

Supporting Informations for:

π -extended phosphepines: redox and optically active P-heterocycles with non-planar framework

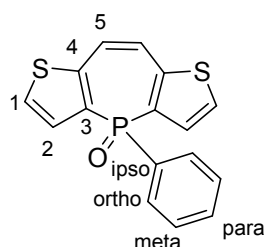
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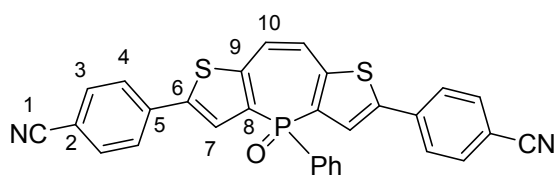
Experimental Part

Experimental Part General. All experiments were performed under an atmosphere of dry argon using standard Schlenk techniques. Commercially available reagents were used as received without further purification. Solvents were freshly purified using MBRAUN SPS-800 drying columns. Separations were performed by gravity column chromatography on basic alumina (Aldrich, Type 5016A, 150 mesh, 58 Å) or silica gel (Merck Geduran 60, 0.063-0.200 mm). ^1H , ^{13}C , and ^{31}P NMR spectra were recorded on Bruker AV III 400 MHz NMR spectrometers equipped with BBO or BBFO probeheads. Assignment of proton and carbon atoms is based on COSY, NOESY, edited-HSQC and HMBC experiments. ^1H and ^{13}C NMR chemical shifts were reported in parts per million (ppm) using residual solvent signal as reference. In the NMR description, C_q corresponds to quaternary carbon; ipso, ortho, meta, para correspond to the respective positions on the exocyclic P-Ph. High-resolution mass spectra were obtained on a Varian MAT 311 or ZabSpec TOF Micromass instrument at CRMPO (Scanmat, UMS 2001). UV-Visible spectra were recorded at room temperature on a VARIAN Cary 5000 spectrophotometer. The UV-Vis emission and excitation spectra measurements were recorded on a FL 920 Edinburgh Instrument equipped with a Hamamatsu R5509-73 photomultiplier for the NIR domain (300-1700 nm) and corrected for the response of the photomultiplier. Quantum yields were calculated relative to quinine sulfate (H_2SO_4 , 0.1 M), $\phi_{\text{ref}} = 0.55$. The electrochemical studies were carried out under argon using an Eco Chemie Autolab PGSTAT 30 potentiostat for cyclic voltammetry with the three-electrode configuration: the working electrode was a platinum disk, the reference electrode was a saturated calomel electrode and the counter-electrode a platinum wire. All potential were internally referenced to the ferrocene/ferrocenium couple. For the measurements, concentrations of 10^{-3} M of the electroactive species were used in freshly distilled and degassed dichloromethane and 0.2 M tetrabutylammonium hexafluorophosphate. Dibromodithienylethenes was prepared according to the literature.¹ Thermogravimetric Analysis and Differential Scanning Calorimetry were performed by using a Mettler-Toledo TGA-DSC-1 apparatus under dry nitrogen flow at a heating rate of $10^\circ\text{C}/\text{min}$.

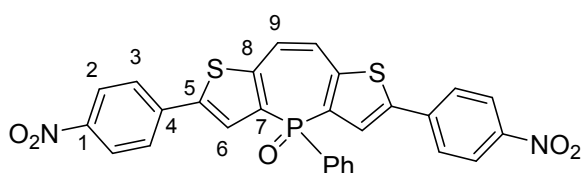


2. Dibromodithienylethene¹ (0.2 g, 0.57 mmol, 1 eq) was degassed under argon and dissolved in 6 ml of dry Et_2O . Then, the mixture was cooled to -78°C and $^t\text{BuLi}$ (1.61 mL, 2.29 mmol, 4 eq) was added dropwise. After 30 min at -78°C , the reaction was allowed to slowly warm up to RT. After 30 min the reaction is cooled to -78°C and PhPCl_2 (0.08 mL, 0.57 mmol, 1 eq) was added dropwise and stirred at -78°C for 1 h and then at RT for one night. A yellow precipitate was formed. The mixture is filtered through basic alumina and washed with CH_2Cl_2 and the solvent were evaporated. **4** (^{31}P NMR: -46.4 ppm) was dissolved in 30 mL of CH_2Cl_2 and directly oxidized with 10 mL of H_2O and NaIO_4 (0.365 g, 1.71 mmol, 3 eq). After 90 min, the organic phase was extracted with water dried over MgSO_4 and the solvent evaporated. The product was purified through silica gel column ($\text{CH}_2\text{Cl}_2/\text{MeOH}$: 95/5) and a yellow solid was obtained ($m = 110$ mg, $\eta = 61\%$). ^1H NMR (400 MHz, CD_2Cl_2) δ 7.55 (m, 2H, H_{ortho}), 7.51 (dd, 2H, $J = 5$ Hz, $J_{\text{H-P}} = 1.5$ Hz, H_1), 7.48 (dd, 1H, $J = 7$ Hz, $J = 1.5$ Hz, H_{para}), 7.41 (ddd, 2H, $J = 1.5$ Hz, $J = 3$ Hz, $J = 7$ Hz, H_{meta}), 7.31 (dd, 2H, $J = 5$ Hz, $J_{\text{H-P}} = 5$ Hz, H_2), 7.02 (s, 2H, H_5). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 145.5 (d, $J_{\text{C-P}} = 7$ Hz, C_4); 134.9 (d, $J_{\text{C-P}} = 112$ Hz, C_{ipso}); 132.2 (d, $J_{\text{C-P}} = 3$ Hz, C_{para}); 131.9 (d, $J_{\text{C-P}} = 13$ Hz, C_2); 131.8 (d, $J_{\text{C-P}} = 106$ Hz, C_3); 131.1 (d, $J_{\text{C-P}} = 11$ Hz, C_{ortho}); 128.8 (d, $J_{\text{C-P}} = 13$ Hz, C_{meta}); 128.7 (d, $J_{\text{C-P}} = 15$ Hz, C_1); 121.7 (s, C_5). ^{31}P NMR (162 MHz, CD_2Cl_2) δ +11.7 (s). HRMS (ESI, $\text{CH}_3\text{OH} / \text{CH}_2\text{Cl}_2$: 70/30) $[\text{M}+\text{Na}]^+(\text{C}_{16}\text{H}_{11}\text{NaPS}_3)$ m/z ; Calcd for : 336.9881 m/z ; Found : 336.9884.

¹ Levine, D. R.; Siegler, M. A.; Tovar, J. D., Thiophene-Fused Borepins As Directly Functionalizable Boron-Containing π -Electron Systems. *J. Am. Chem. Soc.* **2014**, 136, 7132-7139.

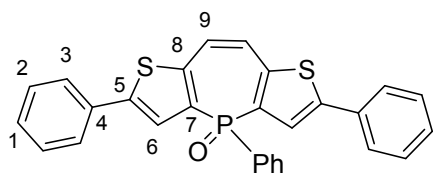


3 (*Direct-Arylation method A*). **2** (110 mg, 0.35 mmol, 1 eq), KOAc (135 mg, 1.4 mmol, 4 eq), Pd(OAc)₂ (0.3 mg, 0.017 mmol, 0.05 eq) and 4-Bromobenzonitrile (4 eq) were dissolved in DMAc (3 mL) under argon. The mixture is heated to 140°C for 20h. DMAc is then evaporated and the product was purified through silica gel column (CH₂Cl₂/AcOEt : 6/4) to afford **6** as a yellow solid (m = 104 mg, η = 58 %). ¹H NMR (400 MHz, CD₂Cl₂) δ 7.76 (d, 2H, J = 5 Hz, H₇), 7.69 (m, 8H, H₃ and H₄), 7.57 (m, 2H, H_{ortho}), 7.50 (m, 1H, H_{para}), 7.43 (m, 2H, H_{meta}), 7.02 (s, 2H, H₁₀). ¹³C NMR (75 MHz, CD₂Cl₂): δ 145.5 (d, J_{C-P} = 7 Hz, C₉); 145.3 (d, J_{C-P} = 7 Hz, C₆); 137.3 (s, C₅); 134.5 (d, J = 112 Hz, C_{ipso}); 133.7 (s, C₃); 131.0 (d, J_{C-P} = 81 Hz, C₈); 132.5 (d, J_{C-P} = 20 Hz, C_{para}); 130.8 (d, J_{C-P} = 11 Hz, C_{ortho}); 129.6 (d, J_{C-P} = 13 Hz, C₇); 129.1 (d, J_{C-P} = 12 Hz, C_{meta}), 126.8 (s, C₄); 122.4 (s, C₁₀); 118.8 (s, C₁); 112.2 (s, C₂). ³¹P NMR (162 MHz, CD₂Cl₂): δ +11.7 (s). HRMS (ESI, CH₂Cl₂ / CH₃OH : 8/2) : [M+Na]⁺(C₃₀H₁₇N₂ONaPS₂), m/z Calcd for : 539.0412, m/z Found : 539.0411.

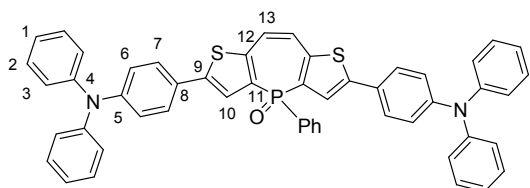


4. (*Direct-Arylation method B*) **2** (80 mg, 0.25 mmol, 1 eq), K₂CO₃ (170.7 mg, 1.02 mmol, 4 eq), Pd(OAc)₂ (5.6 mg, 0.025 mmol, 0.1 eq), 4-iodonitrobenzene (255 mg, 1.02 mmol, 4 eq), PCy₃ (18.8 mg, 0.04 mmol, 0.2 eq), PivOH (8.2 mg, 0.05 mmol, 0.3 eq) are dissolved in 2 mL of DMAc under

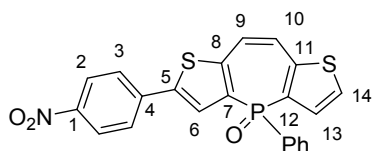
argon. The mixture is heated at 125°C for 20h. DMAc is then evaporated and the product was purified through silica gel column (CH₂Cl₂/AcOEt : 6/4) to afford an orange solid (m = 92 mg, η = 56 %). ¹H NMR (400 MHz, CD₂Cl₂) δ 8.25 (d, 4H, J = 8.8 Hz, H₂), 7.84 (d, 2H, J = 5.2 Hz, H₆), 7.78 (d, 4H, J = 8.8 Hz, J_{H-P} = 5 Hz, H₃), 7.59 (m, 2H, H_{ortho}), 7.52 (m, 1H, H_{para}), 7.45 (m, 2H, H_{meta}), 7.07 (s, 2H, H₉). ¹³C NMR (101 MHz, CD₂Cl₂): δ 147.8 (s, C₁), 145.9 (d, J = 13.6 Hz, C₈), 144.9 (d, J = 14.6 Hz, C₇), 139.2 (s, C₄), 135.3 (s, C₅), 133.0 (d, J = 114.9 Hz, C_{ipso}), 132.7 (d, J = 3.0 Hz, C_{para}), 130.8 (d, J = 9.8 Hz, C_{ortho}), 130.1 (d, J = 12.6 Hz, C₆), 129.1 (d, J = 12.9 Hz, C_{meta}), 127.0 (s, C₃), 124.9 (s, C₂), 122.6 (s, C₉). ³¹P NMR (162 MHz, CD₂Cl₂): δ +12.1 (s); HRMS (ASAP) [M]⁺(C₂₈H₁₇N₂O₅PS₂) m/z Calcd for : 556.0311, m/z Found : 556.0313.



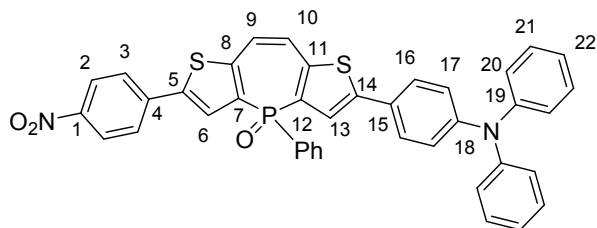
5. **5** was synthesized from **2** according to *Direct-Arylation method B* using 4-Bromobenzene (375 mg, 2.39 mmol, 10 eq) as starting material to afford a yellow solid (m = 66 mg, η = 56 %) after purification on silica gel column (CH₂Cl₂/AcOEt : 6/4). ¹H NMR (400 MHz, CD₂Cl₂) δ 7.64 (m, 2H, H₆), 7.60 (m, 6H, H_{ar}), 7.49 (dd, 1H, J = 1.6 Hz, J = 7.4 Hz, H_{para}), 7.45 (dd, 2H, J = 7.5 Hz, J = 3 Hz, H_{ortho}), 7.39 (m, 4H, H_{ar}), 7.34 (m, 2H, H_{meta}), 6.98 (s, 2H, H₉). ¹³C NMR (101 MHz, CD₂Cl₂): δ 148.0 (d, J_{C-P} = 15 Hz, C₈); 144.6 (d, J_{C-P} = 15 Hz, C₅); 135.0 (d, J = 112 Hz, C_{ipso}); 133.7 (s, C₄); 132.7 (d, J_{C-P} = 7 Hz, C_{para}); 131.4 (d, J_{C-P} = 105.3 Hz, C₇); 131.3 (d, J_{C-P} = 11 Hz, C_{ortho}); 129.9 (s, C₂); 129.4 (s, C₁); 129.3 (d, J_{C-P} = 13 Hz, C₆); 127.9 (d, J_{C-P} = 13 Hz, C_{meta}); 126.9 (s, C₃); 122.1 (s, C₉). ³¹P NMR (162 MHz, CD₂Cl₂): δ +12.1 (s). HRMS (ESI, CH₃OH / CH₂Cl₂ : 90/10) : [M+Na]⁺(C₂₈H₁₉ONaPS₂) m/z Calcd for : 489.0507 m/z; Found : 489.0511.



6. **6** was synthesized from **2** according to *Direct-Arylation method B* using 4-bromotriphenylamine (4 eq.) as starting material to afford a red solid after purification through silica gel column ($\text{CH}_2\text{Cl}_2/\text{AcOEt}$: 9/1) (η = 66 %). ^1H NMR (400 MHz, CD_2Cl_2) δ 7.59 (m, 2H, H_{ortho}), 7.51 (d, 2H, J = 5.1 Hz, H_{10}), 7.46 (m, 5H, H_{para} and H_7), 7.41 (m, 2H, H_{meta}), 7.28 (t, 8H, J = 8.4 Hz, H_2), 7.11 (m, 8H, J = 8.7 Hz, H_3), 7.06 (m, 4H, H_1), 7.01 (d, 4H, J = 8.7 Hz, H_6), 6.92 (s, 2H, H_{13}). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 148.7 (s, C_5), 147.6 (s, C_4), 147.5 (d, $J_{\text{C-P}}$ = 12.9 Hz, C_{12}), 143.2 (d, $J_{\text{C-P}}$ = 17.7 Hz, C_9), 135.4 (d, $J_{\text{C-P}}$ = 112 Hz, C_{ipso}), 132.3 (d, $J_{\text{C-P}}$ = 105.1 Hz, C_{11}), 132.1 (d, $J_{\text{C-P}}$ = 3 Hz, C_{para}), 130.9 (d, $J_{\text{C-P}}$ = 10.8 Hz, C_{ortho}), 129.8 (s, C_2), 128.9 (d, $J_{\text{C-P}}$ = 12.7 Hz, C_{meta}), 127.23 (s, C_7), 126.7 (s, C_8), 126.4 (d, $J_{\text{C-P}}$ = 13 Hz, C_{10}), 125.4 (s, C_3), 124.0 (s, C_1), 123.1 (s, C_6), 121.3 (s, C_{13}). ^{31}P NMR (162 MHz, CD_2Cl_2): δ +12.3 (s). HRMS (ESI, $\text{CH}_3\text{OH}/\text{CH}_2\text{Cl}_2$: 80/20) : $[\text{M}+\text{Na}]^+$ ($\text{C}_{52}\text{H}_{37}\text{N}_2\text{OPS}_2$) m/z Calcd for : 823.1977, m/z Found : 823.1976.



7. **7** was synthesized from **2** according to *Direct-Arylation method B* using 4-iodonitrobenzene (1.5 eq.) as reactant to afford an orange solid (m = 92 mg, η = 55 %). ^1H NMR (400 MHz, CD_2Cl_2) δ 8.22 (d, 2H, J = 8.8 Hz, H_2), 7.77 (d, 1H, J = 5.0 Hz, H_6), 7.75 (d, 2H, J = 8.8 Hz, H_3), 7.59 (d, 1H, J = 6.9 Hz, H_{14}), 7.57 (m, 2H, H_{ortho}), 7.51 (m, 1H, H_{para}), 7.45 (m, 2H, H_{meta}), 7.41 (dd, J = 5 Hz, $J_{\text{H-P}}$ = 5 Hz, 1H, H_{13}), 7.10 (d, 1H, J = 12.3 Hz, H_9), 7.01 (d, 1H, J = 12.3 Hz, H_{10}). ^{13}C NMR (101 MHz, CD_2Cl_2): δ 147.6 (s, C_1), 146.2 (d, J = 13.3 Hz, C_8), 145.2 (d, J = 14.2 Hz, C_7), 144.1 (d, J = 14.6 Hz, C_{12}), 139.3 (s, C_4), 135.3 (s, C_5), 133.9 (d, J = 8.6 Hz, C_{11}), 132.4 (d, J = 4 Hz, C_{para}), 132.3 (d, J = 27.3 Hz, C_{ipso}), 131.9 (d, C_{13}), 130.9 (d, J = 10.8 Hz, C_{ortho}), 130.0 (d, J = 12.9 Hz, C_6), 129.5 (d, J = 15.3 Hz, C_{14}), 129.0 (d, J = 12.7 Hz, C_{meta}), 126.8 (s, C_3), 124.8 (s, C_2), 123.1 (s, C_9), 121.2 (s, C_{10}). ^{31}P NMR (162 MHz, CD_2Cl_2): δ +12.2 (s). HRMS (ASAP) $[\text{M}]^+$ ($\text{C}_{22}\text{H}_{14}\text{NO}_3\text{P}_2\text{S}_2$) m/z Calcd for : 435.0147, m/z Found : 435.0142.



8. **8** was synthesized from **7** according to *Direct-Arylation method B* using 4-bromotriphenylamine (4 eq.) as starting material to afford a red solid after purification through silica gel column ($\text{CH}_2\text{Cl}_2/\text{AcOEt}$: 85/15) (η = 74 %). ^1H NMR (400 MHz, CD_2Cl_2) δ 8.23 (d, 2H, J = 8.9 Hz, H_2), 7.87 (d, 1H, J = 5.1 Hz, H_6), 7.78 (d, 2H, J = 8.9 Hz, H_3), 7.6 (d, 1H, J = 8.9 Hz, H_{13}), 7.59 (m, 2H, H_{ortho}), 7.52 (m, 1H, H_{para}), 7.48 (d, 2H, H_{16}), 7.44 (m, 2H, H_{meta}), 7.29 (t, 4H, J = 8.5 Hz, H_{21}), 7.11 (m, 4H, J = 8.5 Hz, H_{20}), 7.08 (m, 2H, H_{22}), 7.03 (d, 2H, J = 8.8 Hz, H_{17}), 7.02 (d, 1H, J = 12.3 Hz, H_9), 6.96 (d, 1H, J = 12.3 Hz, H_{10}). ^{13}C NMR (101 MHz, CD_2Cl_2): δ 149.0 (s, C_{18}), 148.6 (d, $J_{\text{C-P}}$ = 14.6 Hz, C_7), 147.7 (s, C_1), 147.5 (s, C_{19}), 146.4 (d, $J_{\text{C-P}}$ = 14 Hz, C_{11}), 144.0 (d, $J_{\text{C-P}}$ = 14.3 Hz, C_{12}), 142.8 (d, $J_{\text{C-P}}$ = 14.2 Hz, C_8), 139.4 (s, C_4), 134.8 (d, $J_{\text{C-P}}$ = 112.6 Hz, C_{ipso}), 132.9 (d, $J_{\text{C-P}}$ = 6.7 Hz, C_{14}), 132.5 (d, $J_{\text{C-P}}$ = 3.0 Hz, C_{para}), 131.9 (d, $J_{\text{C-P}}$ = 7.7 Hz, C_5), 130.8 (d, $J_{\text{C-P}}$ = 11 Hz, C_{ortho}), 130.3 (d, $J_{\text{C-P}}$ = 12.8 Hz, C_6), 129.8 (s, C_{21}), 129.0 (d, $J_{\text{C-P}}$ = 12.8 Hz, C_{meta}), 127.3 (s, C_{16}), 126.9 (s, C_3), 126.5 (d, $J_{\text{C-P}}$ = 12.9 Hz, C_{13}), 126.4 (s, C_{15}), 125.4 (s, C_{20}), 124.8 (s, C_2), 124.1 (s, C_{22}), 123.1 (s, C_9), 123.0 (s, C_{17}), 120.8 (s, C_{10}). ^{31}P NMR (162 MHz, CD_2Cl_2): δ +12.8 (s). HRMS (ESI, CH_2Cl_2 / CH_3OH : 90/10) : $[\text{M}+\text{Na}]^+$ ($\text{C}_{40}\text{H}_{27}\text{N}_2\text{O}_3\text{NaPS}_2$) m/z Calcd for : 701.1093, m/z Found : 701.1098.

X-ray Crystallographic Study:

Crystal structure determination: Single crystals suitable for X-Ray crystal analysis were obtained by slow diffusion of vapors of pentane into a dichloromethane solution of the derivatives at room temperature. Excepted compound **5** those single crystal data collection were performed at 150 K with an APEX II Bruker-AXS diffractometer (Centre de Diffractométrie X, Institut des Sciences Chimiques de Rennes, UMR6226 CNRS-Université de Rennes 1, France) with Mo- $K\alpha$ radiation ($\lambda = 0.71073$ Å), all the others diffraction data were collected on a D8 Venture Bruker-AXS diffractometer (Mo- $K\alpha$ radiation). The crystal structures were solved by dual-space algorithm using the SHELXT^{2a} program for all compounds excepted compound **2** that has been solved using direct methods and the *SIR97* program^{2b}. Crystal structures were refined with full-matrix least-square methods based on F^2 (*SHELXL-97*)³ with the aid of the *WINGX*⁴ program. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions.

