	HO-2→LU	277	165584	30.67	HO-1→LU+1
5	273	23083	-2.27	HO-3→LU+1;HO→LU+1	274	25743	-8.75	HO-3→LU+1



## XYZ Cartesian coordinates of optimized structures

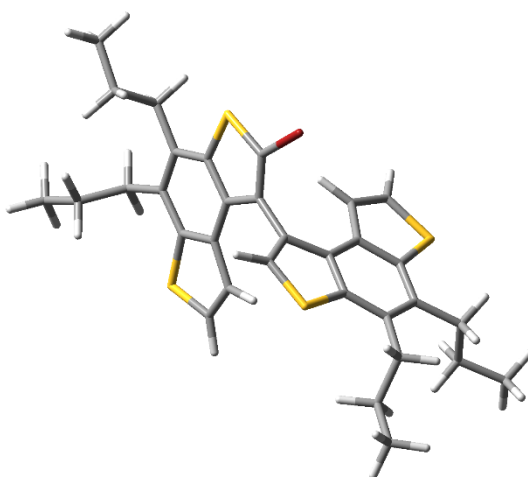
### Calculated P methyl (1) DFT/B3LYP/TZVP

C	4.14265400	0.09705800	0.52597300
C	1.93433000	-1.29223200	-0.64041600
C	4.27932900	-1.25042000	0.19612900
C	2.91292500	0.72445300	0.25314800
C	1.80165100	0.08269000	-0.32230200
C	3.17221700	-1.90955000	-0.36954400
S	3.13578700	-3.61227800	-0.83293500
C	1.48244100	-3.45468500	-1.37629800
H	0.97666500	-4.31711000	-1.78079100
C	0.98732700	-2.20558900	-1.21801800
H	-0.01760000	-1.93354800	-1.49824500
S	2.56943000	2.42828700	0.56973600
C	0.95368200	2.22723400	-0.07120400
C	0.66616600	0.96772100	-0.49947700
Br	-0.20430200	3.72204900	-0.08693300
C	5.27848500	0.87729500	1.13888500
H	5.83898600	0.27743400	1.85605800
H	4.91727200	1.75999200	1.66799700
C	5.56742400	-1.99247600	0.45015500
H	5.62313300	-2.90719400	-0.13982200
H	5.66269900	-2.27718700	1.50284600
C	-0.63905100	0.58611300	-1.08417600
C	-0.91384200	0.77078200	-2.40174100
H	-0.25609400	1.19259400	-3.14527700
S	-2.50884000	0.24696500	-2.86507600
C	-2.85183900	-0.25443400	-1.20751800
C	-3.10002100	-0.90247200	1.42473600
C	-4.06708900	-0.81913600	-0.77357000
C	-1.75062600	-0.00274600	-0.36863300
C	-1.87810000	-0.34541200	1.00028500
C	-4.19814200	-1.14023700	0.57601400
S	-3.05694000	-1.25731200	3.15331400
C	-1.42143600	-0.65125900	3.26297200
H	-0.91834100	-0.66280900	4.21687200
C	-0.93729900	-0.21342000	2.07771100
H	0.05578400	0.19173300	1.96383600
C	-5.47119500	-1.73995900	1.11861200
H	-5.53228700	-1.63266300	2.20153400
H	-6.35457700	-1.26187700	0.69377300
C	-5.19577600	-1.04459000	-1.74818100
H	-5.72131800	-1.97858100	-1.54762500
H	-5.93298700	-0.23664700	-1.69938600
H	-5.53677300	-2.80911000	0.89276600
H	-4.83276300	-1.09017200	-2.77534300
H	6.43804400	-1.38717400	0.19533900
H	5.98443600	1.22161200	0.37623200



Calculated P propyl (*trans*) (1) DFT/B3LYP/TZVP

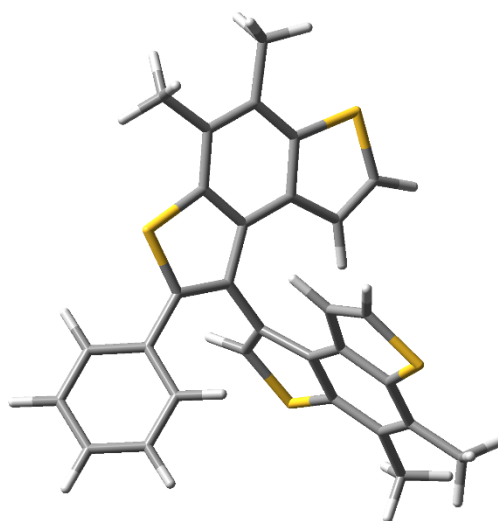
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C	2.94612300	0.62812800	0.20618000
C	1.73536800	0.12788500	-0.30107400
C	2.77764800	-2.04895600	-0.19635800
S	2.45916400	-3.75893700	-0.50178600
C	0.83756700	-3.38989800	-1.03631100
H	0.19182800	-4.19305200	-1.35440600
C	0.55152000	-2.06848600	-0.98942700
H	-0.40513900	-1.66463900	-1.27929400
S	2.86486600	2.38138500	0.41813300
C	1.22251400	2.38636100	-0.18312400
C	0.73928300	1.15940300	-0.51958900
Br	0.30017300	4.03430100	-0.28011500
C	5.32104700	0.53307500	1.03574000
H	5.90029600	-0.14929100	1.65933100
H	5.01849100	1.35030200	1.69948000
C	6.24183800	1.10749100	-0.05837100
H	6.58395600	0.29478400	-0.70390900
H	5.66843100	1.78361400	-0.69785800
C	7.44652000	1.84692400	0.52291600
H	8.05629200	1.18624700	1.14518600
H	7.13186200	2.68912200	1.14472800
H	8.08726100	2.24094100	-0.26858400
C	5.13176200	-2.49066400	0.58186500
H	4.71972000	-3.41861200	0.99179100
H	5.78583300	-2.09109200	1.35817800
C	5.98411300	-2.83868300	-0.65398000
H	5.33620500	-3.23022400	-1.44224900
H	6.43139900	-1.92460000	-1.05254900
C	7.08154100	-3.85424000	-0.33735700
H	6.65807400	-4.79309300	0.02892800
H	7.76306900	-3.47733800	0.43015300
H	7.67572100	-4.08267900	-1.22456700
C	-0.62370500	0.94066100	-1.05389000
C	-0.90451300	1.07869000	-2.37576300
H	-0.21217500	1.34531800	-3.15871000
S	-2.57176100	0.77213100	-2.77174900
C	-2.94153600	0.44001600	-1.07665300
C	-3.21320500	0.03431800	1.59472000
C	-4.22395900	0.10443600	-0.58713300
C	-1.79089000	0.57402100	-0.28091800
C	-1.93332500	0.36368900	1.11325700
C	-4.36344600	-0.10419500	0.78667400
S	-3.18424000	-0.15837900	3.35001500