Table S1: Crystal data and structure refinement

Compound	2	4	5	6	7
CCDC	1856401	1856404	1856402	1856406	1856405
Formula	C ₁₆ H ₁₁ OPS ₂	C ₂₈ H ₁₇ N ₂ O ₅ PS ₂	C ₂₈ H ₁₉ OPS ₂	C ₅₂ H ₃₇ N ₂ OPS ₂	C ₂₂ H ₁₄ NO ₃ PS ₂
MW	314.34	556.52	466.52	800.92	435.43
a (Å)	8.3478(12)	12.6071(11)	15.3061(17)	49.097(3)	8.3846(11)
b (Å)	15.798(2)	13.0276(14)	8.4556(7)	8.6102(5)	14.978(2)
c (Å)	21.359(2)	18.2019(18)	17.0192(17)	21.7918(13)	16.0842(19)
α (°)	90	83.700(18)	90	90	93.086(5)
β (°)	90	82.476(4)	96.521(4)	96.538(2)	102.944(5)
γ (°)	90	65.056(3)	90	90	98.836(5)
V (Å ³)	2816.9(6)	2682.3(5)	2188.4(4)	9152.3(10)	1937.1(4)
Z	8	4	4	8	4
Dc (g.cm ⁻³)	1.482	1.378	1.416	1.163	1.493
Crystal system	orthorhombic	triclinic	monoclinic	monoclinic	triclinic
Space group	P b c a	P -1	P 2 ₁ /n	C 2/c	P -1
T (K)	150(2)	150(2)	150(2)	150(2)	150(2)
Wavelength Mo- $K\alpha$ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
μ (mm ⁻¹)	0.482	0.299	0.336	0.189	0.383
$F(000)$	1296	1144	968	3344	896
θ limit (°)	2.92-27.48	2.93-27.48	2.95-27.47	3.02-27.48	2.53-27.53

^{2a} G. M. Sheldrick, *Acta Cryst.* A71 (2015) 3-8

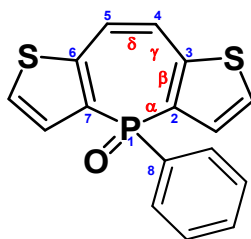
^{2b} Altomare, A., Burla, M. C.; Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. R. Spagna, *J. Appl. Cryst.*, **1999**, 32, 115-119

³ Sheldrick G.M., *Acta Cryst. A*, **2008**, 64, 112-122

⁴ Farrugia, L. J. *J. Appl. Cryst.*, **2012**, 45, 849-854

Index ranges <i>hkl</i>	-10<h<8 -20<k<20 -27<l<27	-16<h<16 -16<k<16 -23<l<23	-19<h<16 -10<k<10 -22<l<22	-63<h<63 -10<k<11 -28<l<28	-10<h<10 -19<k<19 0<l<20
Reflections collected	13001	64263	16338	74591	8892
Reflections [$I > 2\sigma(I)$]	2891	8053	3445	7778	7921
Data / restraints / parameters	3230/0/181	12283/0/685	4960/0/289	10488/0/ 523	8892/0/524
Goodness-of- fit on F^2	1.135	0.999	1.015	1.102	1.034
Final R indices [$I > 2\sigma(I)$]	R1=0.0310 wR2=0.0917	R1= 0.0555 wR2= 0.1198	R1= 0.0433 wR2=0.0970	R1= 0.0798 wR2=0.1749	R1= 0.0400 wR2=0.0897
R indices (all data)	R1= 0.0361 wR2=0.0951	R1=0.1005 wR2=0.1377	R1= 0.0750 wR2=0.1109	R1= 0.1104 wR2= 0.1871	R1= 0.0510 wR2=0.0954
Largest diff peak and hole (e Å ⁻³)	-0.636 and 0.551	-0.454 and 0.375	-0.320 and 0.357	-0.502 and 0.501	-0.351 and 0.434

Table S2 : Bond distances, angles and chemical shifts of compound **2**, **4-6** extracted from X-ray data and ¹H NMR.



Distance (Å)	Compounds			
	2	4	5	6
P1-C7	1.7880(15)	1.787(3)	1.789(2)	1.780(3)
P1-C2	1.7825(16)	1.787(3)	1.791(2)	1.791(3)
P1-C8	1.8014(16)	1.797(3)	1.802(2)	1.803(4)
C4-C5	1.350(2)	1.341(4)	1.340(3)	1.344(5)
C5-C6	1.445(2)	1.437(4)	1.435(3)	1.447(5)
C6-C7	1.390(2)	1.389(4)	1.389(3)	1.383(5)
Angle (°)				
C7-P1-C2	104.21(7)	107.66(13)	104.97(10)	103.47(15)
C2-P1-C8	104.93(7)	105.63(13)	105.10(10)	106.45(16)
C7-P1-C8	106.95(7)	105.42(12)	104.97(10)	108.44(16)

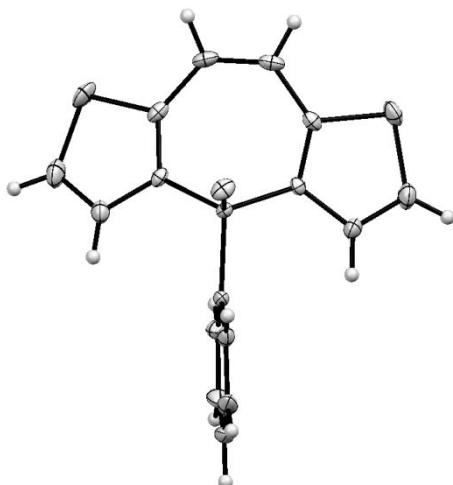


Figure S1: ORTEP representation of **2** with 50% probability ellipsoids

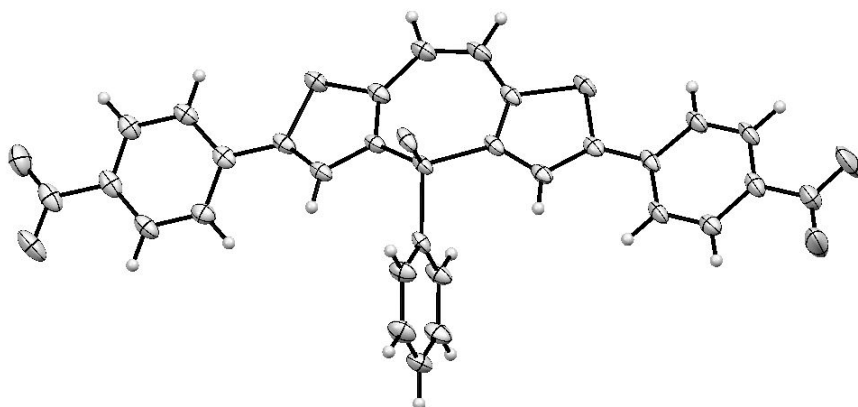


Figure S2: ORTEP representation of **4** with 50% probability ellipsoids

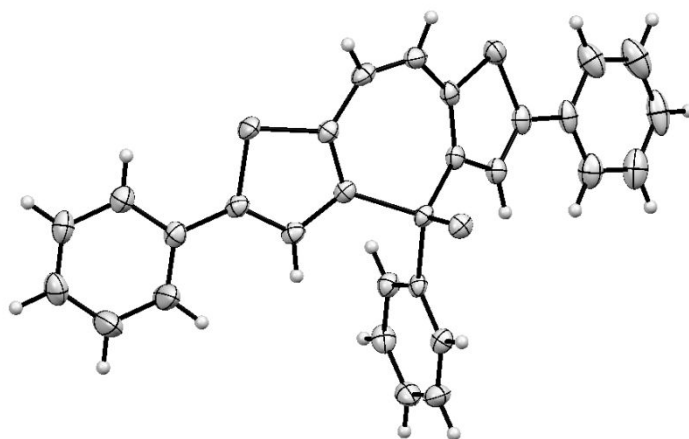


Figure S3: ORTEP representation of **5** with 50% probability ellipsoids

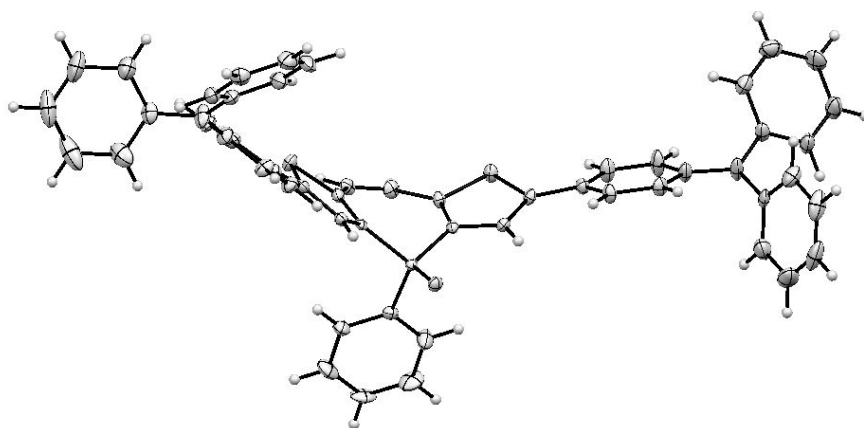


Figure S4: ORTEP representation of **6** with 50% probability ellipsoids

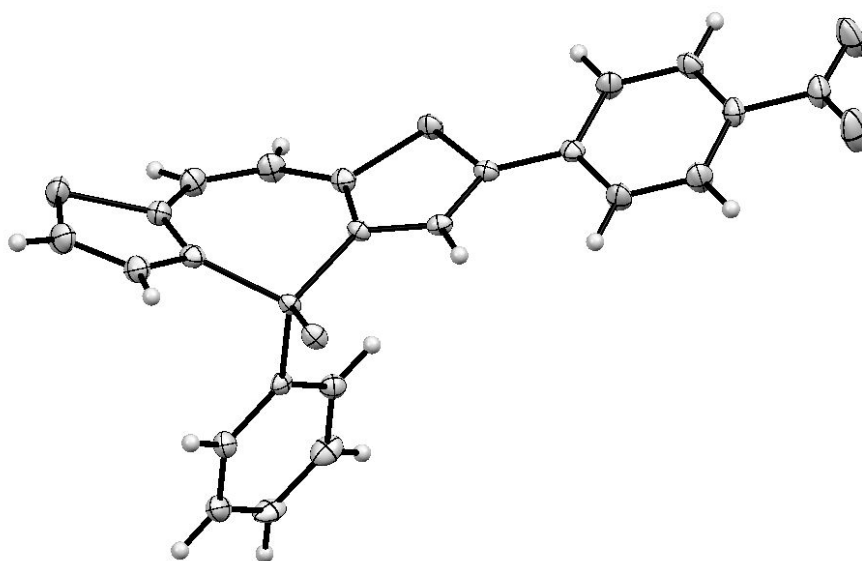


Figure S5: ORTEP representation of **7** with 50% probability ellipsoids

In the case of **3**, single crystals were obtained and several thin yellow plates were tested on the diffractometer, showing a roughly good diffraction power. Finally, a stable crystal was measured, providing a medium quality diffraction data set ($R_{int} \sim 9.3$). Crystal structure were solved and refined, leading to a medium quality structural refinement ($R_1 = 9.26$), even if the structural model is correct, chemical meaningful and unambiguous. Nevertheless, the quality of the data set and structural refinement (B-type alert still remains in the CHECKCIF procedure, due to a large positive residual electronic density of $1.7 \text{ e/\AA}^3$ that could be due to a refinement artefact caused by weak diffraction data below $0.95 \text{ \AA}$ of resolution) prevent its publication.

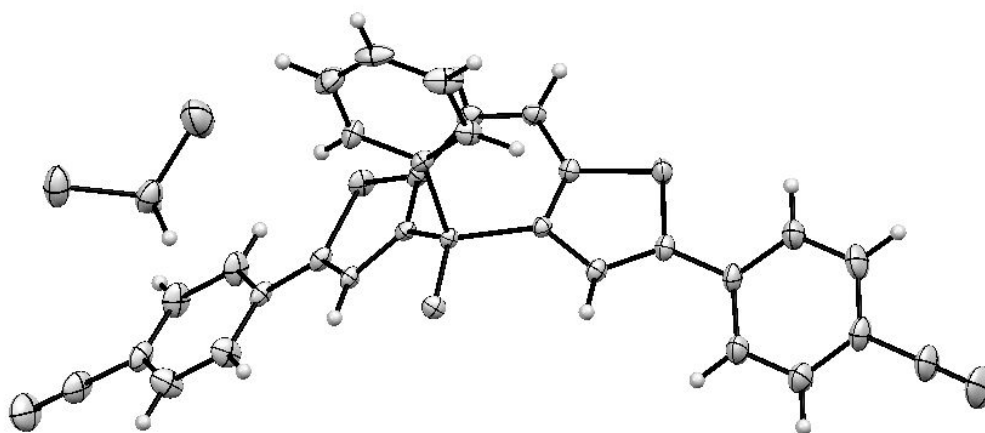


Figure S6: ORTEP representation of **3** with 50% probability ellipsoids

Structural data for **3**

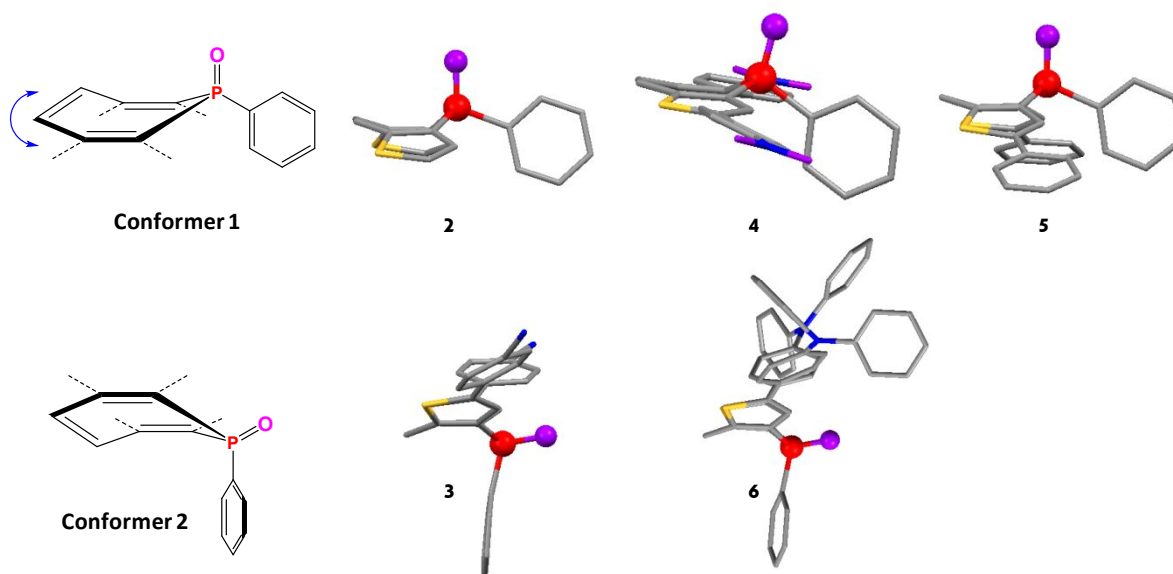
Compound	3
Formula	C ₃₀ H ₁₇ N ₂ O P S ₂ , C H ₂ Cl ₂
MW	601.47
a (Å)	18.6954(18)
b (Å)	8.4480(10)
c (Å)	c = 18.8561(19)
α (°)	90
β (°)	110.034(3)°
γ (°)	90
V (Å ³)	2797.9(5)
Z	4
D _c (g.cm ⁻³)	1.428
Crystal system	monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>
T (K)	150(2)
Wavelength Mo-K α (Å)	0.71073
μ (mm ⁻¹)	0.468
<i>F</i> (000)	1232
θ limit (°)	3.065-27.482
Index ranges <i>hkl</i>	-24< <i>h</i> <24 -10< <i>k</i> <9 -24< <i>l</i> <24
Reflections collected	27269
Reflections [<i>I</i> >2 σ (<i>I</i>)]	4964
Data / restraints / parameters	6376/0/352
Goodness-of-fit on <i>F</i> ²	1.056
Final <i>R</i> indices [<i>I</i> >2 σ (<i>I</i>)]	R1=0.0926 wR2=0.2309
<i>R</i> indices (all data)	R1= 0.1107 wR2=0.2480
Largest diff peak and hole (e Å ⁻³)	-1.259 and 1.732

List of Cartesian coordinates obtained from crystal structure of **3**

P1	8.415100	3.697521	10.334285
S1	12.096960	4.106573	12.515368
S2	5.985484	4.403942	13.809812
O1	8.173763	4.345651	9.015041
C2	8.334403	1.899955	10.261298

C3	7.104084	1.249459	10.428884
H3	6.337409	1.736647	10.706249
C4	7.018714	-0.115738	10.186186
H4	6.194209	-0.565974	10.319900
C5	8.123610	-0.826214	9.750395
H5	8.048603	-1.751490	9.547061
C6	9.332464	-0.181632	9.613989
H6	10.093553	-0.675223	9.332052
C7	9.460560	1.165824	9.877944
H7	10.306446	1.591426	9.801769
C11	9.719801	3.070003	13.366049
H11	10.246168	2.535693	13.949105
C12	10.429888	3.708672	12.283123
C13	10.009031	4.096436	11.020391
C14	11.037066	4.723277	10.271397
H14	10.908349	5.058924	9.392159
C15	12.239402	4.800154	10.937308
C16	13.515893	5.311258	10.435969
C17	13.550161	6.270105	9.419122
H17	12.734446	6.618695	9.076989
C18	14.752073	6.720384	8.901841
H18	14.766273	7.359314	8.198693
C19	15.938142	6.224486	9.422664
C20	15.933003	5.287603	10.451913
H20	16.749805	4.961620	10.809316
C21	14.728271	4.839014	10.946165
H21	14.721071	4.197364	11.647436
C22	17.201818	6.711091	8.900069
N23	18.194777	7.116595	8.494393
C31	8.409302	3.136742	13.653032
H31	8.129116	2.657411	14.424084
C32	7.365657	3.846374	12.936456
C33	7.242644	4.190208	11.589578
C34	6.045692	4.896461	11.299582
H34	5.815554	5.199668	10.429256
C35	5.257018	5.094989	12.397563
C36	3.941659	5.738727	12.451771
C37	3.341762	6.197453	11.266808
H37	3.822090	6.146630	10.449540
C38	2.062283	6.721228	11.273893
H38	1.668525	7.021538	10.462985
C39	1.354661	6.808243	12.460807
C40	1.941340	6.395136	13.651260
H40	1.465768	6.476727	14.469433
C41	3.229521	5.859533	13.645947
H41	3.626279	5.574827	14.460523
C42	0.004618	7.296538	12.430690
N43	-1.081988	7.676698	12.365145
C11	1.113944	1.982492	10.962463
C12	3.770035	1.512192	12.040072
C101	2.636863	2.733773	11.466990
H10A	3.034147	3.221400	10.701963
H10B	2.460099	3.387141	12.189234

Figure S7: view of the conformers of the seven-membered rings observed in the crystals.



Optical spectra

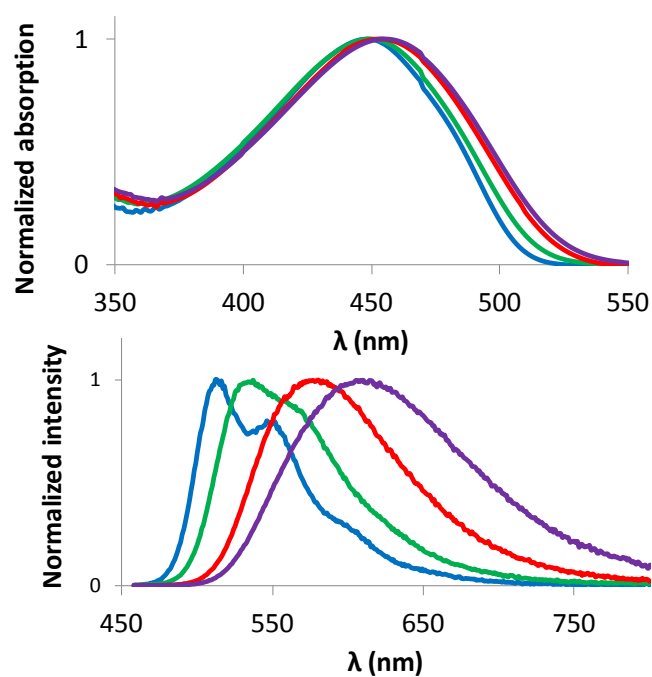


Fig S8: Absorption (up) and emission (down) spectra of **6** in diluted solution ($c = 10^{-6}\text{M}$) of pentane (blue), diethylether (green), DCM (red) and DMF (purple).

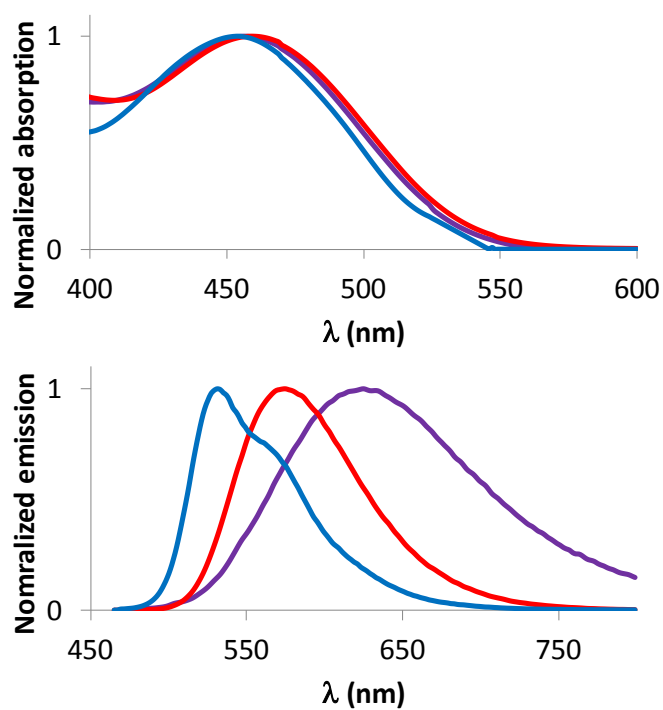


Fig S9: Absorption (up) and emission (down) spectra of **8** in diluted solution ($c = 10^{-6}\text{M}$) of pentane (blue), DCM (red) and DMF (purple).