C	-1.47523800	0.20170300	3.38979400
H	-0.95869000	0.20359900	4.33655600
C	-0.95834800	0.45077900	2.16446400
H	0.08043300	0.69268300	2.00427300
C	-5.67414400	-0.47819000	1.44309900
H	-5.74005600	0.03064700	2.41038300
H	-6.51505300	-0.10496600	0.85682900
C	-5.86212600	-1.99031800	1.67289300
H	-5.01839400	-2.37642000	2.25046600
H	-5.83518300	-2.50732000	0.71026900
C	-7.17053300	-2.31198200	2.39440800
H	-7.20736100	-1.83581100	3.37769200
H	-7.28560600	-3.38772400	2.54277600
H	-8.03559600	-1.96134200	1.82486600
C	-5.36880700	-0.01686800	-1.56895000
H	-6.31795100	0.19539000	-1.07489500
H	-5.25779200	0.75630100	-2.33652800
C	-5.46962600	-1.38699800	-2.26685800
H	-5.61557400	-2.16511500	-1.51336000
H	-4.52063000	-1.61361700	-2.75980400
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H	-7.57261600	-1.24422900	-2.81804600
H	-6.66107800	-2.41856700	-3.76784300
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Calculated P methyl (2) DFT/B3LYP/TZVP

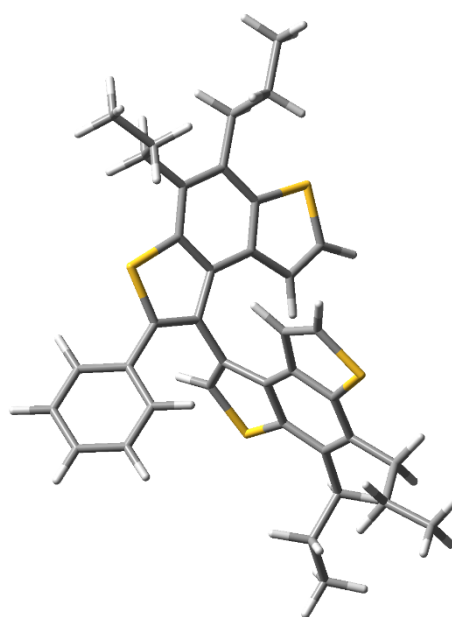
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C	2.93932400	0.78420400	0.26322500
C	1.85593900	0.08141800	-0.29468500
C	3.36154000	-1.80864500	-0.43870900
S	3.44426300	-3.48574500	-0.98280000
C	1.77864700	-3.42323400	-1.50675200
H	1.33231000	-4.29894900	-1.95067900
C	1.19837100	-2.22049600	-1.28884600
H	0.17485900	-2.01010700	-1.55325600
S	2.48193100	2.43987200	0.64271900
C	0.84629900	2.17836700	0.03605200
C	0.66385200	0.89511900	-0.41018900
C	5.31310500	1.07356100	1.09514300
H	5.41551000	0.88007000	2.16788600
C	5.76572500	-1.76209100	0.35480500
H	6.22230700	-1.45602900	1.29646500
H	6.46850500	-1.51251500	-0.44678500
C	-0.60702700	0.42795900	-1.01682100
C	-0.93470900	0.72234500	-2.30182800
H	-0.34922800	1.30004500	-2.99950000
S	-2.46745100	0.06525200	-2.80807800
C	-2.70989800	-0.65545400	-1.21532900
C	-2.82719700	-1.60212400	1.33497100
C	-3.84043600	-1.40482700	-0.83491300
C	-1.62526400	-0.36994400	-0.36537600
C	-1.68674100	-0.86421500	0.96158400
C	-3.90534200	-1.88078800	0.47333200
S	-2.70965200	-2.12308700	3.01748200
C	-1.15552900	-1.33972500	3.17853700
H	-0.63618500	-1.38914900	4.12247400
C	-0.74792200	-0.73034500	2.04114400
H	0.18982700	-0.20333500	1.96033700
C	-5.08652000	-2.68401300	0.95745300
H	-5.14074900	-2.69665200	2.04602000
H	-6.02897700	-2.27728700	0.58895500
C	-4.95468700	-1.65996900	-1.81891700
H	-5.78807300	-0.96619300	-1.66801700
H	-4.61414300	-1.53841000	-2.84743600
H	6.27971300	0.87074100	0.63315000
H	5.67099900	-2.84792200	0.37655300
H	5.11339500	2.13880800	0.97622700
H	-5.35129300	-2.67136500	-1.72508300
H	-5.02573500	-3.72441200	0.62234900
C	-0.09818000	3.30724600	0.08034400



C	-1.87458000	5.48080600	0.18095800
C	0.31184200	4.59091100	-0.30743400
C	-1.41481400	3.13715800	0.52884300
C	-2.29236300	4.21289600	0.57382500
C	-0.56756300	5.66525100	-0.25809000
H	1.32290600	4.74211500	-0.66519500
H	-1.74682000	2.16242000	0.85772500
H	-3.30494900	4.06010100	0.92706200
H	-0.23113200	6.64724400	-0.56793400
H	-2.56081300	6.31788000	0.21920200

### Calculated P propyl (trans) (2) DFT/B3LYP/TZVP

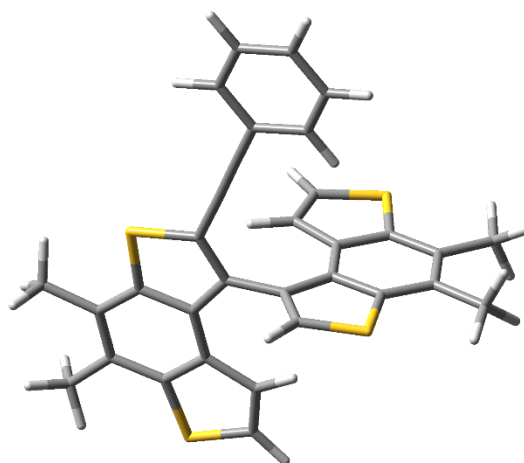
C	4.28466900	0.26969100	-0.21762800
C	1.95084900	-1.06623300	-1.20455900
C	4.39649300	-1.03705000	-0.69726200
C	3.00850800	0.87442400	-0.24202100
C	1.83376400	0.25680000	-0.70316600
C	3.22626300	-1.66149000	-1.18074400
S	3.16784000	-3.28810300	-1.86638600
C	1.45447500	-3.12987300	-2.16540100
H	0.91957900	-3.95005800	-2.61747900
C	0.95699000	-1.93397700	-1.77455800
H	-0.08148900	-1.66874000	-1.88800300
S	2.67905100	2.52181800	0.28298100
C	0.97124400	2.36565600	-0.12744900
C	0.67554300	1.12191700	-0.62187300
C	5.45418500	1.05997300	0.32755400
C	5.69704500	-1.80931400	-0.71511900
H	6.54587600	-1.12672600	-0.77573000
C	-0.67949200	0.74558500	-1.09495700
C	-1.14393100	1.13431400	-2.31076300
H	-0.61966600	1.73149100	-3.04002800
S	-2.75275000	0.56749600	-2.66433900
C	-2.83991100	-0.24091500	-1.09664400
C	-2.67677400	-1.38351400	1.36208900
C	-3.95263400	-0.98090200	-0.63685300
C	-1.64886900	-0.05334400	-0.37407500
C	-1.56695400	-0.64566100	0.91126600
C	-3.86818400	-1.56989500	0.62680900
S	-2.36479100	-2.05377400	2.96611000
C	-0.77450300	-1.33055000	2.99041600
H	-0.14206300	-1.47672200	3.85172400
C	-0.49343200	-0.63221500	1.86606000
H	0.44573900	-0.12602800	1.70727600
C	-4.98622700	-2.38081900	1.24441900
H	-5.60188800	-2.83602800	0.46725900