NMR spectra

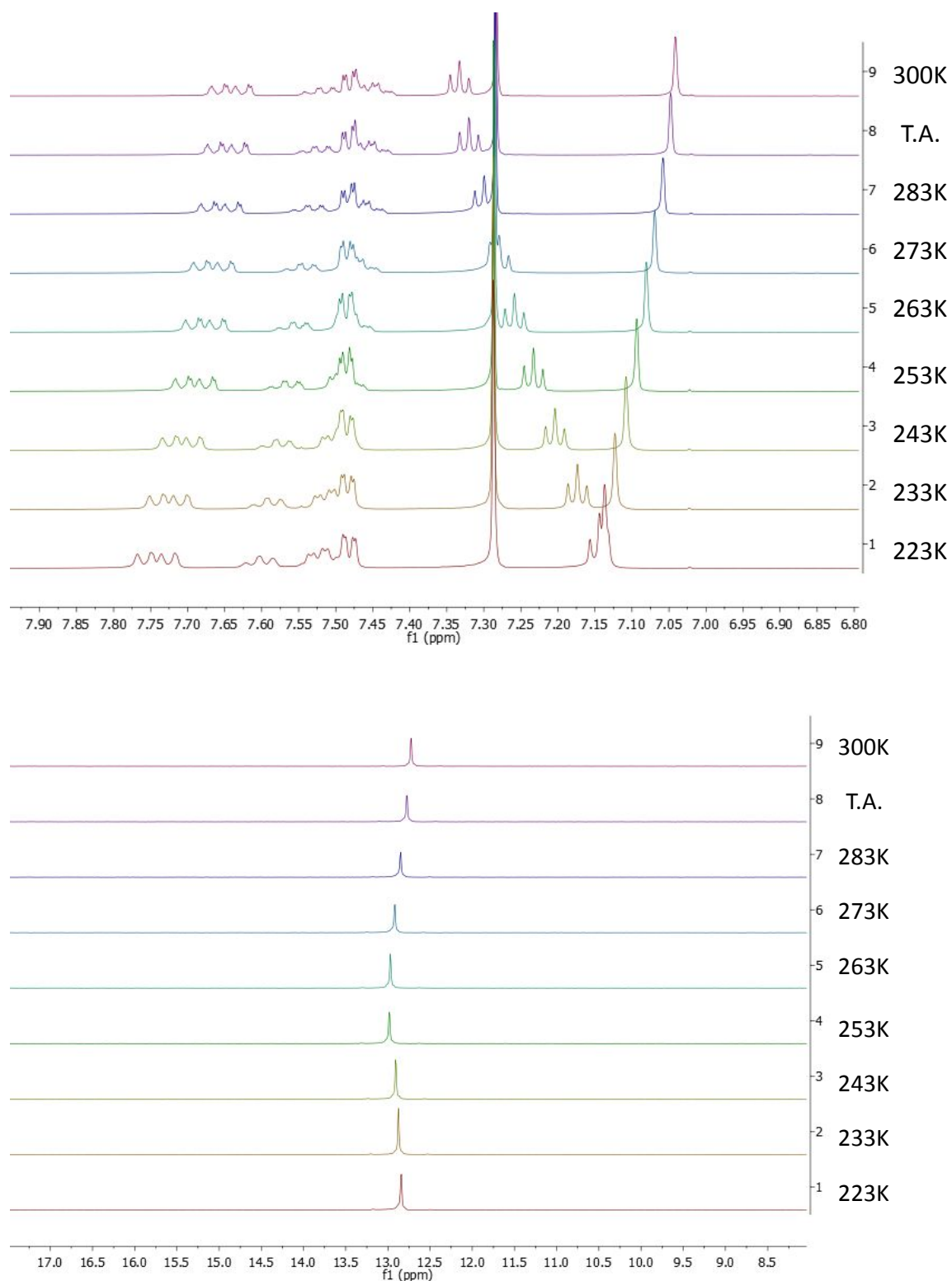


Figure S10 : Variable temperature ¹H NMR (top) and ³¹P NMR (bottom) experiments performed in CDCl₃ for compound **2**.

a)



c)

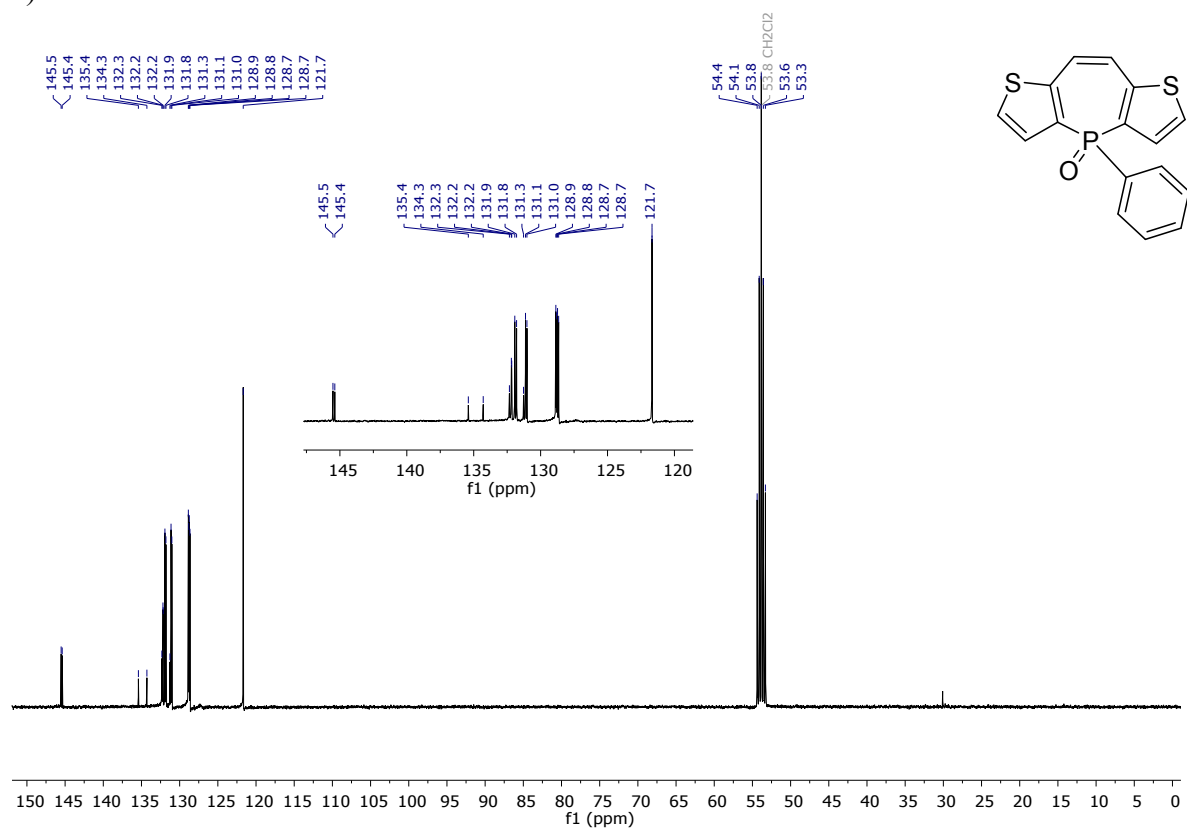
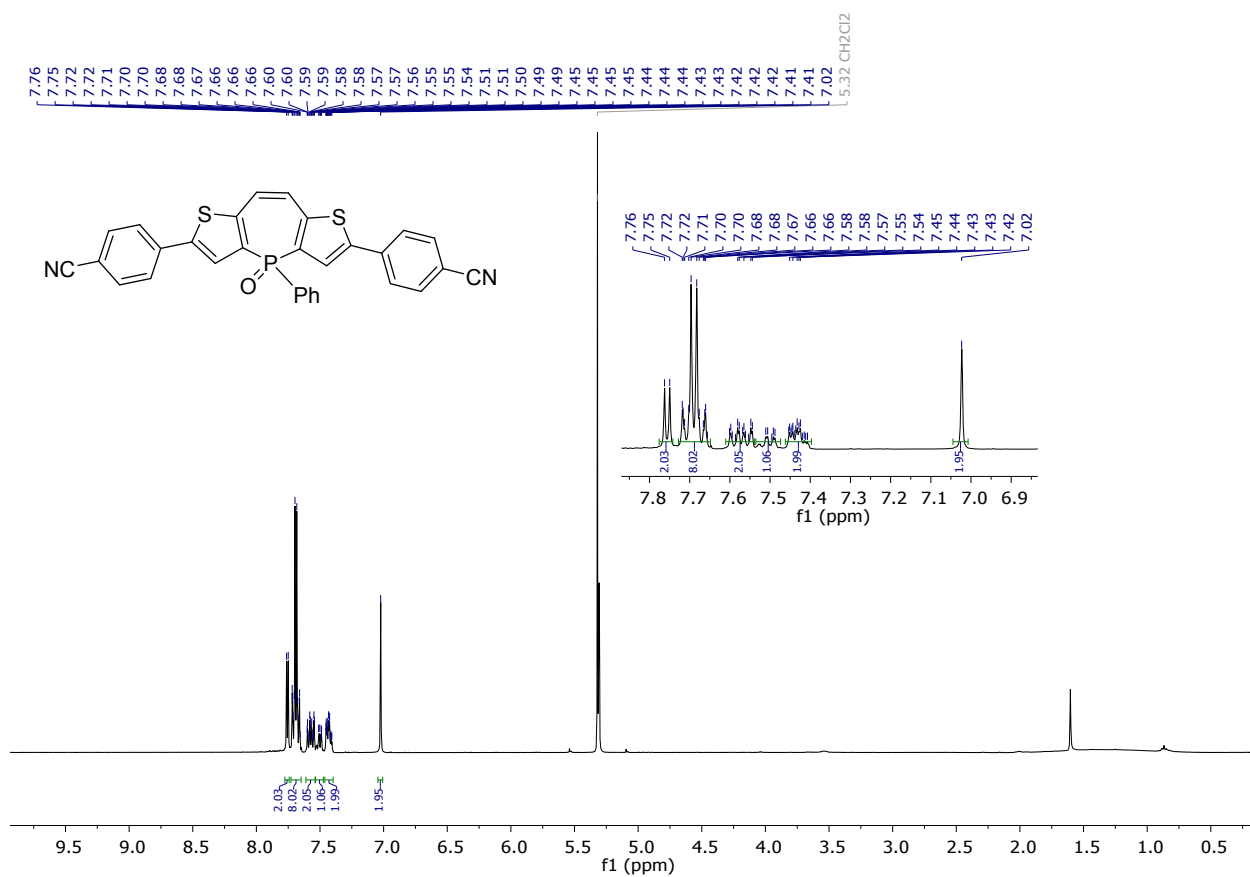


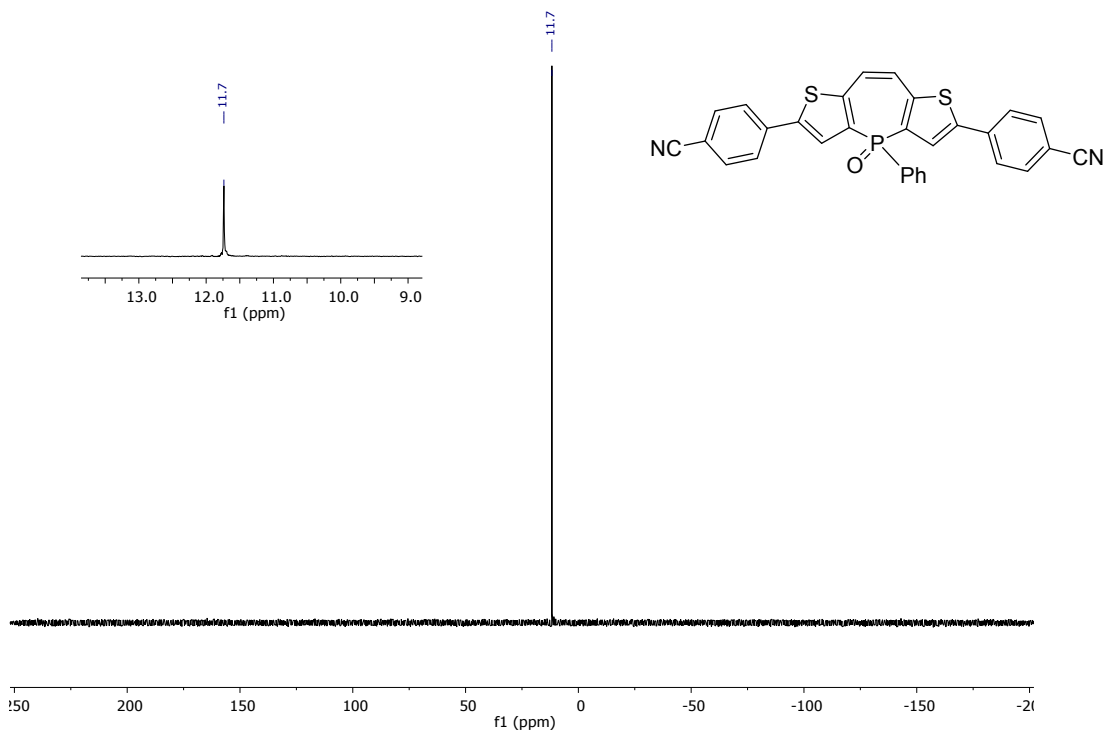
Figure S11: a) ¹H NMR (400 MHz, CD₂Cl₂), b) ¹³P{¹H} NMR and c) ¹³C{¹H} NMR spectra of compound 2.

Compound 3

a)



b)



c)

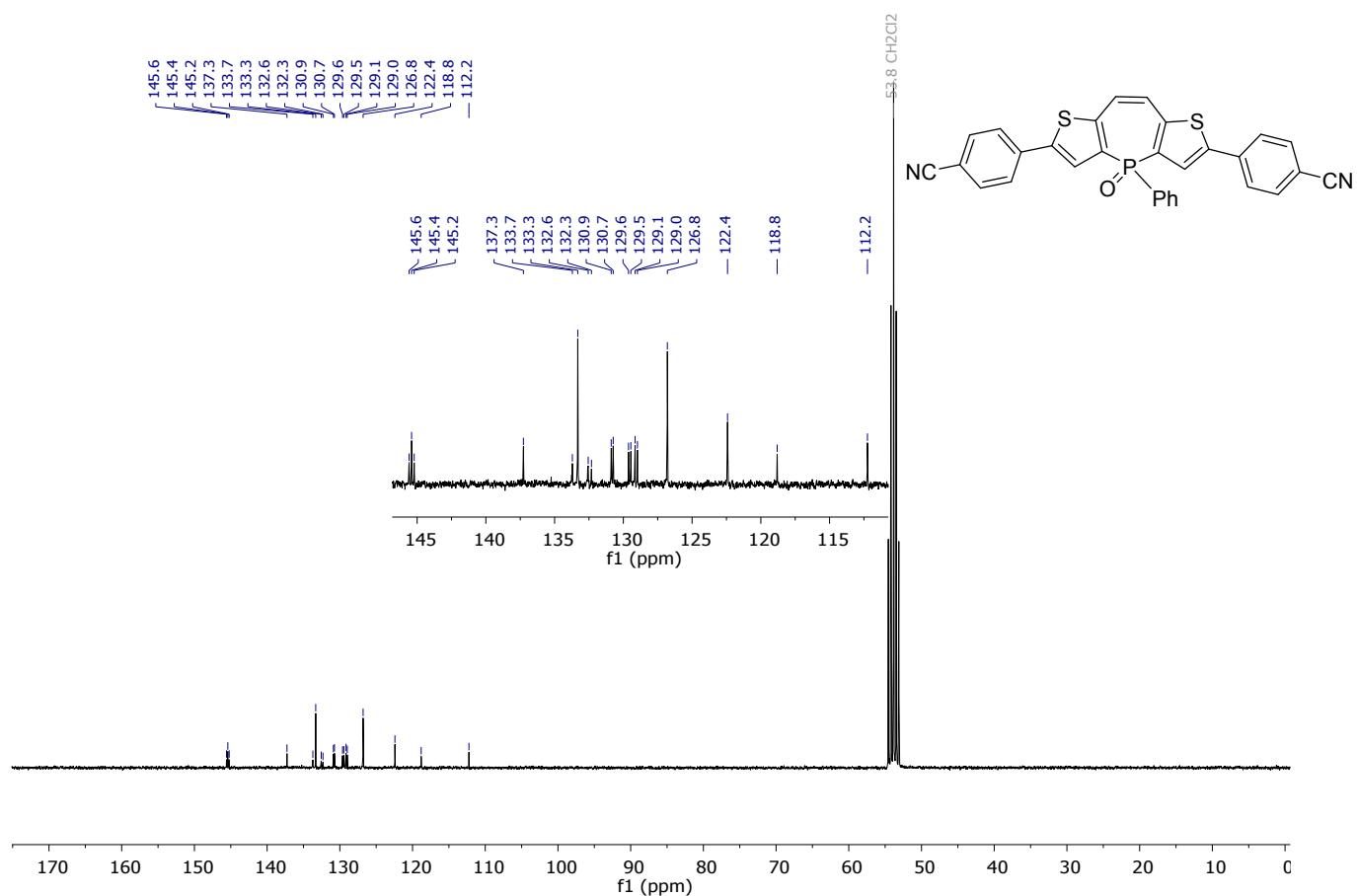
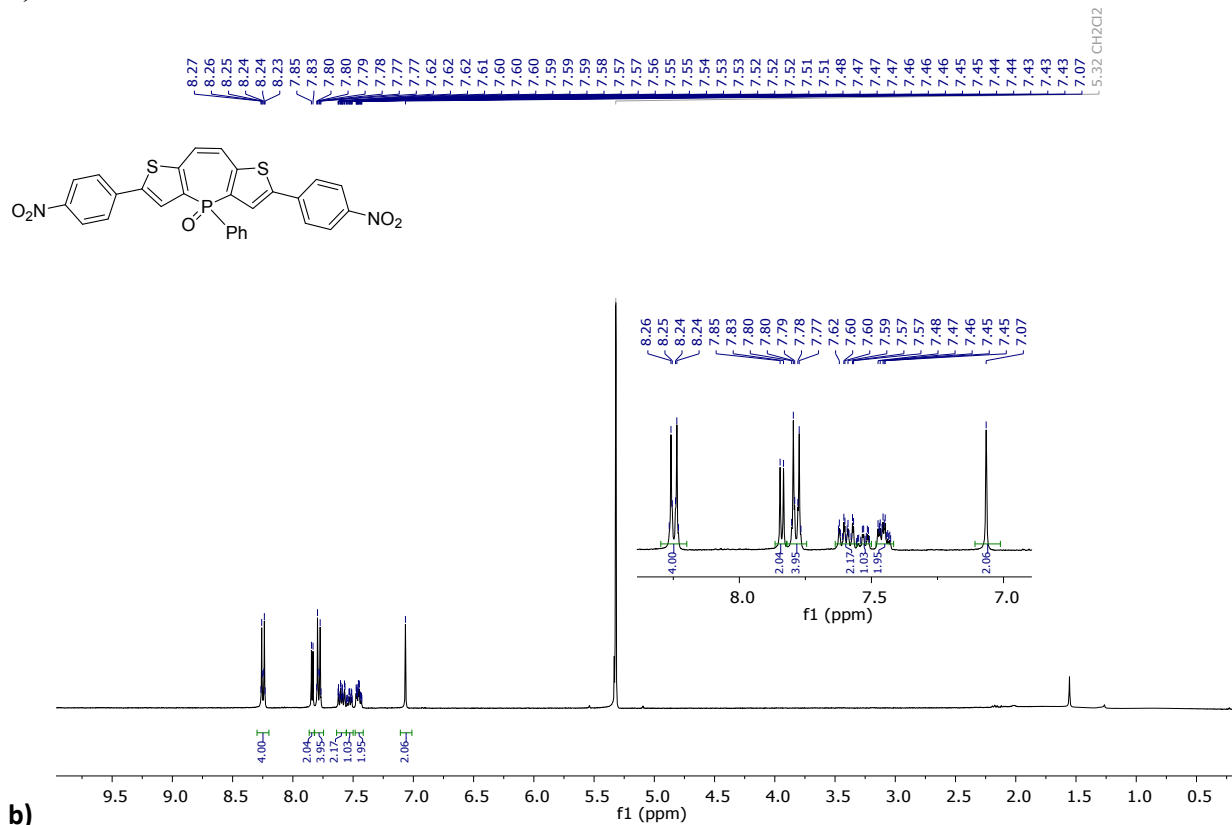


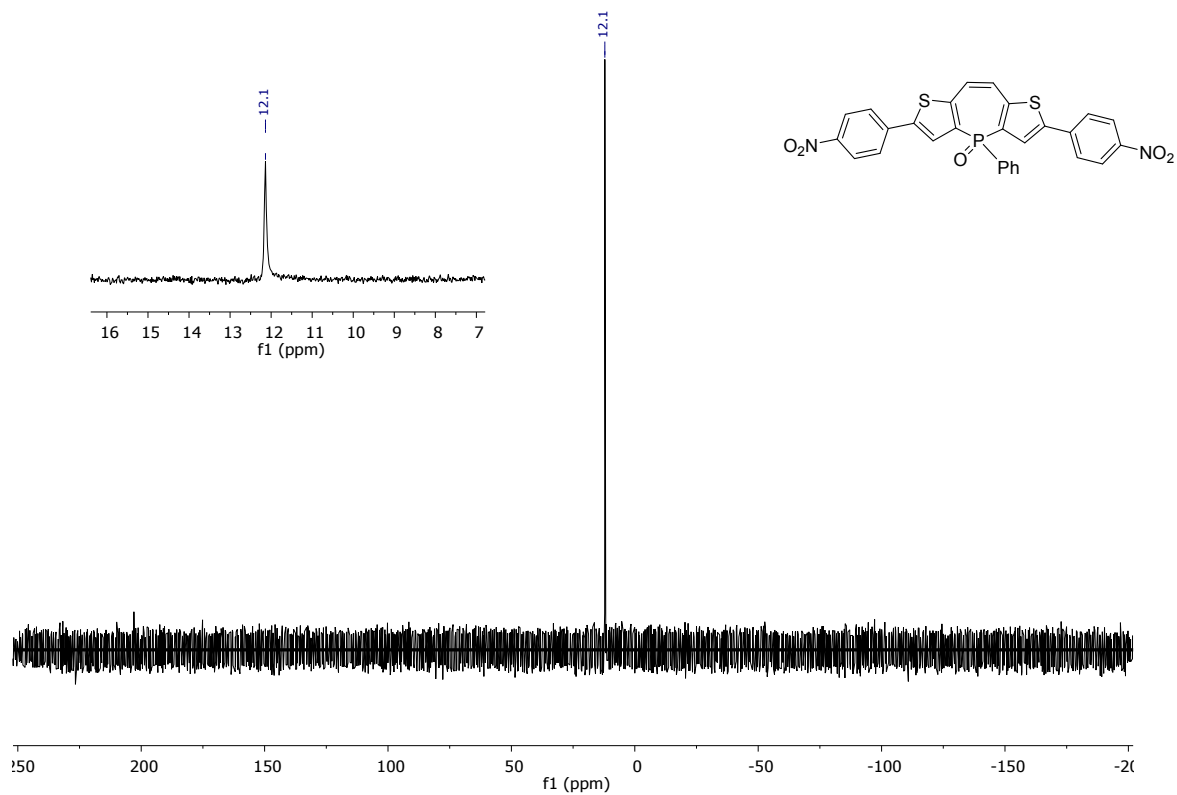
Figure S12: a) ¹H NMR (400 MHz, CD₂Cl₂), b) ¹³P {¹H} NMR and c) ¹³C {¹H} NMR spectra of compound 3.

For compound 4

a)



b)



c)

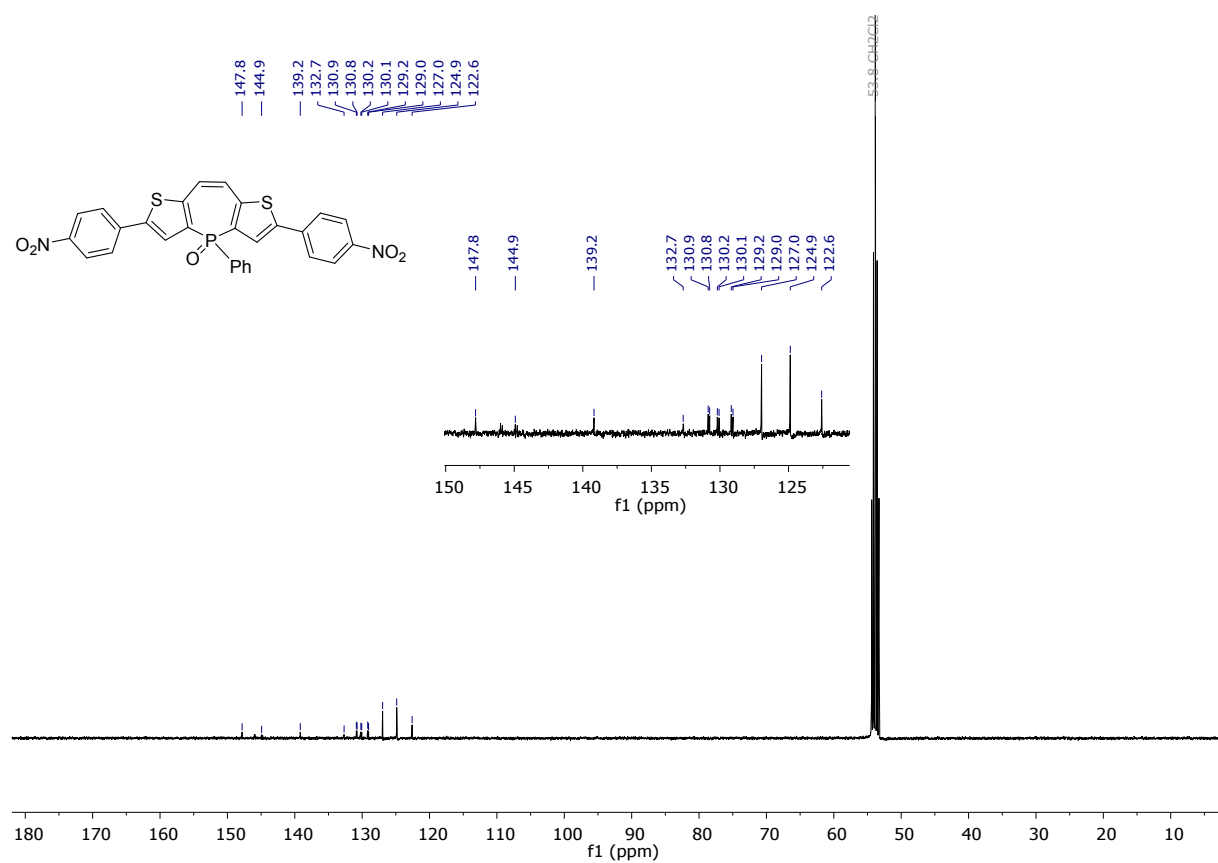
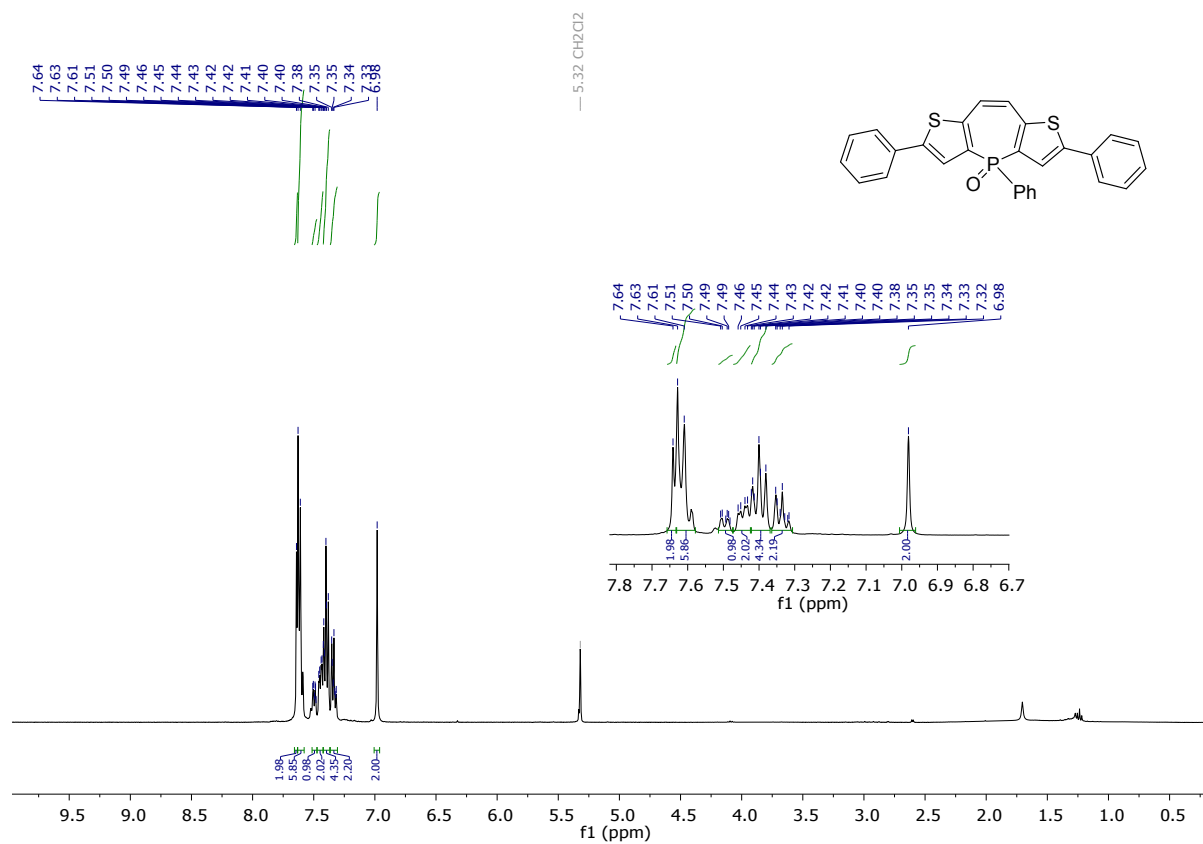


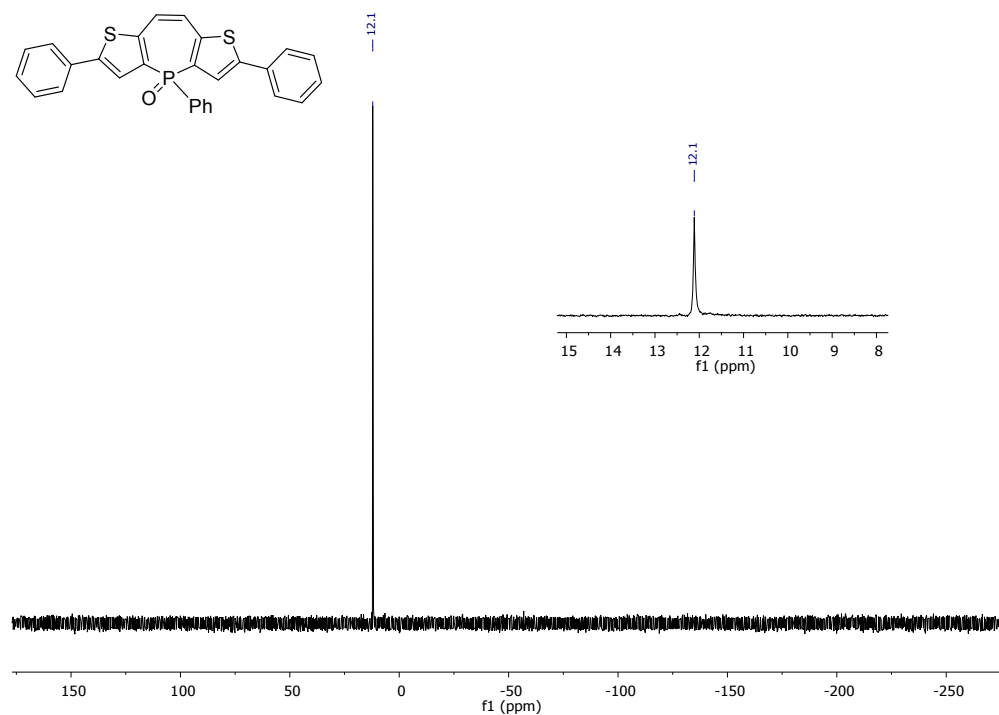
Figure S13: ¹H NMR (400 MHz, CD₂Cl₂), ¹³P{¹H} and ¹³C{¹H} NMR spectra of compound 4

For compound 5

a)



b)



c)

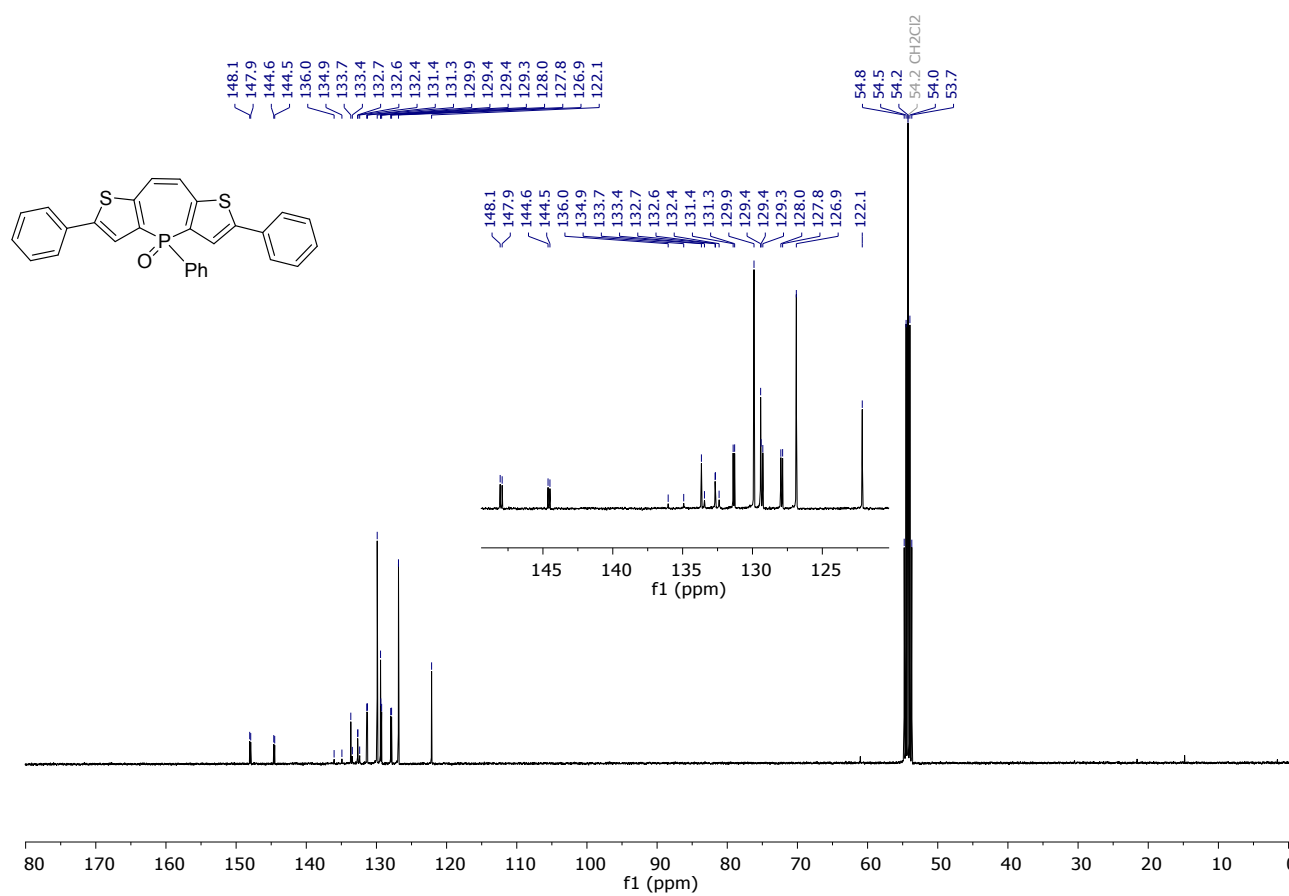
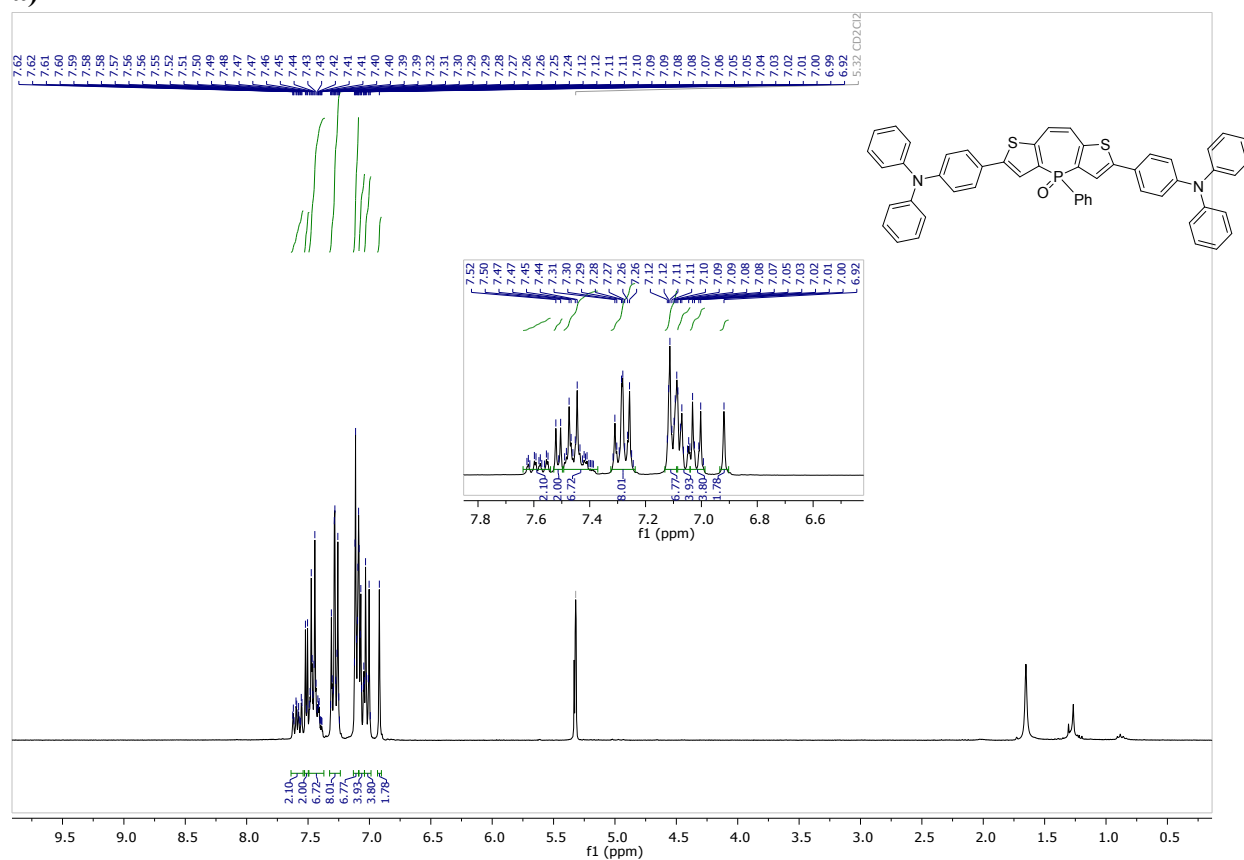


Figure S14: a) ¹H NMR (400 MHz, CD₂Cl₂), b) ¹³P{¹H} NMR and c) ¹³C{¹H} NMR spectra of compound **5**.

For compound 6

a)



c)

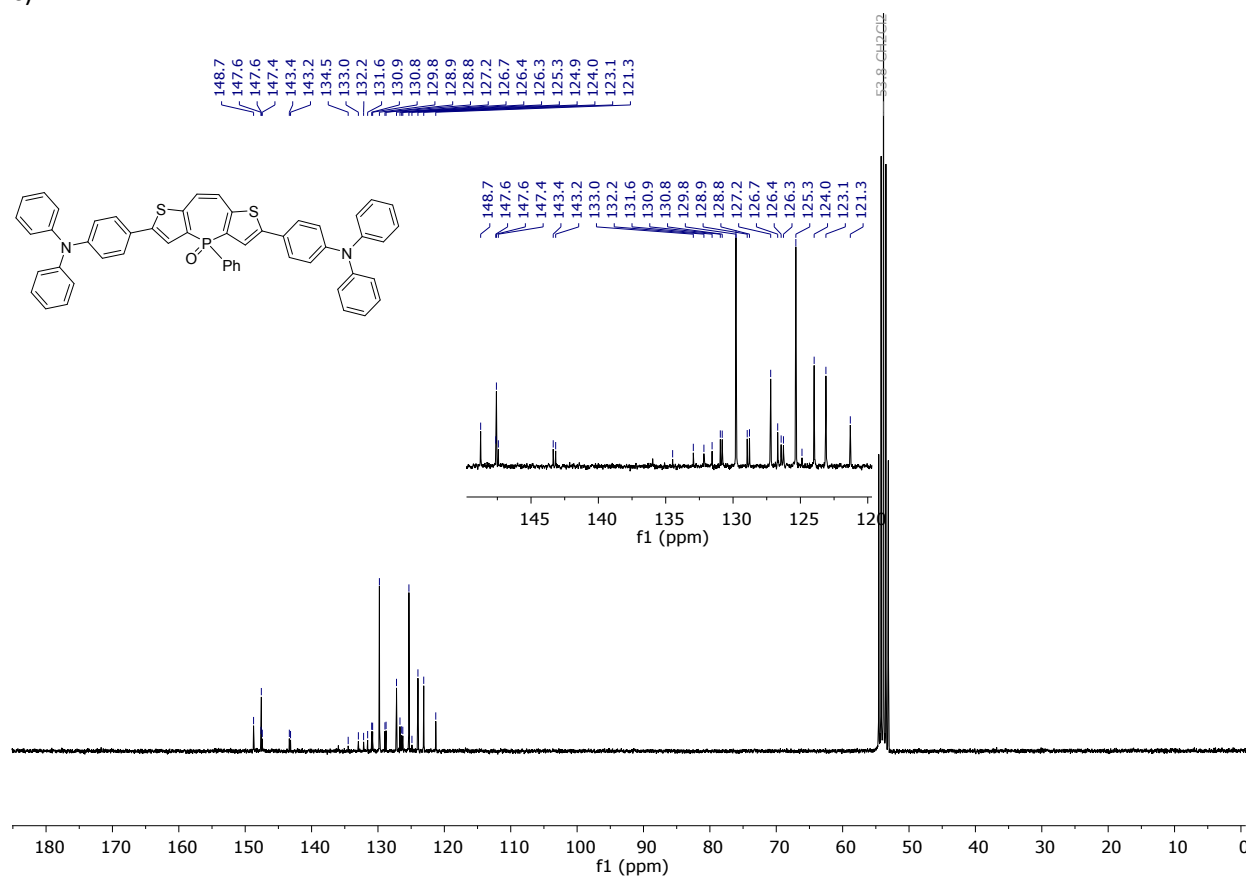
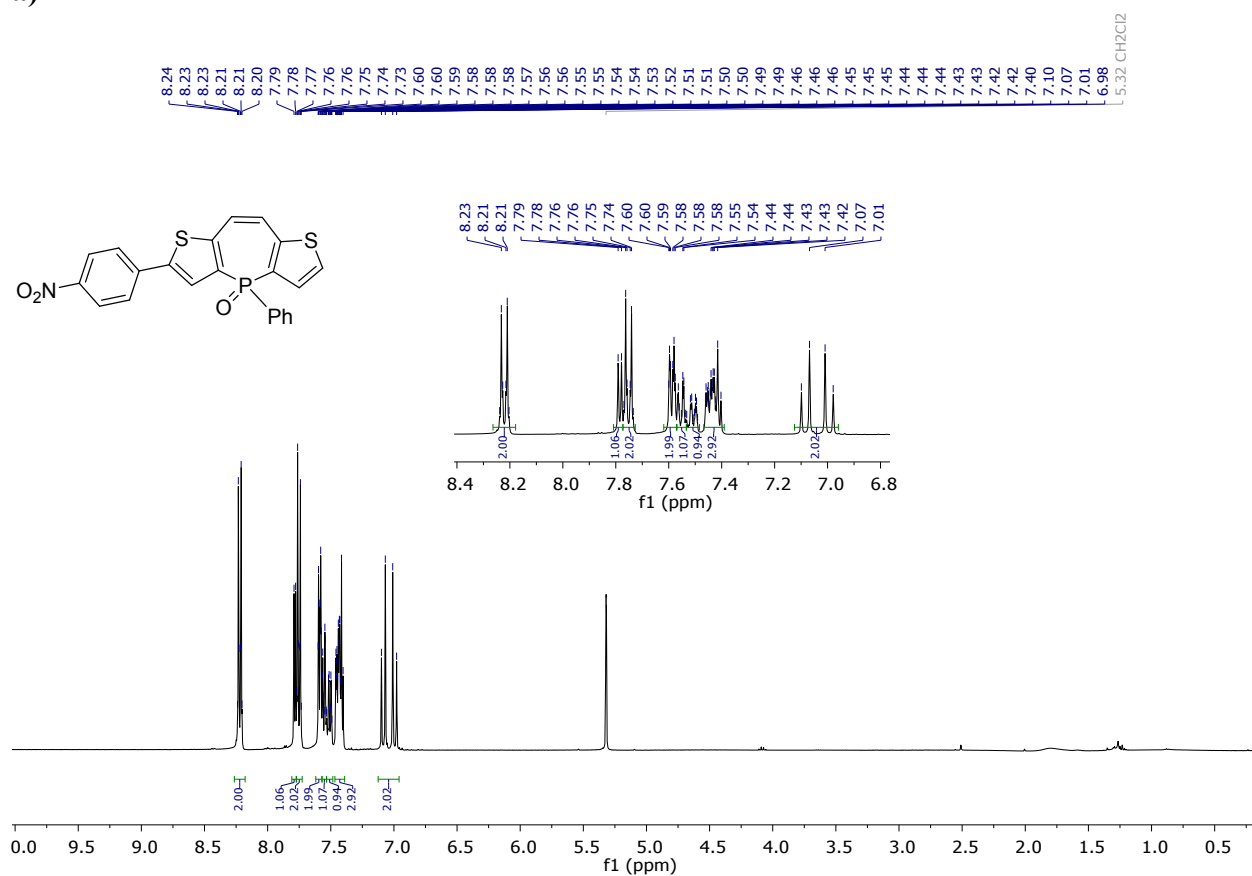


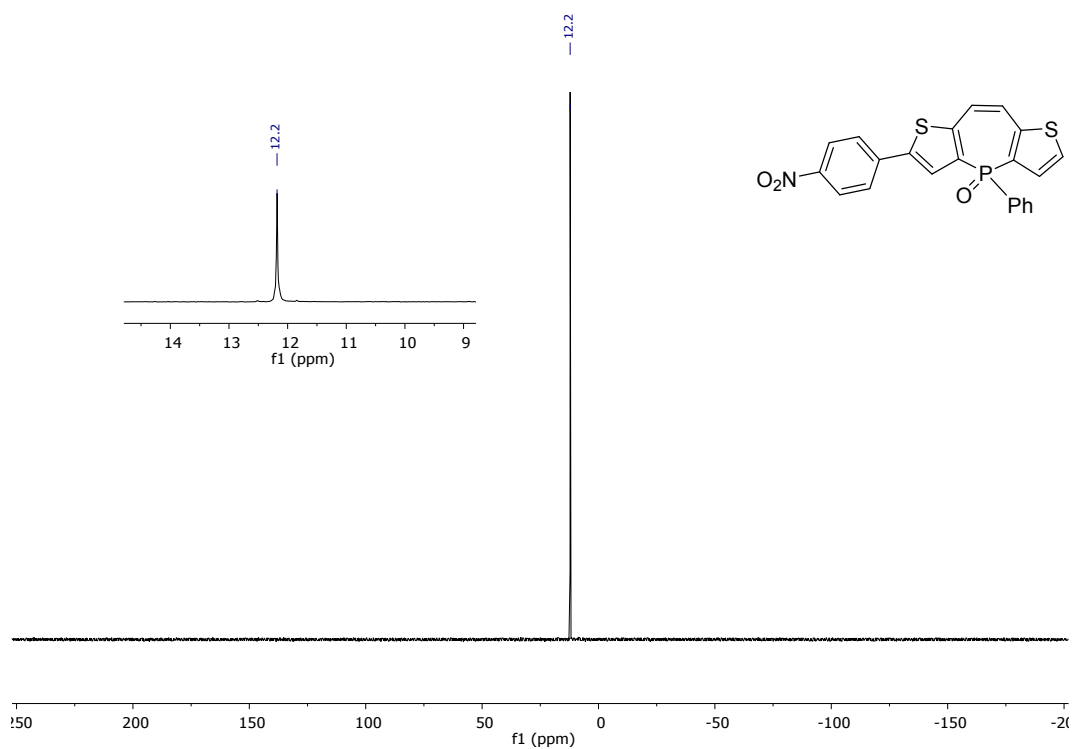
Figure S15: a) ^1H NMR (400 MHz, CD_2Cl_2), b) $^{13}\text{P}\{^1\text{H}\}$ NMR and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound 6.