C	-5.17306200	-1.08675300	-1.52508500
H	-4.84435800	-1.17410700	-2.56604700
H	6.38732600	0.71999400	-0.12395300
H	5.73618000	-2.41111500	-1.62908500
H	5.34442000	2.10624800	0.02313000
H	-5.72027100	-2.00622600	-1.31221800
H	-4.54768800	-3.21598300	1.80049400
C	0.09396800	3.52638400	0.09899400
C	-1.55235200	5.75829800	0.54494300
C	0.51625800	4.81534200	-0.25676800
C	-1.16727700	3.38023500	0.69195400
C	-1.98107400	4.48502500	0.90753500
C	-0.29881300	5.91857000	-0.03645700
H	1.48400800	4.94906400	-0.72440900
H	-1.50469800	2.39995400	0.99809800
H	-2.95117500	4.35003800	1.37028800
H	0.04531400	6.90453900	-0.32444600
H	-2.18849800	6.61794900	0.71637600
C	-6.14515400	0.10421600	-1.41889400
H	-6.51137900	0.17969000	-0.39194000
H	-5.60421200	1.03260800	-1.61913600
C	-7.32705000	-0.02045100	-2.37997500
H	-7.90493300	-0.92785900	-2.18424700
H	-8.00470300	0.83058900	-2.28530800
H	-6.98946000	-0.06145000	-3.41888800
C	-5.89931600	-1.58576000	2.19778400
H	-5.29056300	-1.11581000	2.97441000
H	-6.37356800	-0.77004500	1.64620800
C	-6.97127900	-2.46264900	2.84433600
H	-7.60900500	-1.87945900	3.51191800
H	-7.61494200	-2.92482500	2.09085400
H	-6.52218000	-3.26665200	3.43326800
C	5.59907800	1.01103600	1.86078300
H	5.74674200	-0.02512500	2.17567500
H	4.66538100	1.34092200	2.32365700
C	6.75584900	1.87334000	2.36520600
H	6.84343000	1.82059600	3.45241600
H	7.70913900	1.54824800	1.93951800
H	6.61393200	2.92291700	2.09457100
C	5.89820500	-2.74366500	0.49375400
H	5.89746200	-2.15036000	1.41172800
H	5.04724300	-3.42522000	0.57010600
C	7.19498500	-3.54719900	0.40007400
H	8.06758400	-2.89006200	0.35059500
H	7.31969300	-4.19855600	1.26765300
H	7.20559600	-4.17815100	-0.49254300

### Calculated P methyl (3) DFT/B3LYP/TZVP

C	3.57685400	2.74512600	0.46806800
C	2.95773600	0.20536400	-0.68683100
C	4.61344900	1.88144900	0.11702600
C	2.25415800	2.33115700	0.22355500
C	1.90201400	1.09006200	-0.34358400
C	4.27710000	0.63478900	-0.44434900
S	5.43697000	-0.60021900	-0.93882100
C	4.13855000	-1.64729700	-1.45807700
H	4.37537400	-2.61423700	-1.87294400
C	2.91228600	-1.10642200	-1.26949800
H	1.99966100	-1.61699600	-1.53225700
S	0.82653900	3.30397100	0.56291000
C	-0.22829700	2.02614900	-0.05503800
C	0.47876500	0.92726900	-0.48753900
C	3.85065500	4.09909700	1.07327800
H	4.70558900	4.07445200	1.74887700
C	6.05623900	2.25942000	0.34002100
H	6.33672400	2.15817400	1.39324100
H	6.25115500	3.29231700	0.04848700
C	-0.20338300	-0.25955200	-1.05243700
C	-0.61626200	-0.29761800	-2.34606000
H	-0.50139800	0.48164200	-3.08288900
S	-1.39664600	-1.79102300	-2.79118700
C	-1.17386700	-2.42152100	-1.15706700
C	-0.72588100	-3.10378900	1.44002200
C	-1.59848100	-3.69157800	-0.72031500
C	-0.52432100	-1.47834000	-0.33936700
C	-0.29124500	-1.83417300	1.01222100
C	-1.37798900	-4.03691300	0.61160800
S	-0.34280400	-3.35295700	3.14503600
C	0.37571000	-1.76254900	3.24202500
H	0.78984500	-1.42812500	4.18000300
C	0.33447500	-1.08928900	2.06915100
H	0.73192100	-0.09372600	1.95004000
C	-1.80887600	-5.37595800	1.15555700
H	-1.87113100	-5.36256300	2.24369600
H	-2.78886800	-5.66844700	0.77685000
C	-2.29046900	-4.63599500	-1.67133600
H	-3.37676900	-4.61472900	-1.53660600
H	-2.08764600	-4.37602400	-2.71052400
H	4.06321100	4.84608900	0.30148200
H	6.72896300	1.62572100	-0.23736600
H	2.99487000	4.45946300	1.64545600
H	-1.96423300	-5.66616300	-1.52456900
H	-1.10220000	-6.16513400	0.87928600
C	-1.61647700	2.21479300	-0.04480700

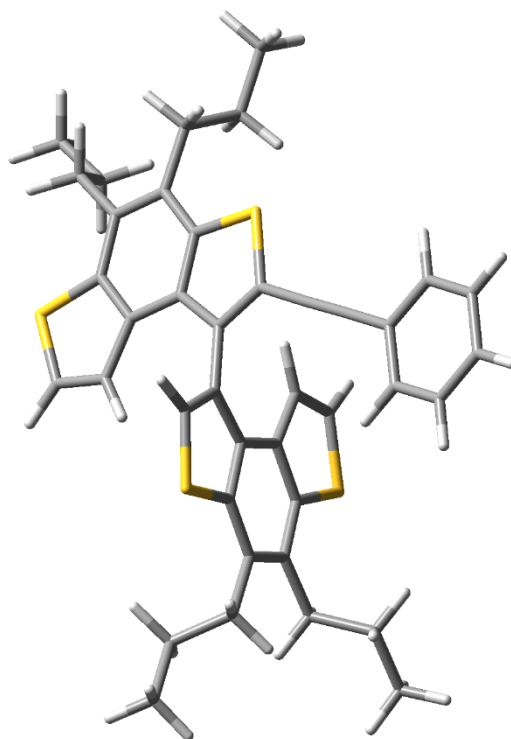


C	-2.81234400	2.40411600	-0.02715800
C	-4.21713900	2.60522500	-0.01529400
C	-6.99085800	2.99818300	0.00397200
C	-5.08403400	1.60600400	-0.49085300
C	-4.76614100	3.80462800	0.46997400
C	-6.14043700	3.99424000	0.47724600
C	-6.45674400	1.80602300	-0.47880600
H	-4.66695500	0.68022600	-0.86512600
H	-4.10447900	4.57805200	0.83797800
H	-6.55031700	4.92332000	0.85416100
H	-7.11362000	1.02778500	-0.84775500
H	-8.06310000	3.14995700	0.01161800