For compound 7

a)



b)



c)

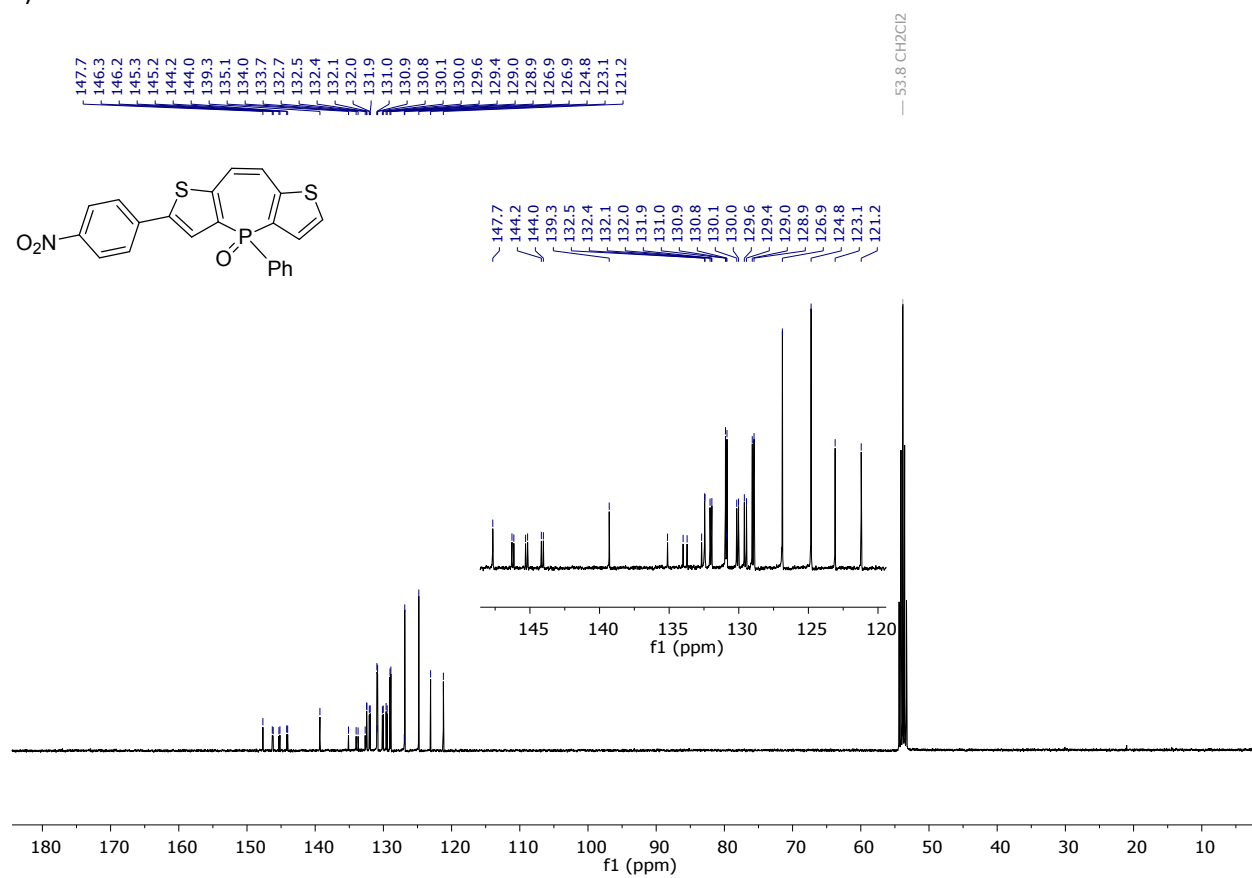
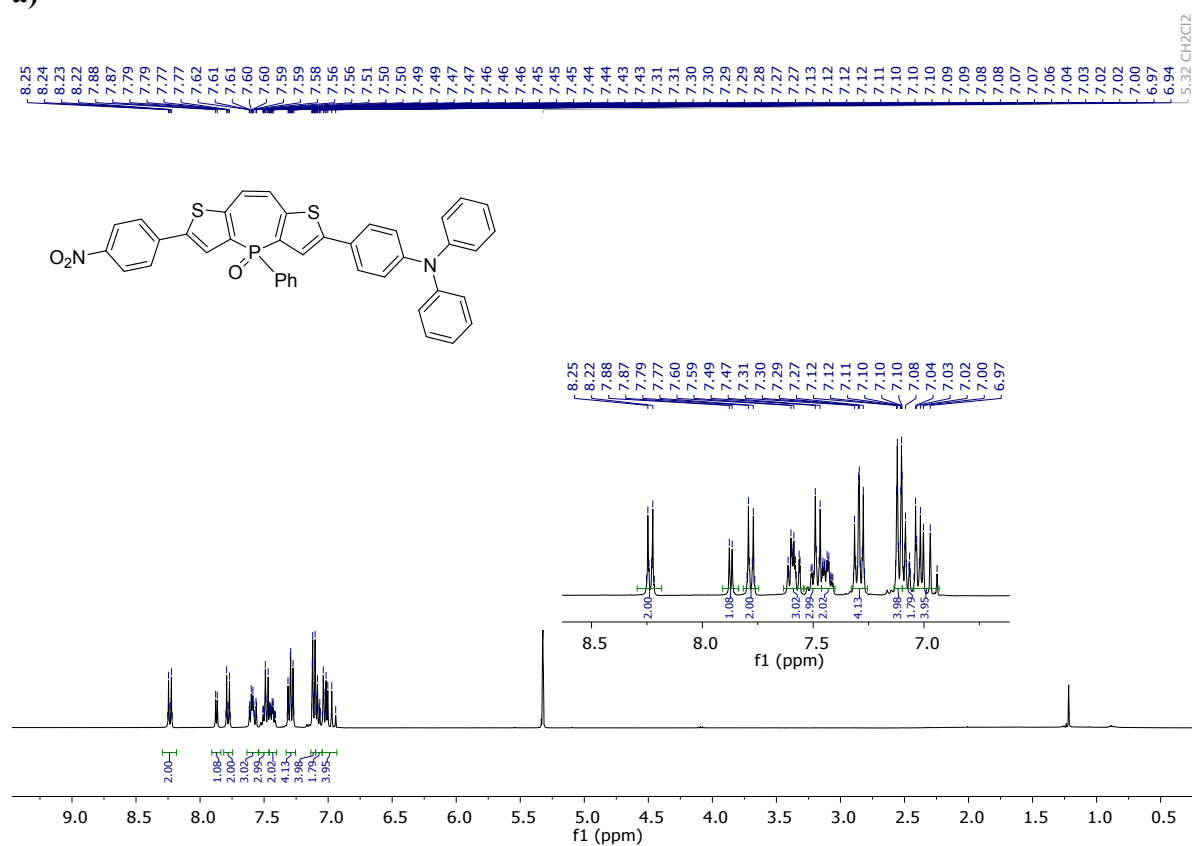


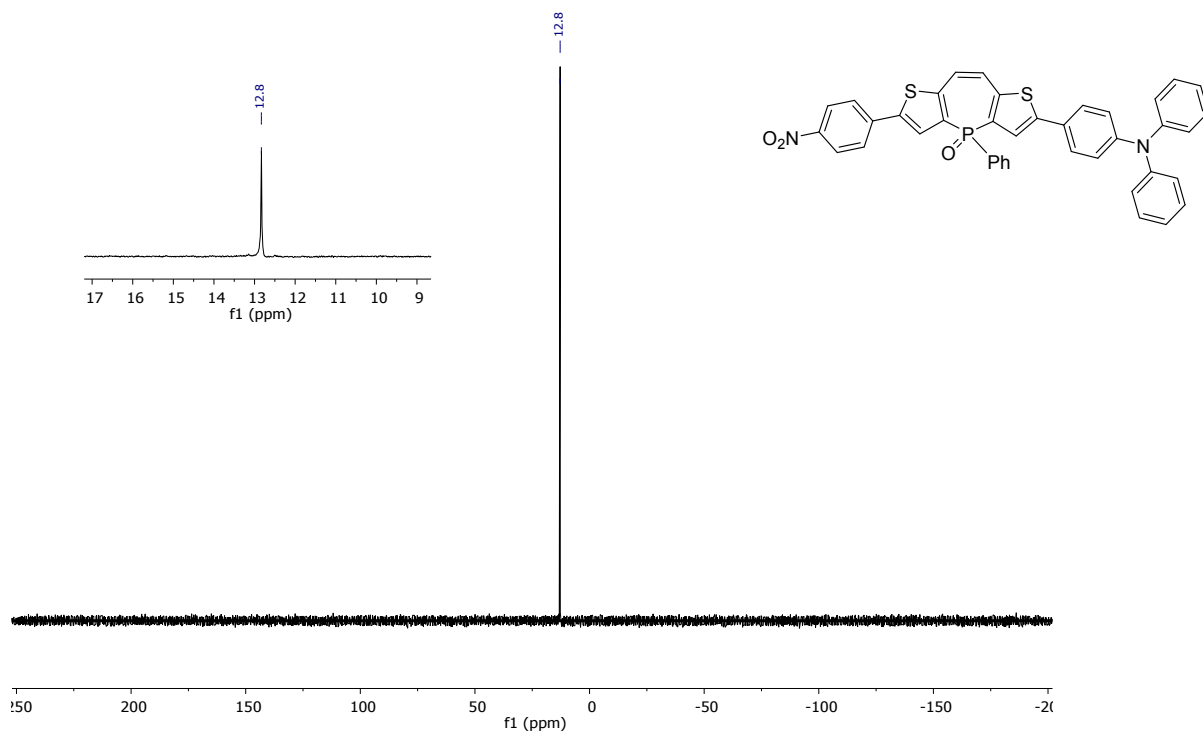
Figure S16: a) ¹H NMR (400 MHz, CD₂Cl₂), b) ¹³P{¹H} NMR and ¹³C{¹H} NMR spectra of compound 7

For compound 8

a)



b)



c)

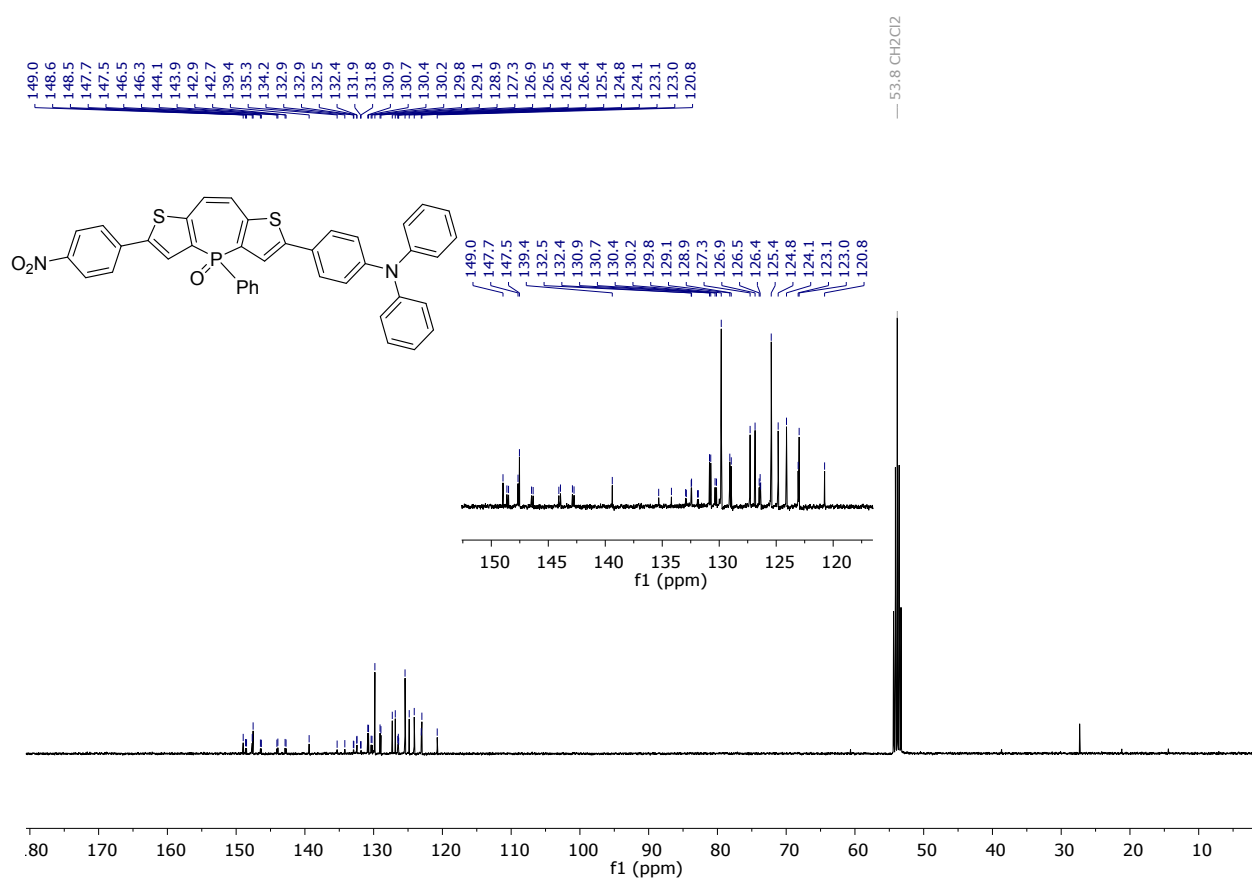


Figure S17: a) ¹H NMR (400 MHz, CD₂Cl₂), b) ¹³P{¹H} and ¹³C{¹H} NMR spectra of **8**

OFETs Fabrication and Characterization

Bottom gate-bottom contacts transistors were fabricated on glass substrates. Substrates were previously cleaned with acetone and rinsed with ethanol. An aluminium layer of 150 nm is then deposited by thermal evaporation and wet etched to define gate electrodes. 420 nm thick SU-8 photoresist (from Microchem) was spin-coated and then exposed to UV light to define gate insulating layer (see MicroChem Su-8 2000 Permanent Epoxy Negative Photoresist Processing Guidelines for Su-8 2000.5, Su-8 2002, So-8 2005, Su-8 2007, Su-8 2010 and Su-8 2015-http://www.microchem.com/pdf/SU-82000DataSheet2000_5thru2015Ver4.pdf). Then, 40 nm thick gold film was thermally evaporated and then wet etched to form source and drain electrodes. Finally, the active layer was deposited by thermal evaporation under a high vacuum of 2.10^{-7} mbar. Substrate temperature was kept constant ($T_{\text{sub}}=30^{\circ}\text{C}$), deposition rate and layer thickness were fixed to 0.1 Å/s and 30 nm respectively.

Devices were stored and characterized in a glove box under nitrogen ambient. All electrical characterizations were performed using Keithley 2636A. Transfer characteristics I_D - V_{GS} were plotted at room temperature. All the measurements were made in the same conditions, the gate-source voltage V_{GS} is varied from 20V to -80V with a -0.5V step, at constant drain-source voltage V_{DS} (-50 V).

As usual, equations for MOSFETs have been used in linear regime. The drain current I_D in linear regime ($V_{DS} \ll V_{GS} - V_{TH}$) is given by:

$$I_D = \frac{W}{L} \mu_{FE} C_{ins} (V_{GS} - V_{TH}) V_{DS} \quad (1)$$

Where W and L are the width and length of the channel, μ_{FE} is the field effect mobility, C_{ins} is the capacitance of the gate insulator per area unit and V_{TH} is the threshold voltage. The first derivative of I_D - V_{GS} curve at constant V_{DS} is the transconductance g_m given by:

$$g_m = \mu_{FE} \frac{W C_{ins} V_{DS}}{L} \quad (2)$$

The threshold voltage V_{TH} is the gate voltage axis intercept of I_D - V_{GS} curve plotted in linear representation. The field effect mobility μ_{FE} is deduced from the extraction of g_m . The given value is the maximum value of μ_{FE} .

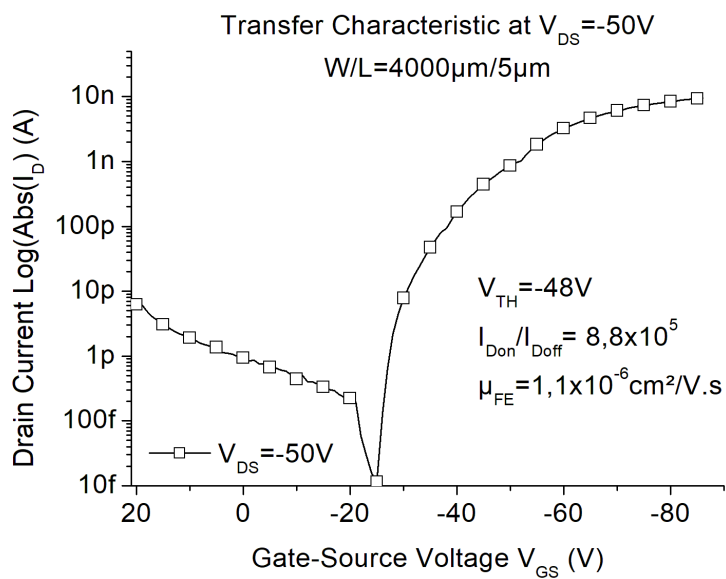


Figure S18: Transfer Characteristic of OFET with $V_{DS} = -50V$

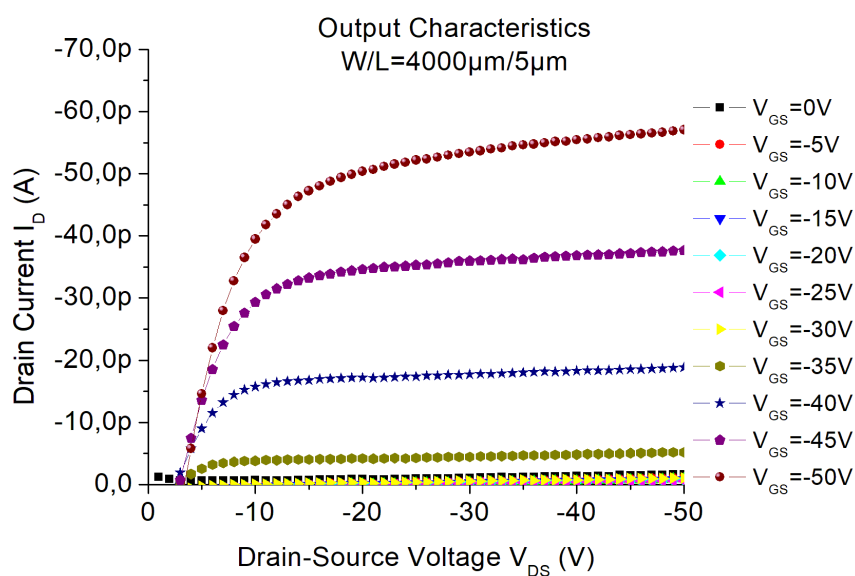


Figure S19 : Output Characteristics of OFET

Thermal Stability

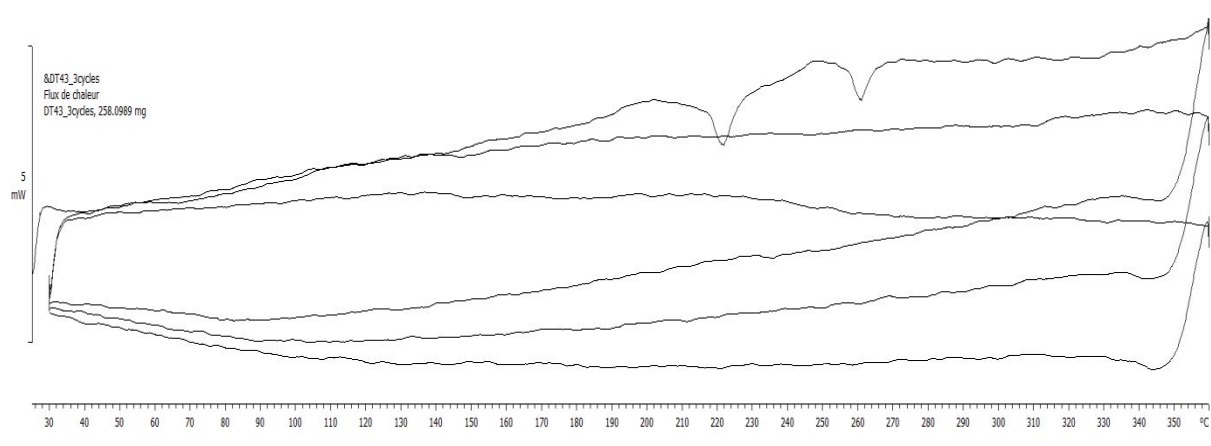


Figure S20: Differential scanning calorimetry experiment performed on **6** (3 cycles).