### Calculated P propyl (trans) (3) DFT/B3LYP/TZVP

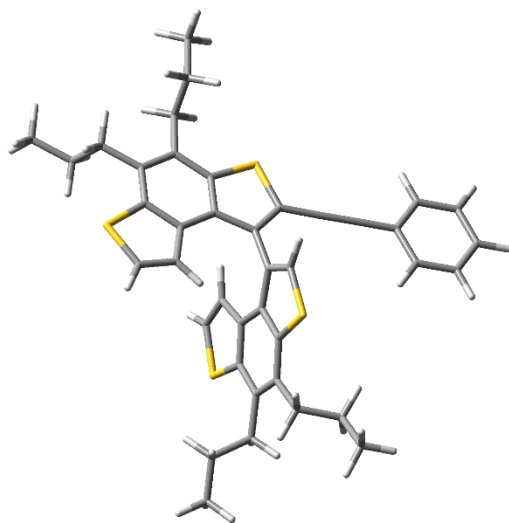
C	4.41265100	0.61815400	-0.27911900
C	2.33667500	-1.18784700	-1.07851600
C	4.73530800	-0.70752500	-0.58031200
C	3.05997600	1.00896300	-0.38472600
C	2.00621100	0.15716500	-0.76674700
C	3.68692000	-1.56793400	-0.97397800
S	3.89221900	-3.26182700	-1.42848000
C	2.18079300	-3.41373900	-1.74170200
H	1.78750300	-4.36159100	-2.07349200
C	1.49772500	-2.26684700	-1.51922100
H	0.43271900	-2.18082300	-1.66353700
S	2.47362200	2.64264100	-0.08310000
C	0.81998000	2.15779500	-0.47592400
C	0.73124700	0.82507400	-0.80783000
C	5.43424300	1.64513000	0.15834500
C	6.14017700	-1.26144200	-0.49566100
H	6.87335200	-0.46878700	-0.65117900
C	-0.55989200	0.20445200	-1.18255500
C	-1.08307900	0.34278400	-2.42859300
H	-0.64679400	0.88109600	-3.25518100
S	-2.61128400	-0.46656500	-2.64242900
C	-2.57745200	-1.02573100	-0.96730200
C	-2.26474600	-1.70955900	1.64533700
C	-3.58542400	-1.80485100	-0.36095100
C	-1.41332300	-0.58112300	-0.31537800
C	-1.25443900	-0.93220700	1.04851400
C	-3.42629600	-2.15326200	0.98013500
S	-1.87789600	-2.04110000	3.33611000
C	-0.38733000	-1.13882200	3.19949700
H	0.25640800	-1.05134000	4.06038000
C	-0.19220900	-0.62200800	1.96445800
H	0.67596500	-0.03782300	1.70326400
C	-4.46456700	-2.94957200	1.73920200
H	-3.96331100	-3.57249400	2.48638900
C	-4.77399700	-2.25692200	-1.18056800
H	-5.65882700	-2.34466100	-0.54765500
H	-5.01636900	-1.48604900	-1.91881000
H	6.41868300	1.39682300	-0.24069100
H	6.28944200	-1.96771600	-1.31894100
H	5.17330500	2.61207200	-0.28491300
H	-4.97300800	-3.64572900	1.06967900
C	-0.21018300	3.10479700	-0.40524200
C	-1.08125700	3.94328500	-0.33912900
C	-2.11776500	4.91006200	-0.26768700
C	-4.16699900	6.81535700	-0.13078100
C	-3.44855400	4.54951900	-0.54175800



C	-1.83330400	6.24280200	0.07630600
C	-2.85178600	7.18247400	0.14268900
C	-4.45928100	5.49721800	-0.47236900
H	-3.67361500	3.52461100	-0.80638200
H	-0.81086600	6.52718300	0.28882800
H	-2.61870100	8.20615800	0.40915000
H	-5.48057400	5.20609000	-0.68559700
H	-4.95922100	7.55181100	-0.07770700
C	6.46127200	-1.98075800	0.82906300
H	5.72527000	-2.77039300	1.00006900
H	6.35145600	-1.27641300	1.65754400
C	7.86868800	-2.57658300	0.84186100
H	8.07679400	-3.07715200	1.78977800
H	8.62928500	-1.80375500	0.70094900
H	7.99380300	-3.31279400	0.04357300
C	5.54866400	1.82252300	1.68475100
H	4.56509500	2.06241100	2.09692400
H	5.84552400	0.87257700	2.13641400
C	6.54795800	2.91239300	2.07163400
H	6.61675800	3.01826900	3.15627900
H	6.25391800	3.88217700	1.66177000
H	7.54948200	2.68491900	1.69640100
C	-5.51573400	-2.07510000	2.44856400
H	-6.03575900	-1.46406400	1.70486900
H	-5.00791100	-1.37428600	3.11626600
C	-6.52915900	-2.90144800	3.23983200
H	-6.03674200	-3.49427700	4.01510300
H	-7.07233100	-3.59320700	2.59009500
H	-7.26495000	-2.26060500	3.73016100
C	-4.54744900	-3.59149400	-1.91559300
H	-4.32328900	-4.37166300	-1.18219600
H	-3.66080200	-3.50610500	-2.54950100
C	-5.74981800	-4.00717100	-2.76268700
H	-5.56668100	-4.95642500	-3.27049100
H	-5.97201100	-3.25905400	-3.52815500
H	-6.64625500	-4.12737400	-2.14824000

Calculated P (3) CONF1 (%POP = 17.3) DFT/B3LYP/TZVP

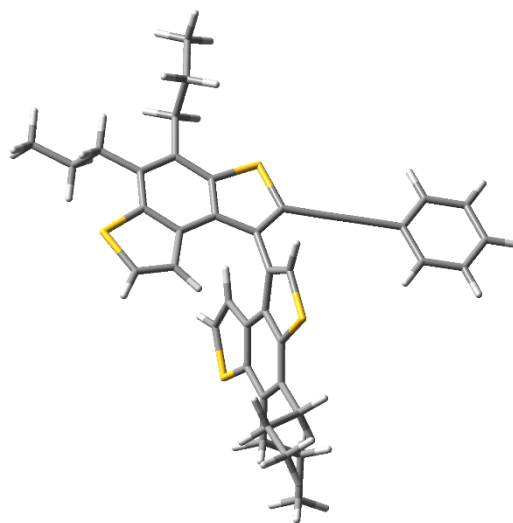
C	4.39472100	0.44854300	0.05935700
C	2.29965100	-1.17591200	-1.01876000
C	4.68363700	-0.84809000	-0.36773700
C	3.06500700	0.90274300	-0.05359800
C	2.00230800	0.13997700	-0.57619600
C	3.62986000	-1.61994500	-0.89882700
S	3.79446200	-3.26813000	-1.50978900
C	2.09461500	-3.31714200	-1.90989500
H	1.68296700	-4.20979700	-2.35363600
C	1.44425900	-2.17054200	-1.60336400
H	0.39102800	-2.02773100	-1.78464500
S	2.51686900	2.50530000	0.43017500
C	0.86492300	2.12789800	-0.07485400
C	0.74979000	0.85030900	-0.57360000
C	5.45765500	1.37931700	0.60063900
C	6.06590000	-1.45007100	-0.24964100
H	6.82741200	-0.67564700	-0.35696300
C	-0.54493800	0.32103300	-1.05989600
C	-1.01239300	0.60753400	-2.30275800
H	-0.52773300	1.21599800	-3.04992700
S	-2.55077200	-0.12856000	-2.66116200
C	-2.59940800	-0.86601400	-1.05681600
C	-2.40255700	-1.84996900	1.46996500
C	-3.64590000	-1.68384200	-0.58074400
C	-1.45395900	-0.52543800	-0.31540500
C	-1.35483000	-1.03383000	1.00380100
C	-3.54197500	-2.19343100	0.71341100
S	-2.09456300	-2.37098400	3.12888400
C	-0.58755100	-1.48613700	3.15499300
H	0.01718400	-1.50166800	4.04787100
C	-0.33084000	-0.84254700	1.99295100
H	0.55334000	-0.24511400	1.83616200
C	-4.58405600	-3.11473500	1.30786500
H	-5.57242400	-2.87630900	0.91092600
C	-4.84583500	-1.95002600	-1.46298100
H	-4.52352700	-1.98530900	-2.50838900
H	-5.25974500	-2.93748000	-1.25090300
H	5.01178900	2.03560800	1.35474400
H	6.22898200	-2.14141400	-1.08203800
H	6.22664400	0.81051700	1.12637200
H	-4.64857600	-2.93565000	2.38551400
C	-0.13826500	3.09366500	0.07935600
C	-0.98357400	3.94889700	0.22189900
C	-1.98873500	4.93798300	0.38124600
C	-3.97555500	6.88862500	0.69155000
C	-3.31567700	4.67391300	-0.00016700



C	-1.67628600	6.19753500	0.92107000
C	-2.66388500	7.16001100	1.07261500
C	-4.29546500	5.64352900	0.15586400
H	-3.56220100	3.70550200	-0.41542600
H	-0.65669800	6.40746400	1.21735500
H	-2.40940700	8.12649500	1.49024100
H	-5.31420300	5.42686600	-0.14162000
H	-4.74365300	7.64252800	0.81174900
C	6.29812800	-2.20452600	1.07338800
H	5.53345700	-2.97777700	1.18426700
H	6.15677500	-1.51418600	1.91021900
C	7.68774000	-2.83592400	1.15225200
H	7.82972200	-3.36130200	2.09896100
H	8.47335200	-2.07967500	1.07147800
H	7.84026500	-3.55814900	0.34600500
C	6.12590700	2.24984000	-0.48033700
H	6.59297000	1.60016700	-1.22634800
H	5.35672600	2.81748200	-1.01064600
C	7.16783000	3.20674800	0.09809200
H	7.62945100	3.80957900	-0.68670100
H	7.96567700	2.66282000	0.61113300
H	6.71744200	3.89202200	0.82094300
C	-4.29351100	-4.60876100	1.07077000
H	-3.30188300	-4.84796200	1.46375400
H	-4.24860800	-4.79954300	-0.00560200
C	-5.33852700	-5.51941700	1.71469300
H	-5.11333400	-6.57190800	1.53009400
H	-6.33810800	-5.31971300	1.31890000
H	-5.37679900	-5.37340400	2.79735400
C	-5.96165600	-0.89718400	-1.32490700
H	-5.54829800	0.09307100	-1.53417000
H	-6.30381900	-0.87068600	-0.28619800
C	-7.14471800	-1.17021800	-2.25325200
H	-6.83450500	-1.16531700	-3.30147100
H	-7.92345300	-0.41388300	-2.13463700
H	-7.59515400	-2.14492100	-2.04668800

Calculated P (3) CONF2 (%POP = 16.6) DFT/B3LYP/TZVP

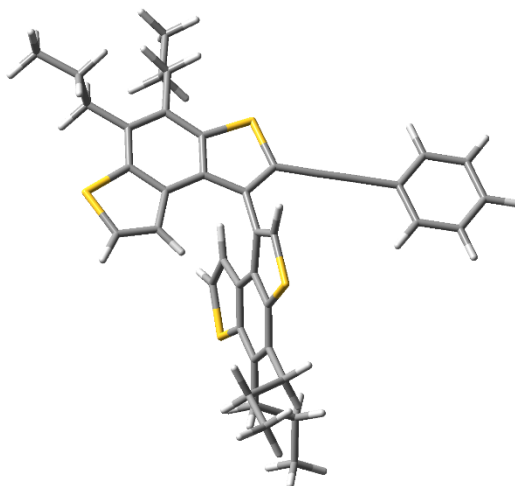
C	4.40861000	0.38415300	0.12767400
C	2.31547800	-1.28440500	-0.88469200
C	4.68878300	-0.94226700	-0.20292400
C	3.08816300	0.84596100	-0.04647000
C	2.02682800	0.06236200	-0.54030900
C	3.63636000	-1.73568400	-0.70405200
S	3.79101200	-3.42409600	-1.19614200
C	2.09979600	-3.47943400	-1.63047400
H	1.68541300	-4.39558300	-2.02052600
C	1.45909400	-2.30631300	-1.41850200
H	0.41212900	-2.16287700	-1.63260800
S	2.55144900	2.48429700	0.31487500
C	0.90619400	2.09357900	-0.20136700
C	0.78462400	0.78655800	-0.61512800
C	5.47237500	1.33676100	0.62776900
C	6.05943200	-1.55185900	-0.01138100
H	6.83412000	-0.79676600	-0.15578700
C	-0.50645200	0.24260700	-1.09481600
C	-0.94241700	0.45271500	-2.36409100
H	-0.43117700	1.00149800	-3.13922900
S	-2.48835000	-0.27565000	-2.70504700
C	-2.58569000	-0.89978700	-1.05550700
C	-2.46905300	-1.69842200	1.54064200
C	-3.66323900	-1.65416500	-0.54517700
C	-1.44689500	-0.53523600	-0.31522900
C	-1.38970300	-0.94649000	1.03984900
C	-3.60478100	-2.06114800	0.78755700
S	-2.20450800	-2.11357000	3.23647900
C	-0.66958900	-1.27778200	3.22909600
H	-0.07803200	-1.25433600	4.13058100
C	-0.37437200	-0.72264800	2.03112000
H	0.53356300	-0.16980300	1.84863800
C	-4.72353000	-2.83613900	1.44797600
H	-4.29918000	-3.50859100	2.19983200
C	-4.81577900	-2.01939100	-1.45467500
H	-5.74218800	-2.09068300	-0.88206700
H	-4.97694300	-1.21054200	-2.17424900
H	5.01926700	2.04991300	1.32365000
H	6.23070000	-2.30246400	-0.78897300
H	6.22120900	0.79639800	1.20961500
H	-5.21793600	-3.48304800	0.72099800
C	-0.08773100	3.07883400	-0.13652000
C	-0.92708100	3.94926800	-0.07267200
C	-1.92605000	4.95503400	-0.00528500
C	-3.90097100	6.93779200	0.12377300
C	-3.24503900	4.67728600	-0.40430800