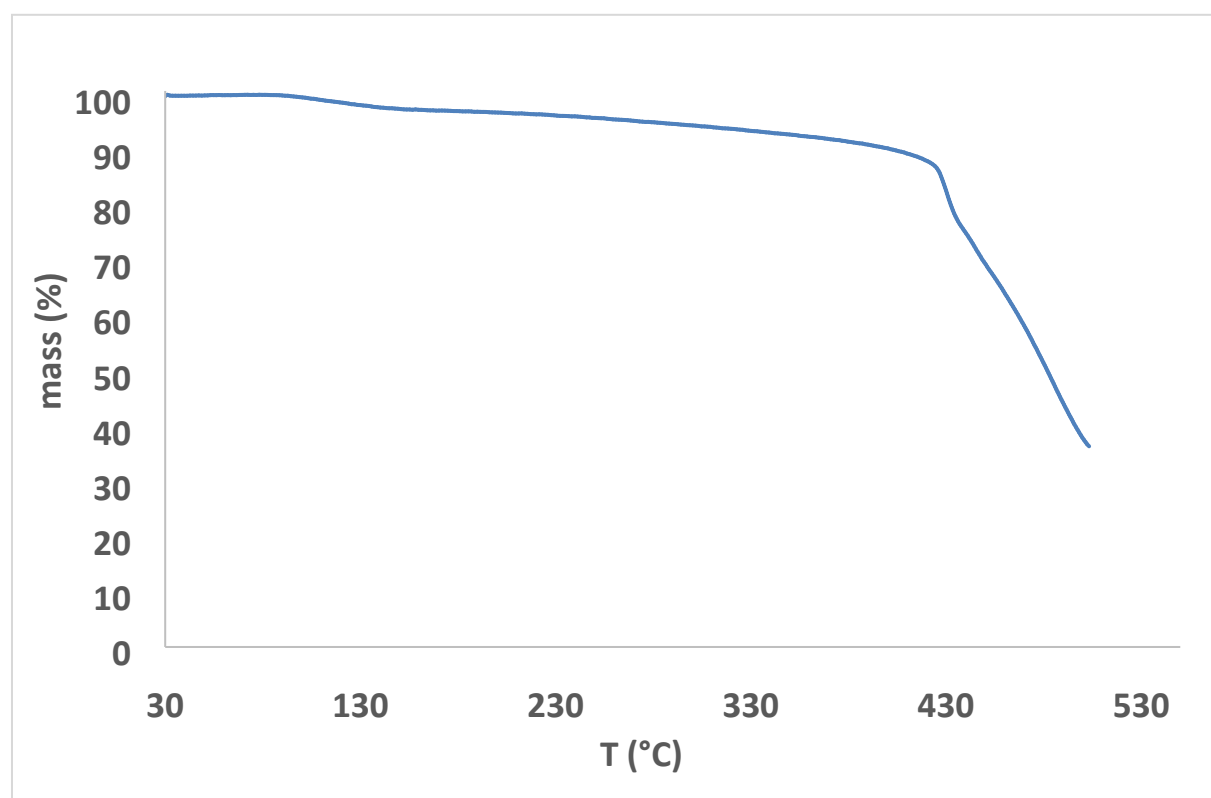


Figure S21: Thermogravimetric analyses (TGA) measurements performed on **6**.

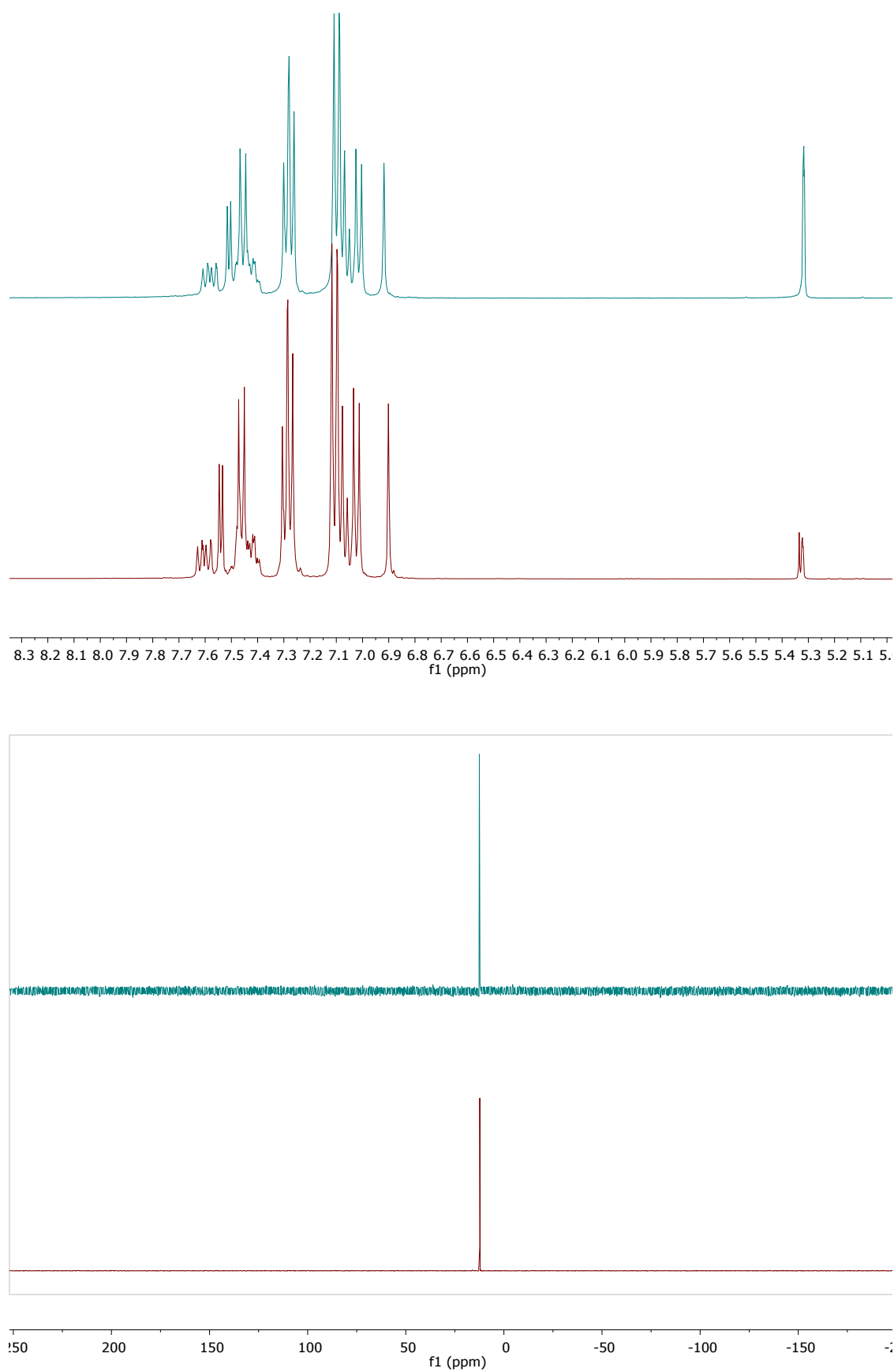


Figure S22 : ^1H (400 MHz, CD_2Cl_2) (up) and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of **6** before (red) and after (blue) sublimation

Theoretical calculations

All calculations were carried out with the Gaussian 09 program package. Full geometry optimization was performed for all molecules at the B3LYP/6-31G*, CAM-B3LYP/6-31G* and M06-2X/6-31G* levels of theory and subsequently harmonic vibrational frequencies were calculated at the same level to establish the nature of the stationary point obtained, for minima no negative eigenvalue of the Hessian was present. TD-DFT calculations have been carried out at the same level of theory, TD-DFT optimization was only carried-out at with the CAM-B3LYP method, as these calculations are more time-demanding. Molecular orbitals have been visualized with the VMD program.

Table S3 : Relative energy and TD-DFT absorption data of the different conformers of **2-8** at the B3LYP/6-31G* level of theory

Compound	Relative energy (kcal/mol)	Experimental λ_{abs} (nm)	Theoretical λ_{abs} (nm)	Intensity	Transition	Coefficient
2 ax- $\perp$	0.00	347	369	0.302	HOMO $\rightarrow$ LUMO	0.699
2 ax- $\parallel$	0.90	347	353	0.305	HOMO $\rightarrow$ LUMO	0.700
2 eq	0.38	347	348	0.369	HOMO $\rightarrow$ LUMO	0.698
3 ax- $\perp$	0.00	410	452	1.158	HOMO $\rightarrow$ LUMO	0.705
3 ax- $\parallel$	0.95	410	442	1.122	HOMO $\rightarrow$ LUMO	0.706
3 eq	0.72	410	438	1.278	HOMO $\rightarrow$ LUMO	0.705
4 ax- $\perp$	0.00	425	471	1.159	HOMO $\rightarrow$ LUMO	0.706
4 ax- $\parallel$	0.95	425	462	1.081	HOMO $\rightarrow$ LUMO	0.706
4 eq	0.68	425	463	1.190	HOMO $\rightarrow$ LUMO	0.706
5 ax- $\perp$	0.00	402	438	0.864	HOMO $\rightarrow$ LUMO	0.704
5 ax- $\parallel$	0.91	402	424	0.857	HOMO $\rightarrow$ LUMO	0.705
5 eq	0.54	402	416	0.998	HOMO $\rightarrow$ LUMO	0.705
6 ax- $\perp$	0.00	454	523	1.317	HOMO $\rightarrow$ LUMO	0.703
6 ax- $\parallel$	0.91	454	508	1.313	HOMO $\rightarrow$ LUMO	0.702
6 eq	0.61	454	496	1.473	HOMO $\rightarrow$ LUMO	0.702
8 ax- $\perp$	0.00	459	588	0.555	HOMO $\rightarrow$ LUMO	0.703
8 ax- $\parallel$	0.98	459	582	0.462	HOMO $\rightarrow$ LUMO	0.703
8 eq	0.64	459	574	0.492	HOMO $\rightarrow$ LUMO	0.703

Table S4 : Relative energy and TD-DFT absorption data of the different conformers of **2-8** at the CAM-B3LYP/6-31G* level of theory

Compound	Relative energy (kcal/mol)	Experimental λ_{abs} (nm)	Theoretical λ_{abs} (nm)	Intensity	Transition			Coefficient
2 ax- $\perp$	0.00	347	327	0.330	HOMO	→	LUMO	0.693
2 ax- $\parallel$	0.75	347	314	0.320	HOMO	→	LUMO	0.693
2 eq	0.59	347	310	0.393	HOMO	→	LUMO	0.692
3 ax- $\perp$	0.00	410	376	1.156	HOMO	→	LUMO	0.680
3 ax- $\parallel$	0.82	410	365	1.146	HOMO	→	LUMO	0.676
3 eq	0.91	410	363	1.320	HOMO	→	LUMO	0.677
4 ax- $\perp$	0.00	425	380	1.188	HOMO	→	LUMO	0.661
4 ax- $\parallel$	0.82	425	369	1.172	HOMO	→	LUMO	0.654
4 eq	0.88	425	367	1.340	HOMO	→	LUMO	0.654
5 ax- $\perp$	0.00	402	370	0.876	HOMO	→	LUMO	0.686
5 ax- $\parallel$	0.77	402	357	0.869	HOMO	→	LUMO	0.684
5 eq	0.68	402	352	1.012	HOMO	→	LUMO	0.685
6 ax- $\perp$	0.00	454	400	1.588	HOMO	→	LUMO	0.607
6 ax- $\parallel$	0.76	454	388	1.600	HOMO	→	LUMO	0.604
6 eq	0.72	454	381	1.818	HOMO	→	LUMO	0.608
8 ax- $\perp$	0.00	459	400	1.290	HOMO	→	LUMO	0.481
8 ax- $\parallel$	0.83	459	389	1.266	HOMO	→	LUMO	0.458
8 eq	0.79	459	384	1.450	HOMO	→	LUMO	0.457

Table S5 : TD-DFT emission data of the different conformers of **2-8** at the CAM-B3LYP/6-31G* level of theory

Compound	Experimental λ_{em} (nm)	Theoretical λ_{em} (nm)	Intensity	Transition			Coefficient
2 ax- $\perp$	424	415	0.355	HOMO	$\leftarrow$	LUMO	0.699
2 ax- $\parallel$	424	413	0.341	HOMO	$\leftarrow$	LUMO	0.699
2 eq	424	415	0.355	HOMO	$\leftarrow$	LUMO	-0.699
3 ax- $\perp$	473	491	1.240	HOMO	$\leftarrow$	LUMO	0.692
3 ax- $\parallel$	473	490	1.216	HOMO	$\leftarrow$	LUMO	0.692
3 eq	473	468	1.432	HOMO	$\leftarrow$	LUMO	-0.692
4 ax- $\perp$	525	493	1.263	HOMO	$\leftarrow$	LUMO	0.687
4 ax- $\parallel$	525	492	1.237	HOMO	$\leftarrow$	LUMO	-0.686
4 eq	525	471	1.453	HOMO	$\leftarrow$	LUMO	0.686
5 ax- $\perp$	468	482	0.984	HOMO	$\leftarrow$	LUMO	0.695
5 ax- $\parallel$	468	480	0.965	HOMO	$\leftarrow$	LUMO	-0.695
5 eq	468	457	1.138	HOMO	$\leftarrow$	LUMO	-0.695
6 ax- $\perp$	580	522	1.666	HOMO	$\leftarrow$	LUMO	0.671
6 ax- $\parallel$	580	518	1.654	HOMO	$\leftarrow$	LUMO	-0.671
6 eq	580	495	1.912	HOMO	$\leftarrow$	LUMO	0.671
8 ax- $\perp$	575	521	1.486	HOMO	$\leftarrow$	LUMO	-0.636
8 ax- $\parallel$	575	519	1.464	HOMO	$\leftarrow$	LUMO	0.635
8 eq	575	498	1.671	HOMO	$\leftarrow$	LUMO	-0.631

Table S6 : Relative energy and TD-DFT absorption data of the different conformers of **2-8** at the M06-2X/6-31G* level of theory

Compound	Relative energy (kcal/mol)	Experimental λ_{abs} (nm)	Theoretical λ_{abs} (nm)	Intensity	Transition			Coefficient
2 ax- $\perp$	0.00	347	327	0.318	HOMO	→	LUMO	0.696
2 ax- $\parallel$	0.29	347	311	0.313	HOMO	→	LUMO	0.696
2 eq	0.53	347	304	0.388	HOMO	→	LUMO	0.695
3 ax- $\perp$	0.00	410	378	1.139	HOMO	→	LUMO	0.687
3 ax- $\parallel$	0.33	410	365	1.137	HOMO	→	LUMO	0.684
3 eq	0.73	410	359	1.303	HOMO	→	LUMO	0.685
4 ax- $\perp$	0.00	425	379	1.147	HOMO	→	LUMO	0.677
4 ax- $\parallel$	0.35	425	367	1.146	HOMO	→	LUMO	0.671
4 eq	0.69	425	363	1.299	HOMO	→	LUMO	0.671
5 ax- $\perp$	0.00	402	370	0.852	HOMO	→	LUMO	0.692
5 ax- $\parallel$	0.29	402	356	0.855	HOMO	→	LUMO	0.690
5 eq	0.54	402	347	1.003	HOMO	→	LUMO	0.690
6 ax- $\perp$	0.00	454	408	1.605	HOMO	→	LUMO	0.631
6 ax- $\parallel$	0.33	454	390	1.578	HOMO	→	LUMO	0.621
6 eq	0.70	454	383	1.830	HOMO	→	LUMO	0.627
8 ax- $\perp$	0.00	459	409	1.204	HOMO	→	LUMO	0.546
8 ax- $\parallel$	0.40	459	397	1.176	HOMO	→	LUMO	0.528
8 eq	0.65	459	389	1.354	HOMO	→	LUMO	0.524

Table S7 : Isomerisation barriers of **2** in kcal/mol

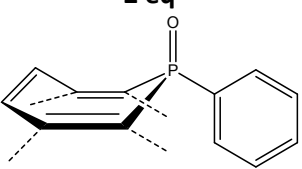
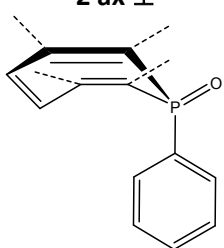
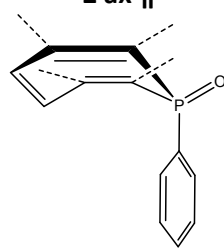
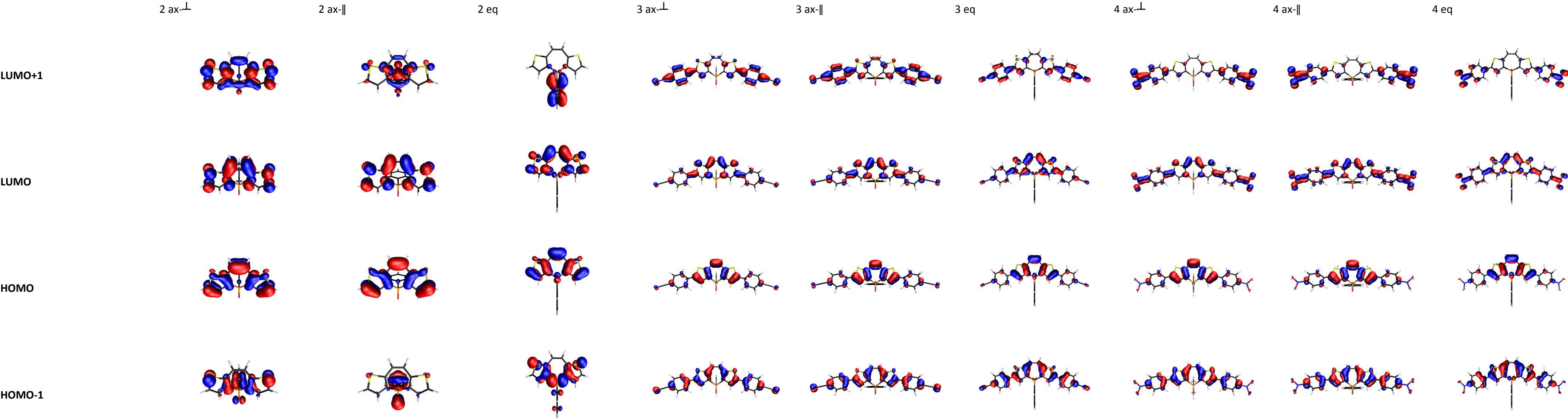
	2 eq 	TS1	2 ax-⊥ 	TS2	2 ax- 
B3LYP/ 6-31G*	0.39	1.75	0.00	1.03	0.87
CAM-B3LYP/ 6-31G*	0.61	2.26	0.00	0.94	0.73
M06-2X/ 6-31G*	0.61	2.58	0.00	0.60	0.25

Figure S23: Geometry change between the ground state and excited state geometries of the most stable conformers of **2-8** at the CAM-B3LYP/6-31G* level of theory

	Ground state	Excited state
2 ax-⊥		
3 ax-⊥		
4 ax-⊥		

	Ground state	Excited state
5 ax- $\perp$		
6 ax- $\perp$		
8 ax- $\perp$		

Table S8 : Kohn-Sham orbitals of the different conformers of **2-8** at the B3LYP/6-31G* level of theory



5 ax- $\perp$ 5 ax- $\parallel$

5 eq

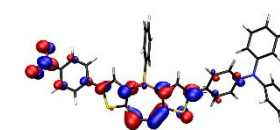
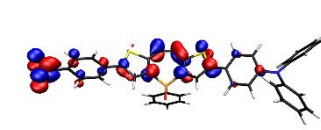
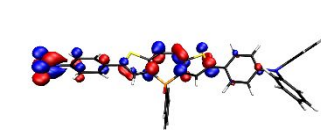
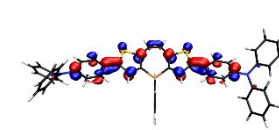
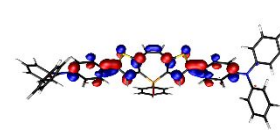
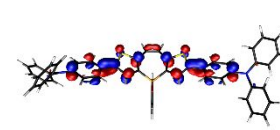
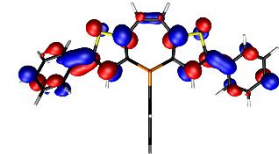
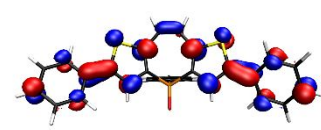
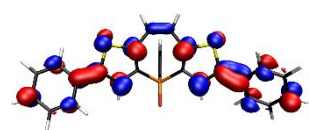
6 ax- $\perp$ 6 ax- $\parallel$

6 eq

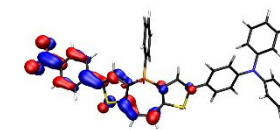
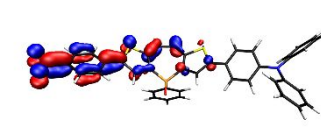
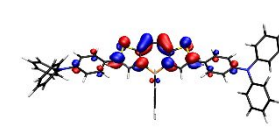
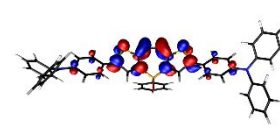
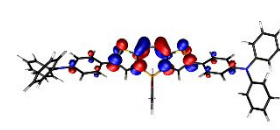
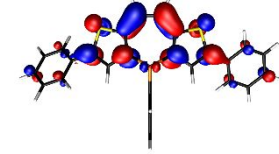
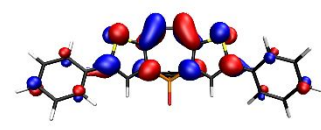
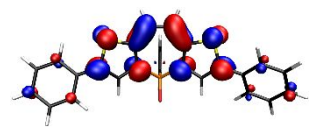
8 ax- $\perp$ 8 ax- $\parallel$