C	-1.61546300	6.24458600	0.45955400
C	-2.59716800	7.22290100	0.52146000
C	-4.21894400	5.66300000	-0.33815600
H	-3.49011500	3.68591400	-0.76235300
H	-0.60199500	6.46510700	0.76884400
H	-2.34427800	8.21253000	0.88193100
H	-5.23154900	5.43564400	-0.64830900
H	-4.66448800	7.70416400	0.17386800
C	6.25195600	-2.21355800	1.36653600
H	5.47420500	-2.96737500	1.51414600
H	6.10195700	-1.46394300	2.14909600
C	7.63044600	-2.85512100	1.52157800
H	7.74413400	-3.31388600	2.50597100
H	8.42823800	-2.11639900	1.40573600
H	7.79046000	-3.63447600	0.77198700
C	6.17695100	2.12076100	-0.49554300
H	6.65118800	1.41441300	-1.18321300
H	5.42788900	2.65935700	-1.08197000
C	7.21927300	3.10278200	0.03835700
H	7.70694200	3.64271800	-0.77590800
H	7.99755900	2.58640300	0.60690200
H	6.76268300	3.84312000	0.70044700
C	-5.77842700	-1.94019100	2.12425900
H	-6.22219300	-1.27888600	1.37418900
H	-5.28379100	-1.28860700	2.84925500
C	-6.87601500	-2.74649400	2.81785400
H	-6.46098600	-3.38940400	3.59847300
H	-7.40662600	-3.38809300	2.10896600
H	-7.61254900	-2.09020600	3.28613800
C	-4.60067800	-3.33385700	-2.22832000
H	-4.45715400	-4.15070800	-1.51493300
H	-3.67273200	-3.26470600	-2.80225900
C	-5.76359900	-3.66195400	-3.16426600
H	-5.58959100	-4.59856000	-3.69809500
H	-5.90440400	-2.87595200	-3.91083500
H	-6.70155700	-3.76453700	-2.61172800

Calculated P (3) CONF3 (%POP = 12.6) DFT/B3LYP/TZVP

C	4.40634900	0.46105900	0.15077900
C	2.35081400	-1.33559100	-0.70765300
C	4.71429800	-0.88409600	-0.05620000
C	3.07998400	0.88026000	-0.07805700
C	2.03582000	0.03278300	-0.49748900
C	3.67782900	-1.74319500	-0.47565000
S	3.86257500	-3.47115700	-0.78679600
C	2.17340200	-3.60141500	-1.21297500
H	1.77474900	-4.56143400	-1.50041800
C	1.51250900	-2.42345400	-1.12760700
H	0.46255100	-2.32264500	-1.35116200
S	2.51465200	2.53808400	0.10801800
C	0.88280600	2.07113100	-0.38683400
C	0.78551100	0.72682600	-0.66564700
C	5.43176100	1.46154500	0.63712000
C	6.11352700	-1.43038100	0.11951300
H	6.05335500	-2.46505300	0.47061400
C	-0.48928800	0.11873700	-1.11085800
C	-0.90306700	0.19420800	-2.40253400
H	-0.38305600	0.66870000	-3.21973100
S	-2.43427700	-0.58403700	-2.69598400
C	-2.55684600	-1.03948400	-0.99383100
C	-2.48113400	-1.57201100	1.67117900
C	-3.63630600	-1.75135800	-0.42929100
C	-1.43611800	-0.58850600	-0.27384100
C	-1.40029600	-0.86118400	1.11648800
C	-3.59887300	-2.02188200	0.93841700
S	-2.24373700	-1.81260300	3.40437000
C	-0.71727000	-0.96388200	3.34001200
H	-0.14251500	-0.84400900	4.24469400
C	-0.40557000	-0.52781400	2.09776900
H	0.50022500	0.01412100	1.87620000
C	-4.72141100	-2.74103100	1.65329300
H	-4.30351800	-3.33166100	2.47433500
C	-4.76856800	-2.21823900	-1.31749700
H	-5.70440500	-2.24262200	-0.75641100
H	-4.92433500	-1.48666700	-2.11658600
H	6.42411900	1.19569100	0.26881600
H	6.63830500	-0.88336300	0.90476100
H	5.21153600	2.44235200	0.20396000
H	-5.19647700	-3.46167800	0.98520200
C	-0.12566300	3.04237600	-0.43725300
C	-0.97858300	3.90110300	-0.47395100
C	-1.99367800	4.89170100	-0.52256400
C	-4.00081700	6.84363400	-0.62137400
C	-1.70228200	6.23305900	-0.22036200