8 eq

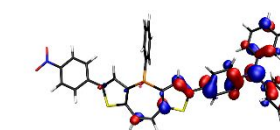
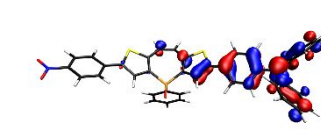
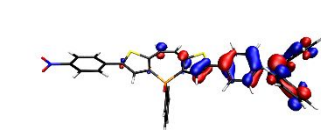
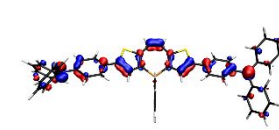
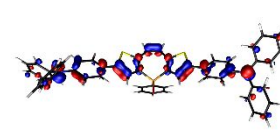
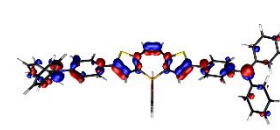
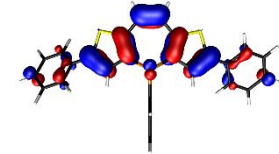
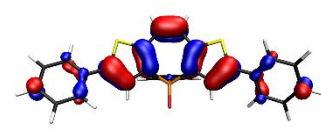
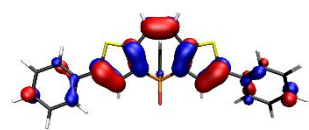
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LUMO



HOMO



HOMO-1

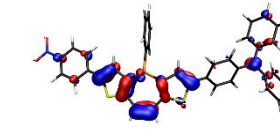
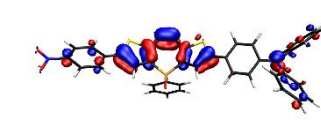
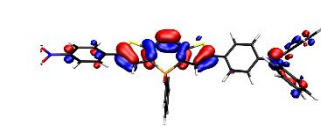
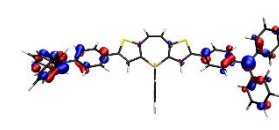
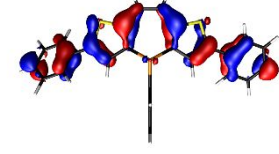
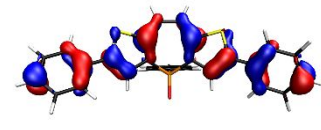
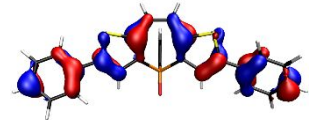
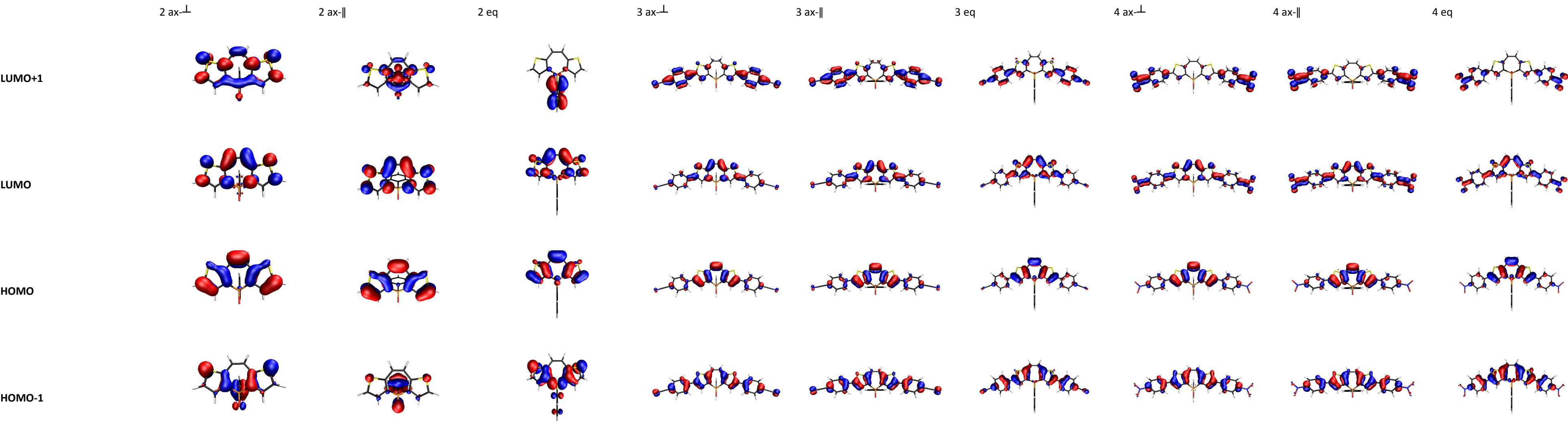


Table S9 : Kohn-Sham orbitals of the different conformers of **2-8** at the CAM-B3LYP/6-31G* level of theory



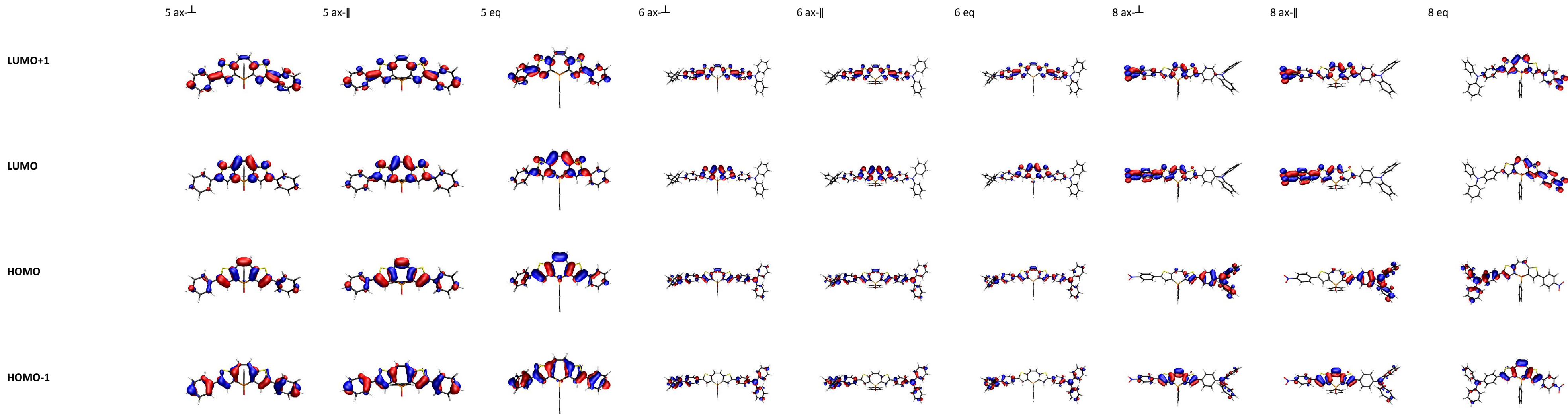


Table S10 : Kohn-Sham orbitals of the different conformers of **2-8** at the M06-2X/6-31G* level of theory

5 ax- $\perp$ 5 ax- $\parallel$

5 eq

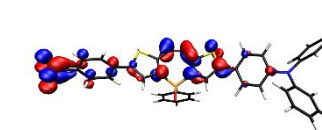
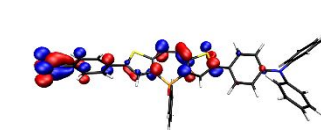
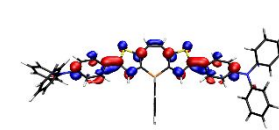
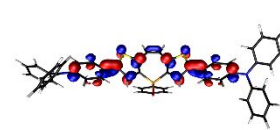
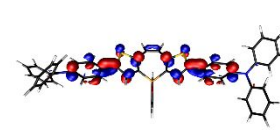
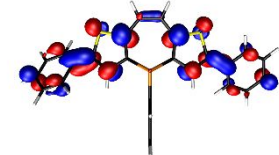
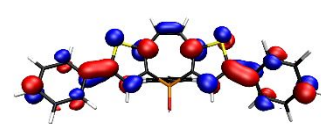
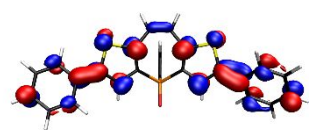
6 ax- $\perp$ 6 ax- $\parallel$

6 eq

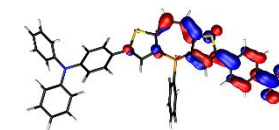
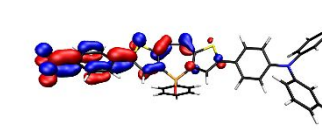
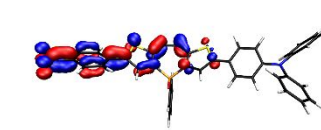
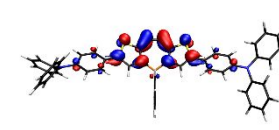
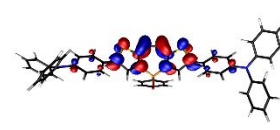
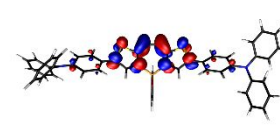
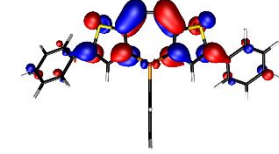
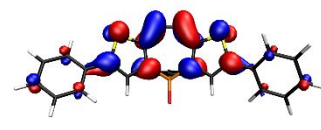
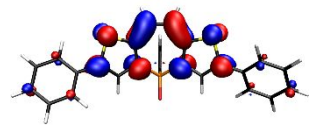
8 ax- $\perp$ 8 ax- $\parallel$

8 eq

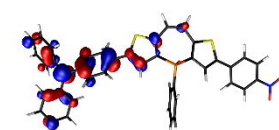
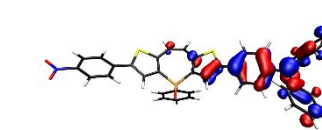
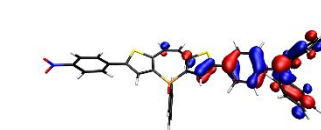
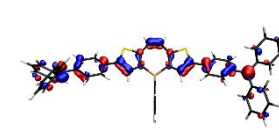
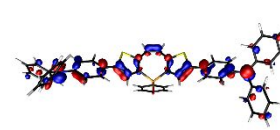
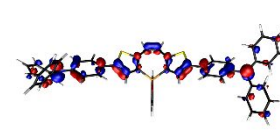
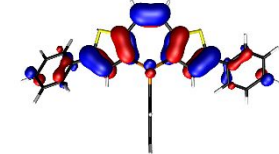
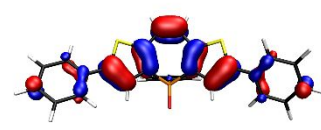
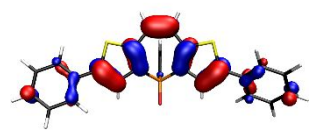
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LUMO



HOMO



HOMO-1

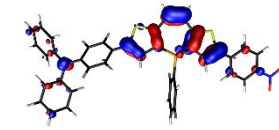
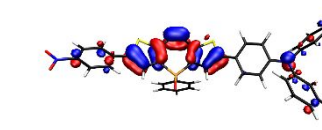
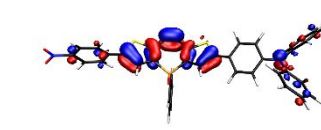
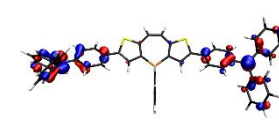
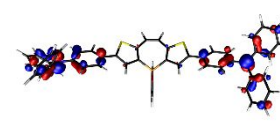
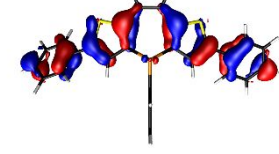
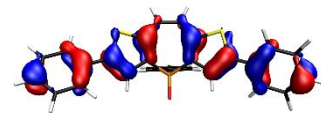
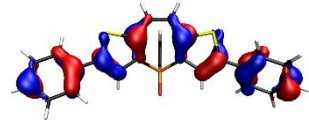


Table S11 : Energy of the Kohn-Sham orbitals of the different conformers of **2-8** at the B3LYP/6-31G* level of theory

(eV)	2 ax- $\perp$	2 ax- $\parallel$	2 eq	3 ax- $\perp$	3 ax- $\parallel$	3 eq	4 ax- $\perp$	4 ax- $\parallel$	4 eq	5 ax- $\perp$	5 ax- $\parallel$	5 eq	6 ax- $\perp$	6 ax- $\parallel$	6 eq	8 ax- $\perp$	8 ax- $\parallel$	8 eq
HOMO-1	-6.78	-6.74	-6.71	-6.74	-6.73	-6.77	-6.93	-6.91	-6.95	-6.20	-6.19	-6.23	-5.03	-5.04	-5.06	-5.81	-5.83	-5.81
HOMO	-5.76	-5.80	-5.74	-5.91	-5.94	-5.92	-6.03	-6.07	-6.04	-5.37	-5.40	-5.38	-4.79	-4.81	-4.82	-5.08	-5.08	-5.11
LUMO	-2.07	-1.96	-1.91	-2.85	-2.81	-2.79	-3.10	-3.07	-3.07	-2.21	-2.14	-2.10	-2.08	-2.01	-1.98	-2.71	-2.70	-2.70
LUMO+1	-0.54	-0.75	-0.74	-2.01	-2.04	-2.04	-2.65	-2.67	-2.69	-1.06	-1.10	-1.06	-0.99	-1.03	-1.01	-2.09	-2.04	-2.02

Table S12 : Energy of the Kohn-Sham orbitals of the different conformers of **2-8** at the CAM-B3LYP/6-31G* level of theory

(eV)	2 ax- $\perp$	2 ax- $\parallel$	2 eq	3 ax- $\perp$	3 ax- $\parallel$	3 eq	4 ax- $\perp$	4 ax- $\parallel$	4 eq	5 ax- $\perp$	5 ax- $\parallel$	5 eq	6 ax- $\perp$	6 ax- $\parallel$	6 eq	8 ax- $\perp$	8 ax- $\parallel$	8 eq
HOMO-1	-8.21	-8.27	-8.18	-8.08	-8.06	-8.11	-8.26	-8.23	-8.28	-7.56	-7.54	-7.59	-6.27	-6.27	-6.31	-7.14	-7.18	-7.15
HOMO	-7.16	-7.22	-7.14	-7.22	-7.26	-7.23	-7.32	-7.37	-7.33	-6.70	-6.74	-6.72	-6.05	-6.08	-6.10	-6.29	-6.30	-6.33
LUMO	-0.87	-0.72	-0.68	-1.67	-1.60	-1.59	-1.87	-1.82	-1.83	-1.04	-0.93	-0.90	-0.96	-0.85	-0.82	-1.52	-1.49	-1.49
LUMO+1	0.76	0.54	0.57	-0.76	-0.80	-0.80	-1.35	-1.37	-1.39	0.22	0.16	0.20	0.25	0.20	0.22	-0.83	-0.76	-0.75

Table S13 : Energy of the Kohn-Sham orbitals of the different conformers of **2-8** at the M06-2X/6-31G* level of theory

(eV)	2 ax- $\perp$	2 ax- $\parallel$	2 eq	3 ax- $\perp$	3 ax- $\parallel$	3 eq	4 ax- $\perp$	4 ax- $\parallel$	4 eq	5 ax- $\perp$	5 ax- $\parallel$	5 eq	6 ax- $\perp$	6 ax- $\parallel$	6 eq	8 ax- $\perp$	8 ax- $\parallel$	8 eq
HOMO-1	-8.15	-8.28	-8.16	-8.05	-8.00	-8.05	-8.22	-8.17	-8.22	-7.51	-7.49	-7.53	-6.21	-6.22	-6.25	-7.09	-7.14	-7.12
HOMO	-7.10	-7.17	-7.11	-7.16	-7.22	-7.20	-7.28	-7.34	-7.31	-6.65	-6.71	-6.69	-5.99	-6.04	-6.05	-6.23	-6.24	-6.27
LUMO	-1.22	-1.06	-0.97	-2.04	-1.96	-1.94	-2.20	-2.15	-2.14	-1.40	-1.29	-1.23	-1.34	-1.22	-1.18	-1.85	-1.81	-1.80
LUMO+1	0.40	0.16	0.15	-1.12	-1.17	-1.17	-1.61	-1.64	-1.65	-0.17	-0.23	-0.20	-0.16	-0.21	-0.17	-1.12	-1.07	-1.04

Detailed TD-DFT results

2 ax- $\perp$ (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
369	0.3015	HOMO $\rightarrow$ LUMO	0.699
300	0.049	HOMO-5 $\rightarrow$ LUMO	-0.116
		HOMO-4 $\rightarrow$ LUMO	-0.111
		HOMO-1 $\rightarrow$ LUMO	0.653
		HOMO $\rightarrow$ LUMO+1	0.155
293	0.003	HOMO-5 $\rightarrow$ LUMO	0.204
		HOMO-4 $\rightarrow$ LUMO	0.107
		HOMO-2 $\rightarrow$ LUMO	0.638
		HOMO-1 $\rightarrow$ LUMO	0.134
		HOMO $\rightarrow$ LUMO+1	0.107
293	0.0002	HOMO-6 $\rightarrow$ LUMO	-0.191
		HOMO-3 $\rightarrow$ LUMO	0.679

2 ax- $\parallel$ (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
353	0.305	HOMO $\rightarrow$ LUMO	0.700
303	0.0081	HOMO-5 $\rightarrow$ LUMO	0.112
		HOMO-1 $\rightarrow$ LUMO	0.696
291	0.0025	HOMO-6 $\rightarrow$ LUMO	-0.101
		HOMO-3 $\rightarrow$ LUMO	-0.367
		HOMO-2 $\rightarrow$ LUMO	-0.364
		HOMO $\rightarrow$ LUMO+1	0.410
		HOMO $\rightarrow$ LUMO+2	0.196
286	0.0014	HOMO-6 $\rightarrow$ LUMO	0.222
		HOMO-4 $\rightarrow$ LUMO	-0.130
		HOMO-3 $\rightarrow$ LUMO	0.540
		HOMO-2 $\rightarrow$ LUMO	-0.308
		HOMO $\rightarrow$ LUMO+1	0.196

2 eq (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
348	0.3686	HOMO $\rightarrow$ LUMO	0.698
295	0.0276	HOMO-3 $\rightarrow$ LUMO	-0.102
		HOMO-1 $\rightarrow$ LUMO	0.627
		HOMO $\rightarrow$ LUMO+2	0.273
286	0.0333	HOMO-6 $\rightarrow$ LUMO	0.104
		HOMO-2 $\rightarrow$ LUMO	0.673
		HOMO $\rightarrow$ LUMO+1	-0.170

283	0.0031	HOMO-2 → LUMO	0.163
		HOMO → LUMO+1	0.684

3 ax- $\perp$ (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
452	1.1577	HOMO → LUMO	0.705
364	0.0028	HOMO-1 → LUMO	0.498
		HOMO → LUMO+1	0.488
331	0.1307	HOMO-5 → LUMO	-0.105
		HOMO-3 → LUMO	0.129
		HOMO-2 → LUMO	0.303
		HOMO-1 → LUMO	0.430
		HOMO → LUMO+1	-0.429
323	0.0509	HOMO-3 → LUMO	-0.389
		HOMO-2 → LUMO	0.537
		HOMO-1 → LUMO	-0.133
		HOMO → LUMO+1	0.156

3 ax- $\parallel$ (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
442	1.1217	HOMO → LUMO	0.706
363	0.0014	HOMO-1 → LUMO	-0.480
		HOMO → LUMO+1	0.506
334	0.0167	HOMO-2 → LUMO	0.698
328	0.2812	HOMO-4 → LUMO	0.148
		HOMO-1 → LUMO	0.491
		HOMO → LUMO+1	0.471

3 eq (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
438	1.2783	HOMO → LUMO	0.705
361	0.0014	HOMO-1 → LUMO	0.413
		HOMO → LUMO+1	0.561
329	0.1124	HOMO-2 → LUMO	-0.343
		HOMO-1 → LUMO	0.486
		HOMO → LUMO+1	-0.345
		HOMO → LUMO+6	-0.101
318	0.0433	HOMO-2 → LUMO	0.594
		HOMO-1 → LUMO	0.263
		HOMO → LUMO+1	-0.239

4 ax- $\perp$ (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
471	1.1593	HOMO $\rightarrow$ LUMO	0.706
402	0.0305	HOMO-1 $\rightarrow$ LUMO	-0.184
		HOMO $\rightarrow$ LUMO+1	0.676
353	0.0063	HOMO $\rightarrow$ LUMO+2	0.695
350	0.1102	HOMO-1 $\rightarrow$ LUMO	0.648
		HOMO $\rightarrow$ LUMO+1	0.176
		HOMO $\rightarrow$ LUMO+3	-0.129

4 ax- $\parallel$ (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
462	1.0809	HOMO $\rightarrow$ LUMO	0.706
400	0.0434	HOMO-1 $\rightarrow$ LUMO	0.189
		HOMO $\rightarrow$ LUMO+1	0.675
349	0.1917	HOMO-1 $\rightarrow$ LUMO	0.653
		HOMO $\rightarrow$ LUMO+1	-0.189
		HOMO $\rightarrow$ LUMO+3	0.145
346	0.008	HOMO-2 $\rightarrow$ LUMO	0.682
		HOMO-2 $\rightarrow$ LUMO+2	-0.108
		HOMO $\rightarrow$ LUMO+2	-0.129

4 eq (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
463	1.1902	HOMO $\rightarrow$ LUMO	0.706
405	0.02	HOMO-1 $\rightarrow$ LUMO	-0.143
		HOMO $\rightarrow$ LUMO+1	0.687
347	0.0826	HOMO-2 $\rightarrow$ LUMO	0.163
		HOMO-1 $\rightarrow$ LUMO	0.646
		HOMO $\rightarrow$ LUMO+1	0.129
		HOMO $\rightarrow$ LUMO+3	-0.148
344	0.0736	HOMO $\rightarrow$ LUMO+2	0.689

5 ax- $\perp$ (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
438	0.8637	HOMO $\rightarrow$ LUMO	0.704
350	0.0203	HOMO-1 $\rightarrow$ LUMO	0.618
		HOMO $\rightarrow$ LUMO+1	-0.325
311	0.0463	HOMO-8 $\rightarrow$ LUMO	0.108
		HOMO-7 $\rightarrow$ LUMO	-0.101

		HOMO-2 → LUMO	0.574
		HOMO-1 → LUMO	0.176
		HOMO → LUMO+1	0.324
306	0.1003	HOMO-10 → LUMO	0.119
		HOMO-3 → LUMO	-0.273
		HOMO-2 → LUMO	-0.306
		HOMO-1 → LUMO	0.251
		HOMO → LUMO+1	0.481

5 ax-|| (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
424	0.8567	HOMO → LUMO	0.705
347	0.0204	HOMO-1 → LUMO	0.593
		HOMO → LUMO+1	-0.367
315	0.0077	HOMO-2 → LUMO	0.697
306	0.1955	HOMO-6 → LUMO	-0.103
		HOMO-4 → LUMO	0.124
		HOMO-1 → LUMO	0.348
		HOMO → LUMO+1	0.571
		HOMO → LUMO+2	0.107