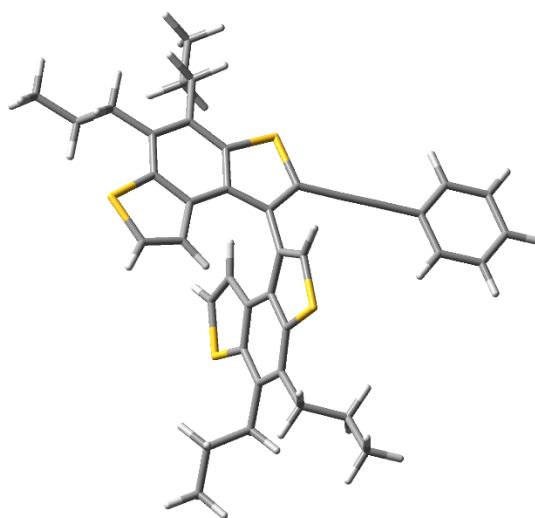


C	-3.30990400	4.54642100	-0.87532200
C	-4.29980300	5.51717400	-0.92254900
C	-2.69990600	7.19581700	-0.27075300
H	-0.69099800	6.50582700	0.05223800
H	-3.54024000	3.51504300	-1.10831200
H	-5.31006800	5.23759200	-1.19540900
H	-2.46170000	8.22589800	-0.03527500
H	-4.77678400	7.59810600	-0.65932600
C	6.95674400	-1.39332000	-1.16937500
H	7.03778000	-0.35902700	-1.51637300
H	6.43098900	-1.93827800	-1.95771800
C	8.35238600	-1.98481600	-0.97400100
H	8.93146300	-1.94451000	-1.89890900
H	8.29837800	-3.03100700	-0.66178800
H	8.91164900	-1.43997300	-0.20850800
C	5.48411700	1.59804000	2.17056400
H	4.49033900	1.86221700	2.54185300
H	5.72433700	0.62520200	2.60954000
C	6.50187700	2.64035800	2.63281100
H	6.52311400	2.71617500	3.72193900
H	6.26214500	3.63031900	2.23607300
H	7.51127800	2.38587000	2.29827600
C	-5.79717900	-1.79591600	2.22105700
H	-6.23487700	-1.21675700	1.40259800
H	-5.32219800	-1.07046900	2.88661700
C	-6.89809700	-2.54387900	2.97237400
H	-6.48994200	-3.10204100	3.81901000
H	-7.40924300	-3.25835500	2.32124800
H	-7.64971900	-1.85404400	3.36182300
C	-4.52764400	-3.60052900	-1.95304700
H	-4.39014200	-4.34128100	-1.15985400
H	-3.59002100	-3.57878900	-2.51488900
C	-5.67034200	-4.03179000	-2.87191500
H	-6.61732000	-4.08917300	-2.32829000
H	-5.47837100	-5.01467800	-3.30729700
H	-5.80434300	-3.32494500	-3.69495300



Calculated P (3) CONF4 (%POP = 8.0) DFT/B3LYP/TZVP

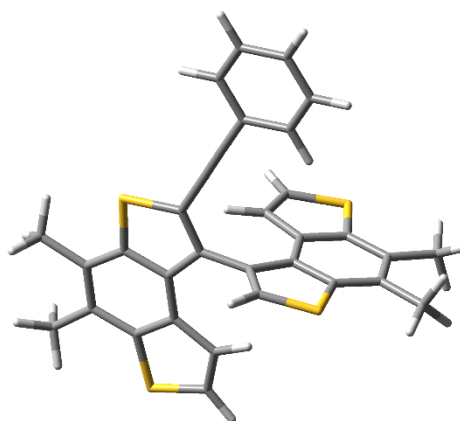
C	4.38305300	0.73818100	-0.33235300
C	2.32321900	-1.05012800	-1.20975000
C	4.72372700	-0.55590800	-0.73425800
C	3.02090700	1.10693100	-0.37864500
C	1.97467400	0.26243400	-0.79592300
C	3.68276200	-1.40816600	-1.16370400
S	3.90968900	-3.06106100	-1.74198500
C	2.19441600	-3.22648500	-2.02577900
H	1.81154700	-4.15648500	-2.41526100
C	1.49486200	-2.11282000	-1.70672200
H	0.42515500	-2.03979700	-1.82006700
S	2.41101000	2.70278500	0.05120800
C	0.75779600	2.21264700	-0.33708600
C	0.68654600	0.90511300	-0.76062600
C	5.39500400	1.75313400	0.15297500
C	6.14068700	-1.08478300	-0.72159500
H	6.85437400	-0.26798900	-0.83781900
C	-0.60064800	0.28503600	-1.14955500
C	-1.15334300	0.49513300	-2.37261700
H	-0.74714100	1.09872300	-3.16888700
S	-2.66456000	-0.33839900	-2.61288300
C	-2.58055700	-1.01188700	-0.98217300
C	-2.18677700	-1.87989100	1.56397700
C	-3.55049100	-1.86565400	-0.41562700
C	-1.41642100	-0.57941700	-0.32220100
C	-1.21506600	-1.02721900	1.00728500
C	-3.34542100	-2.31568900	0.88850300
S	-1.75748000	-2.31451500	3.22080600
C	-0.30452200	-1.34780500	3.12607000
H	0.34895300	-1.29352200	3.98233700
C	-0.15023600	-0.73940900	1.92751400
H	0.68821600	-0.10144700	1.69675900
C	-4.29850800	-3.26753000	1.57681200
H	-5.31949800	-3.09981200	1.22934700
C	-4.78095300	-2.23255000	-1.21583700
H	-4.51591400	-2.29424500	-2.27599300
H	-5.12648800	-3.23098200	-0.94192200
H	6.37403400	1.55412700	-0.28505000
H	6.28322200	-1.72835800	-1.59587900
H	5.10476200	2.74306200	-0.21490900
H	-4.31271300	-3.04845600	2.64889000
C	-0.28748800	3.13133000	-0.17442300
C	-1.16990100	3.94717900	-0.02619600
C	-2.21871600	4.88832100	0.14218900
C	-4.29203600	6.74341000	0.47174500
C	-1.94472700	6.19835900	0.57140600



C	-3.55131700	4.52500500	-0.11890800
C	-4.57401300	5.44769700	0.04610400
C	-2.97510300	7.11316500	0.73307100
H	-0.92095500	6.48480100	0.77449600
H	-3.76826900	3.51741300	-0.44864100
H	-5.59660000	5.15457500	-0.15798000
H	-2.74997600	8.11945200	1.06466600
H	-5.09355500	7.46037800	0.59944100
C	6.50803400	-1.88816700	0.54133000
H	5.79198400	-2.70326200	0.67304200
H	6.40463900	-1.24599300	1.41965600
C	7.92669700	-2.45348400	0.47974700
H	8.16758500	-3.01476100	1.38493200
H	8.66842300	-1.65676400	0.37631800
H	8.04663000	-3.12910700	-0.37117700
C	5.54316000	1.82569500	1.68505900
H	4.56550700	2.01551200	2.13561200
H	5.86922500	0.85296000	2.06185200
C	6.53034000	2.90659000	2.12464200
H	6.62345800	2.93786900	3.21218200
H	6.20773100	3.89624900	1.79083400
H	7.52663800	2.72693500	1.71148500
C	-3.93721500	-4.75188500	1.37952700
H	-2.91308300	-4.92029300	1.72270300
H	-3.94202100	-4.98367500	0.31031600
C	-4.89090000	-5.69134100	2.11700900
H	-5.92081300	-5.56308800	1.77276000
H	-4.87681400	-5.50352600	3.19378300
H	-4.61670600	-6.73656100	1.95940500
C	-5.94446200	-1.23618200	-1.05425600
H	-5.59984000	-0.23505800	-1.32671700
H	-6.22818900	-1.18352000	0.00091500
C	-7.16104600	-1.61186900	-1.89972900
H	-7.97278300	-0.89374600	-1.76593400
H	-7.54402900	-2.59936500	-1.62812800
H	-6.91134600	-1.63574600	-2.96371900

### Calculated P methyl (3) DFT/CAM-B3LYP/TZVP (Ground state)

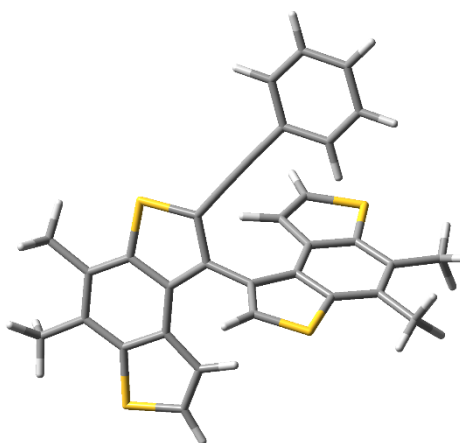
C	3.50977400	2.78657100	0.45195700
C	2.91063500	0.26092400	-0.70822300
C	4.54366200	1.94109700	0.09209100
C	2.19090600	2.36292200	0.21405200
C	1.85424400	1.13099300	-0.35448800
C	4.21836600	0.69588400	-0.47397100
S	5.38012100	-0.51598900	-0.97781600
C	4.09779100	-1.56890000	-1.49330400
H	4.34019900	-2.53104300	-1.91497300
C	2.87252500	-1.04773300	-1.29818300
H	1.96386800	-1.56563300	-1.55866200
S	0.76287400	3.31047100	0.56786600
C	-0.27170400	2.03536600	-0.04670200
C	0.43186900	0.95469500	-0.48955300
C	3.77452000	4.13381300	1.06484600
H	4.61326100	4.10126600	1.75854400
C	5.98031600	2.32749800	0.30790800
H	6.27802200	2.17792000	1.34903700
H	6.15457900	3.37469600	0.06417900
C	-0.23454100	-0.23852700	-1.04871600
C	-0.68324800	-0.28213200	-2.32075900
H	-0.61289600	0.50599800	-3.05327000
S	-1.42806000	-1.78862100	-2.74742900
C	-1.13794800	-2.41727900	-1.13605100
C	-0.58800000	-3.09791800	1.43195400
C	-1.50816500	-3.69996900	-0.69381200
C	-0.49653300	-1.46902600	-0.33610300
C	-0.20973100	-1.82337200	1.00002700
C	-1.23639700	-4.04320600	0.61785700
S	-0.14630300	-3.34529500	3.11030500
C	0.52409600	-1.74412300	3.19772800
H	0.95817600	-1.40203500	4.12336400
C	0.42701800	-1.06508700	2.04030900
H	0.79037000	-0.05770600	1.91618500
C	-1.60756900	-5.39312900	1.16594800
H	-1.64608100	-5.38418300	2.25415000
H	-2.58399500	-5.71672200	0.80776400
C	-2.19769300	-4.65647100	-1.62694100
H	-3.27833000	-4.66296800	-1.46166400
H	-2.02975800	-4.38840300	-2.66913700
H	4.00830100	4.87887300	0.29975400
H	6.65028200	1.73266100	-0.31084500
H	2.90934200	4.49698300	1.61825200
H	-1.83985300	-5.67626400	-1.49168100
H	-0.88018200	-6.15404200	0.87107400
C	-1.66975800	2.20059500	-0.02590600



C	-2.86152600	2.35595300	-0.00417500
C	-4.27638800	2.51779300	0.01116500
C	-7.04456300	2.82735700	0.03564700
C	-5.10601600	1.50195400	-0.46926000
C	-4.85283600	3.69046400	0.50389500
C	-6.22733200	3.84020600	0.51424100
C	-6.47949000	1.65994900	-0.45509900
H	-4.66108700	0.59273000	-0.85070600
H	-4.21287700	4.47875200	0.87698800
H	-6.66369900	4.75312800	0.89856000
H	-7.11333200	0.86641100	-0.82937500
H	-8.12012600	2.94754100	0.04538600

### Calculated P methyl (3) DFT/CAM-B3LYP/TZVP (Excited state)

C	4.28175500	2.00392400	0.39046500
C	3.33473800	-0.57937900	-0.35080900
C	5.19623900	0.93764300	0.24632300
C	2.94498300	1.77042500	0.14281600
C	2.40591900	0.50977200	-0.25982100
C	4.69105600	-0.31294000	-0.10556900
S	5.64673600	-1.77871700	-0.25529700
C	4.23015700	-2.70165700	-0.62216900
H	4.31510600	-3.76058500	-0.80528600
C	3.10089800	-1.95236600	-0.63869100
H	2.12872600	-2.36689800	-0.84943900
S	1.67701300	2.99672500	0.27846000
C	0.44965500	1.82457400	-0.20204200
C	1.02546700	0.53096600	-0.44980200
C	4.77119000	3.36535700	0.79592000
H	5.47338400	3.30500200	1.62751000
C	6.65736500	1.14748200	0.49991400
H	6.86542000	1.25109900	1.56942200
H	7.02058500	2.05480100	0.01502000
C	0.18612700	-0.55941500	-0.95542000
C	0.28037600	-0.99495800	-2.23484100
H	0.96365100	-0.63007200	-2.98508700
S	-0.85839600	-2.23292700	-2.64159100
C	-1.52351400	-2.19038400	-1.01823100
C	-2.31337400	-1.93183600	1.56305900
C	-2.57581500	-3.00281700	-0.56079600
C	-0.86422000	-1.24374000	-0.23029200
C	-1.25888200	-1.12781800	1.12007600
C	-2.99017500	-2.85782600	0.75128300
S	-2.64959800	-1.64494400	3.25926600
C	-1.37628100	-0.46404500	3.33794500
H	-1.17878500	0.03959100	4.27047700



C	-0.73894300	-0.29251900	2.16551200
H	0.07357200	0.40306200	2.03120300
C	-4.11286300	-3.68281100	1.31535000
H	-4.56880500	-3.19549100	2.17621600
H	-4.89854900	-3.84942900	0.58014300
C	-3.23305900	-3.99301600	-1.48259000
H	-4.19639300	-3.62249000	-1.84239900
H	-2.61676400	-4.19679300	-2.35683400
H	5.28595800	3.86245900	-0.03016000
H	7.25445800	0.31536000	0.13107700
H	3.95184700	4.01152000	1.10599100
H	-3.41432200	-4.94450400	-0.98377600
H	-3.75697400	-4.66262100	1.64511100
C	-0.85309600	2.17628800	-0.34093300
C	-2.04116200	2.47143300	-0.45673900
C	-3.39152100	2.76236900	-0.59005400
C	-6.12220700	3.32901300	-0.86432300
C	-4.30992500	1.74997900	-0.95928100
C	-3.88849500	4.06747500	-0.36184100
C	-5.23116000	4.33484100	-0.49880200
C	-5.64871200	2.04006100	-1.09179500
H	-3.94101500	0.74744400	-1.13129900
H	-3.19716600	4.84999500	-0.07894500
H	-5.59590000	5.33861800	-0.32052100
H	-6.33868100	1.25492600	-1.37460000
H	-7.17655100	3.54835000	-0.97016600