5 eq (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
416	0.9983	HOMO → LUMO	0.705
340	0.0105	HOMO-1 → LUMO	0.569
		HOMO → LUMO+1	-0.399
308	0.059	HOMO-2 → LUMO	0.537
		HOMO-1 → LUMO	0.228
		HOMO → LUMO+1	0.337
		HOMO → LUMO+2	-0.127
		HOMO → LUMO+7	0.107
305	0.0015	HOMO-2 → LUMO	0.195
		HOMO → LUMO+2	0.669

6 ax-⊥ (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
523	1.3168	HOMO → LUMO	0.703
464	0.0703	HOMO-1 → LUMO	0.701
384	0.1979	HOMO-2 → LUMO	0.696
359	0.1165	HOMO-3 → LUMO	0.152
		HOMO → LUMO+1	0.677

6 ax-|| (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
508	1.3133	HOMO → LUMO	0.702
452	0.0974	HOMO-1 → LUMO	0.700
374	0.2222	HOMO-2 → LUMO	0.692
362	0.1575	HOMO-3 → LUMO	-0.139
		HOMO → LUMO+1	0.680

6 eq (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
496	1.4732	HOMO → LUMO	0.702
444	0.0502	HOMO-1 → LUMO	0.701
370	0.2704	HOMO-2 → LUMO	0.691
358	0.0738	HOMO-3 → LUMO	-0.123
		HOMO → LUMO+1	0.682

8 ax-⊥ (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
588	0.5552	HOMO → LUMO	0.703
457	0.5059	HOMO-1 → LUMO	0.236
		HOMO → LUMO+1	0.657
437	0.3249	HOMO-1 → LUMO	0.659
		HOMO → LUMO+1	-0.241
368	0.0711	HOMO-2 → LUMO	0.221
		HOMO-1 → LUMO+1	0.638
		HOMO → LUMO+2	0.150

8 ax-|| (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
582	0.4622	HOMO → LUMO	0.703
451	0.6219	HOMO-1 → LUMO	-0.264
		HOMO → LUMO+1	0.646
430	0.2773	HOMO-1 → LUMO	0.649
		HOMO → LUMO+1	0.268
362	0.1645	HOMO-2 → LUMO	-0.299
		HOMO-1 → LUMO+1	0.565
		HOMO → LUMO+2	-0.260

8 eq (ground state, B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
574	0.4918	HOMO $\rightarrow$ LUMO	0.703
444	0.7925	HOMO-1 $\rightarrow$ LUMO	0.327
		HOMO $\rightarrow$ LUMO+1	0.616
431	0.1664	HOMO-1 $\rightarrow$ LUMO	0.620
		HOMO $\rightarrow$ LUMO+1	-0.330
359	0.2114	HOMO-2 $\rightarrow$ LUMO	0.259
		HOMO-1 $\rightarrow$ LUMO+1	0.590
		HOMO $\rightarrow$ LUMO+2	-0.249

2 ax- $\perp$ (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
327	0.3301	HOMO $\rightarrow$ LUMO	0.693
253	0.0713	HOMO-5 $\rightarrow$ LUMO	-0.245
		HOMO-1 $\rightarrow$ LUMO	0.597
		HOMO $\rightarrow$ LUMO+1	-0.220
239	0.0064	HOMO-7 $\rightarrow$ LUMO	0.111
		HOMO-5 $\rightarrow$ LUMO	0.291
		HOMO-3 $\rightarrow$ LUMO	0.403
		HOMO-2 $\rightarrow$ LUMO	0.418
		HOMO-2 $\rightarrow$ LUMO+2	-0.140
239	0.0956	HOMO-6 $\rightarrow$ LUMO	-0.156
		HOMO-4 $\rightarrow$ LUMO	0.656
		HOMO-1 $\rightarrow$ LUMO+1	0.101

2 ax- $\perp$ (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
415	0.3545	HOMO $\leftarrow$ LUMO	0.699

2 ax- $\parallel$ (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
314	0.3198	HOMO $\rightarrow$ LUMO	0.693
248	0.0144	HOMO-3 $\rightarrow$ LUMO	-0.332
		HOMO-2 $\rightarrow$ LUMO	0.453
		HOMO $\rightarrow$ LUMO+1	0.327
		HOMO $\rightarrow$ LUMO+2	0.222
		HOMO $\rightarrow$ LUMO+7	0.107
238	0.0381	HOMO-7 $\rightarrow$ LUMO	0.234
		HOMO-5 $\rightarrow$ LUMO	-0.132

		HOMO-1 → LUMO	0.630
235	0.0524	HOMO-4 → LUMO	0.492
		HOMO-2 → LUMO	0.337
		HOMO → LUMO+1	-0.302
		HOMO → LUMO+2	-0.110

2 ax-|| (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
413	0.3405	HOMO ← LUMO	0.699

2 eq (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
310	0.3927	HOMO → LUMO	0.692
252	0.0267	HOMO-1 → LUMO	0.544
		HOMO → LUMO+2	-0.399
		HOMO → LUMO+6	-0.116
235	0.1378	HOMO-5 → LUMO	0.203
		HOMO-1 → LUMO	0.382
		HOMO → LUMO+2	0.520
233	0.0745	HOMO-3 → LUMO	0.669
		HOMO-1 → LUMO+2	-0.128

2 eq (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
415	0.3545	HOMO ← LUMO	-0.699

3 ax-⊥ (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
376	1.1556	HOMO-1 → LUMO+1	0.120
		HOMO → LUMO	0.680
287	0.2345	HOMO-1 → LUMO	0.581
		HOMO → LUMO+1	0.349
272	0.0339	HOMO-2 → LUMO	-0.136
		HOMO-1 → LUMO	-0.299
		HOMO-1 → LUMO+2	0.161
		HOMO → LUMO+1	0.539
		HOMO → LUMO+3	0.115
		HOMO → LUMO+6	-0.161
258	0.061	HOMO-6 → LUMO+1	0.108
		HOMO-5 → LUMO	-0.332

		HOMO-2 → LUMO	0.530
		HOMO-1 → LUMO	-0.125
		HOMO → LUMO+1	0.105

3 ax- $\perp$ (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
491	1.24	HOMO ← LUMO	0.692

3 ax- $\parallel$ (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
365	1.1462	HOMO-1 → LUMO+1	0.136
		HOMO → LUMO	0.676
287	0.3434	HOMO-1 → LUMO	0.557
		HOMO → LUMO+1	0.390
271	0.0127	HOMO-4 → LUMO	0.117
		HOMO-1 → LUMO	-0.338
		HOMO-1 → LUMO+2	-0.163
		HOMO → LUMO+1	0.514
		HOMO → LUMO+3	0.141
		HOMO → LUMO+6	-0.153
253	0.062	HOMO-10 → LUMO	0.179
		HOMO-5 → LUMO	0.216
		HOMO-4 → LUMO+1	-0.124
		HOMO-2 → LUMO	0.417
		HOMO-1 → LUMO+1	0.272
		HOMO → LUMO+2	-0.307

3 ax- $\parallel$ (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
490	1.2163	HOMO ← LUMO	0.692

3 eq (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
363	1.3197	HOMO-1 → LUMO+1	-0.137
		HOMO → LUMO	0.677
285	0.1839	HOMO-1 → LUMO	0.510
		HOMO → LUMO+1	-0.448
272	0.0097	HOMO-2 → LUMO	0.221
		HOMO-1 → LUMO	0.360
		HOMO-1 → LUMO+2	0.137

		HOMO → LUMO+1	0.442
		HOMO → LUMO+4	0.188
		HOMO → LUMO+6	-0.187
256	0.0215	HOMO-4 → LUMO	0.152
		HOMO-2 → LUMO	0.555
		HOMO-1 → LUMO	-0.202
		HOMO → LUMO+1	-0.162
		HOMO → LUMO+4	0.102

3 eq (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
468	1.4323	HOMO-1 ← LUMO+1	0.103
		HOMO ← LUMO	-0.692

4 ax- $\perp$ (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
380	1.1877	HOMO-1 → LUMO+1	0.122
		HOMO → LUMO	0.661
		HOMO → LUMO+2	0.174
311	0.0017	HOMO-12 → LUMO+1	0.438
		HOMO-12 → LUMO+3	-0.173
		HOMO-12 → LUMO+8	-0.103
		HOMO-11 → LUMO	-0.310
		HOMO-11 → LUMO+2	0.351
		HOMO-11 → LUMO+9	0.116
311	0	HOMO-12 → LUMO	-0.312
		HOMO-12 → LUMO+2	0.355
		HOMO-12 → LUMO+9	0.117
		HOMO-11 → LUMO+1	0.439
		HOMO-11 → LUMO+3	-0.173
		HOMO-11 → LUMO+8	-0.103
298	0.2277	HOMO-9 → LUMO+1	0.103
		HOMO-1 → LUMO	0.414
		HOMO → LUMO+1	0.522
		HOMO → LUMO+3	0.111

4 ax- $\perp$ (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
493	1.2634	HOMO ← LUMO	0.687
		HOMO ← LUMO+2	-0.101

4 ax-|| (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
369	1.1719	HOMO-1 $\rightarrow$ LUMO+1	0.142
		HOMO $\rightarrow$ LUMO	0.654
		HOMO $\rightarrow$ LUMO+2	0.188
311	0.0023	HOMO-12 $\rightarrow$ LUMO+1	0.437
		HOMO-12 $\rightarrow$ LUMO+3	0.158
		HOMO-12 $\rightarrow$ LUMO+4	-0.104
		HOMO-11 $\rightarrow$ LUMO	-0.328
		HOMO-11 $\rightarrow$ LUMO+2	0.339
		HOMO-11 $\rightarrow$ LUMO+8	0.140
311	0.0001	HOMO-12 $\rightarrow$ LUMO	-0.331
		HOMO-12 $\rightarrow$ LUMO+2	0.342
		HOMO-12 $\rightarrow$ LUMO+8	0.142
		HOMO-11 $\rightarrow$ LUMO+1	0.436
		HOMO-11 $\rightarrow$ LUMO+3	0.158
		HOMO-11 $\rightarrow$ LUMO+4	-0.104
298	0.3256	HOMO-1 $\rightarrow$ LUMO	0.422
		HOMO $\rightarrow$ LUMO+1	0.520
		HOMO $\rightarrow$ LUMO+3	-0.100

4 ax-|| (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
492	1.2369	HOMO $\leftarrow$ LUMO	-0.686
		HOMO $\leftarrow$ LUMO+2	0.106

4 eq (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
367	1.3402	HOMO-1 $\rightarrow$ LUMO+1	-0.140
		HOMO $\rightarrow$ LUMO	0.654
		HOMO $\rightarrow$ LUMO+2	0.187
311	0.0015	HOMO-12 $\rightarrow$ LUMO+1	0.439
		HOMO-12 $\rightarrow$ LUMO+3	0.162
		HOMO-12 $\rightarrow$ LUMO+8	-0.128
		HOMO-11 $\rightarrow$ LUMO	0.336
		HOMO-11 $\rightarrow$ LUMO+2	-0.332
		HOMO-11 $\rightarrow$ LUMO+9	-0.138
311	0.0002	HOMO-12 $\rightarrow$ LUMO	0.339
		HOMO-12 $\rightarrow$ LUMO+2	-0.336
		HOMO-12 $\rightarrow$ LUMO+9	-0.139
		HOMO-11 $\rightarrow$ LUMO+1	0.439
		HOMO-11 $\rightarrow$ LUMO+3	0.162

		HOMO-11 → LUMO+8	-0.128
298	0.1493	HOMO-1 → LUMO	-0.372
		HOMO → LUMO+1	0.552
		HOMO → LUMO+3	-0.112

4 eq (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
471	1.4534	HOMO-1 ← LUMO+1	0.105
		HOMO ← LUMO	0.686
		HOMO ← LUMO+2	-0.101

5 ax- $\perp$ (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
370	0.8761	HOMO-1 → LUMO+1	0.107
		HOMO → LUMO	0.686
281	0.1319	HOMO-11 → LUMO	0.110
		HOMO-1 → LUMO	0.660
		HOMO → LUMO+1	0.143
262	0.064	HOMO-2 → LUMO	-0.187
		HOMO → LUMO+1	0.611
		HOMO → LUMO+3	0.103
		HOMO → LUMO+7	-0.149
254	0.0476	HOMO-8 → LUMO	-0.171
		HOMO-7 → LUMO	0.233
		HOMO-2 → LUMO	0.546
		HOMO-1 → LUMO	-0.106
		HOMO → LUMO+1	0.193

5 ax- $\perp$ (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
482	0.9837	HOMO ← LUMO	0.695

5 ax- $\parallel$ (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
357	0.8687	HOMO-1 → LUMO+1	0.121
		HOMO → LUMO	0.684
278	0.2037	HOMO-11 → LUMO	-0.104
		HOMO-1 → LUMO	0.651
		HOMO → LUMO+1	0.182
264	0.0528	HOMO-1 → LUMO	-0.123

		HOMO-1 → LUMO+3	0.129
		HOMO → LUMO+1	0.619
		HOMO → LUMO+2	-0.122
		HOMO → LUMO+7	0.144
247	0.0149	HOMO-6 → LUMO	0.395
		HOMO-4 → LUMO	-0.116
		HOMO-3 → LUMO	0.392
		HOMO-1 → LUMO	0.110
		HOMO-1 → LUMO+3	-0.114
		HOMO → LUMO+1	-0.137
		HOMO → LUMO+2	-0.196

5 ax-|| (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
480	0.9654	HOMO ← LUMO	-0.695

5 eq (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
352	1.0121	HOMO-1 → LUMO+1	0.124
		HOMO → LUMO	0.685
274	0.1185	HOMO-11 → LUMO	0.101
		HOMO-2 → LUMO	0.103
		HOMO-1 → LUMO	0.643
		HOMO → LUMO+1	0.158
264	0.0324	HOMO-2 → LUMO	-0.212
		HOMO → LUMO+1	0.601
		HOMO → LUMO+4	0.132
		HOMO → LUMO+7	-0.156
249	0.0328	HOMO-2 → LUMO	0.575
		HOMO-1 → LUMO	-0.160
		HOMO → LUMO+1	0.212

5 eq (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
457	1.1381	HOMO ← LUMO	-0.695

6 ax- $\perp$ (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
400	1.5883	HOMO-2 → LUMO	-0.294
		HOMO-1 → LUMO+1	-0.157

		HOMO → LUMO	0.607
330	0.2352	HOMO-3 → LUMO	-0.174
		HOMO-1 → LUMO	0.597
		HOMO-1 → LUMO+2	-0.119
		HOMO → LUMO+1	-0.266
296	0.2563	HOMO-2 → LUMO	0.494
		HOMO-1 → LUMO+1	-0.322
		HOMO-1 → LUMO+8	-0.104
		HOMO → LUMO	0.139
		HOMO → LUMO+2	-0.246
		HOMO → LUMO+7	-0.127
281	0.0101	HOMO-3 → LUMO	-0.119
		HOMO-2 → LUMO+1	-0.103
		HOMO-2 → LUMO+8	0.117
		HOMO-1 → LUMO	0.151
		HOMO-1 → LUMO+2	0.137
		HOMO-1 → LUMO+3	-0.204
		HOMO-1 → LUMO+4	-0.251
		HOMO-1 → LUMO+7	0.103
		HOMO → LUMO+1	0.351
		HOMO → LUMO+3	0.336

6 ax- $\perp$ (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
522	1.6663	HOMO-2 $\leftarrow$ LUMO	-0.158
		HOMO-1 $\leftarrow$ LUMO+1	-0.119
		HOMO $\leftarrow$ LUMO	0.671

6 ax- $\parallel$ (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
388	1.6002	HOMO-2 → LUMO	-0.286
		HOMO-1 → LUMO+1	-0.175
		HOMO → LUMO	0.604
327	0.3387	HOMO-3 → LUMO	-0.171
		HOMO-1 → LUMO	0.582
		HOMO-1 → LUMO+5	-0.141
		HOMO → LUMO+1	-0.295
291	0.1984	HOMO-2 → LUMO	0.485
		HOMO-1 → LUMO+1	-0.337
		HOMO-1 → LUMO+9	0.122
		HOMO → LUMO	0.111
		HOMO → LUMO+5	-0.277
281	0.0019	HOMO-2 → LUMO+3	0.103

		HOMO-1 → LUMO+3	-0.364
		HOMO-1 → LUMO+4	0.159
		HOMO → LUMO+1	0.206
		HOMO → LUMO+2	0.130
		HOMO → LUMO+3	0.373
		HOMO → LUMO+4	0.170

6 ax-|| (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
518	1.6542	HOMO-2 ← LUMO	0.153
		HOMO-1 ← LUMO+1	0.121
		HOMO ← LUMO	-0.671

6 eq (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
381	1.818	HOMO-2 → LUMO	-0.272
		HOMO-1 → LUMO+1	-0.181
		HOMO → LUMO	0.608
323	0.1875	HOMO-3 → LUMO	-0.159
		HOMO-1 → LUMO	0.572
		HOMO-1 → LUMO+5	0.141
		HOMO → LUMO+1	-0.310
289	0.1666	HOMO-2 → LUMO	0.492
		HOMO-1 → LUMO+1	-0.333
		HOMO-1 → LUMO+8	-0.133
		HOMO → LUMO+5	0.254
281	0.0059	HOMO-2 → LUMO+3	0.120
		HOMO-1 → LUMO+3	-0.279
		HOMO-1 → LUMO+4	0.331
		HOMO → LUMO+3	0.444

6 eq (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
495	1.9118	HOMO-2 ← LUMO	-0.145
		HOMO-1 ← LUMO+1	-0.133
		HOMO ← LUMO	0.671

8 ax-⊥ (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
400	1.2898	HOMO-1 → LUMO	0.379

		HOMO-1 → LUMO+1	-0.140
		HOMO → LUMO	0.481
		HOMO → LUMO+1	-0.269
321	0.1895	HOMO-2 → LUMO	0.237
		HOMO-1 → LUMO	0.483
		HOMO → LUMO	-0.227
		HOMO → LUMO+1	0.264
		HOMO → LUMO+2	-0.214
311	0.0005	HOMO-16 → LUMO	0.452
		HOMO-16 → LUMO+1	0.444
		HOMO-16 → LUMO+2	0.172
		HOMO-16 → LUMO+4	0.136
		HOMO-16 → LUMO+10	0.148
297	0.1121	HOMO-1 → LUMO+1	0.320
		HOMO → LUMO	0.405
		HOMO → LUMO+1	0.362
		HOMO → LUMO+2	-0.248

8 ax-⊥ (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
521	1.4857	HOMO-1 ← LUMO	0.222
		HOMO ← LUMO	-0.636
		HOMO ← LUMO+1	-0.163

8 ax-|| (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
389	1.2658	HOMO-1 → LUMO	-0.371
		HOMO-1 → LUMO+1	0.156
		HOMO → LUMO	0.458
		HOMO → LUMO+1	-0.304
318	0.2763	HOMO-2 → LUMO	0.252
		HOMO-1 → LUMO	0.466
		HOMO → LUMO	0.170
		HOMO → LUMO+1	-0.301
		HOMO → LUMO+2	0.219
311	0.0034	HOMO-16 → LUMO	0.487
		HOMO-16 → LUMO+1	0.401
		HOMO-16 → LUMO+2	0.196
		HOMO-16 → LUMO+10	0.142
296	0.1857	HOMO-1 → LUMO	0.102
		HOMO-1 → LUMO+1	-0.261
		HOMO → LUMO	0.455
		HOMO → LUMO+1	0.317

		HOMO → LUMO+2	-0.261
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8 ax-|| (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
519	1.4643	HOMO-1 ← LUMO	-0.220
		HOMO ← LUMO	0.635
		HOMO ← LUMO+1	0.172

8 eq (ground state, CAM-B3LYP/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
384	1.4497	HOMO-1 → LUMO	-0.369
		HOMO-1 → LUMO+1	0.152
		HOMO → LUMO	0.457
		HOMO → LUMO+1	-0.308
316	0.1494	HOMO-2 → LUMO	-0.237
		HOMO-1 → LUMO	0.458
		HOMO → LUMO	0.137
		HOMO → LUMO+1	-0.323
		HOMO → LUMO+2	-0.229
		HOMO → LUMO+6	-0.112
311	0.0038	HOMO-16 → LUMO	0.501
		HOMO-16 → LUMO+1	0.388
		HOMO-16 → LUMO+2	-0.184
		HOMO-16 → LUMO+9	-0.178
295	0.1619	HOMO-1 → LUMO	0.125
		HOMO-1 → LUMO+1	-0.288
		HOMO → LUMO	0.464
		HOMO → LUMO+1	0.298
		HOMO → LUMO+2	0.231

8 eq (excited state, CAM-B3LYP/6-31G*)

λ_e (nm)	Intensity	Transition	Coefficient
498	1.6712	HOMO-1 ← LUMO	0.217
		HOMO ← LUMO	-0.631
		HOMO ← LUMO+1	-0.188

2 ax-⊥ (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
327	0.3184	HOMO → LUMO	0.696
253	0.0712	HOMO-5 → LUMO	0.221

		HOMO-1 → LUMO	0.610
		HOMO → LUMO+1	0.232
240	0.0175	HOMO-5 → LUMO	-0.233
		HOMO-3 → LUMO	0.465
		HOMO-2 → LUMO	0.389
		HOMO → LUMO+1	0.153
240	0.1169	HOMO-4 → LUMO	0.674

2 ax-|| (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
311	0.3125	HOMO → LUMO	0.696
249	0.0145	HOMO-3 → LUMO	0.264
		HOMO-1 → LUMO	0.482
		HOMO → LUMO+1	-0.324
		HOMO → LUMO+2	-0.247
236	0.0541	HOMO-6 → LUMO	-0.121
		HOMO-5 → LUMO	-0.315
		HOMO-2 → LUMO	0.589
235	0.0373	HOMO-7 → LUMO	0.107
		HOMO-4 → LUMO	0.467
		HOMO-3 → LUMO	-0.440
		HOMO → LUMO+1	-0.159

2 eq (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
304	0.3879	HOMO → LUMO	0.695
251	0.0165	HOMO-1 → LUMO	0.499
		HOMO → LUMO+2	-0.460
234	0.1288	HOMO-4 → LUMO	-0.185
		HOMO-3 → LUMO	0.124
		HOMO-2 → LUMO	0.217
		HOMO-1 → LUMO	0.424
		HOMO → LUMO+2	0.420
		HOMO → LUMO+4	0.113
230	0.0671	HOMO-5 → LUMO	0.633
		HOMO-1 → LUMO+2	-0.131
		HOMO → LUMO+1	-0.215

3 ax-⊥ (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
378	1.1394	HOMO-1 → LUMO+1	-0.101

		HOMO → LUMO	0.687
287	0.2058	HOMO-1 → LUMO HOMO → LUMO+1	0.613 -0.301
277	0.0359	HOMO-1 → LUMO HOMO-1 → LUMO+2 HOMO → LUMO+1 HOMO → LUMO+6	0.266 0.150 0.591 -0.138
260	0.0767	HOMO-6 → LUMO+1 HOMO-5 → LUMO HOMO-2 → LUMO	0.107 0.305 0.577

3 ax-|| (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
365	1.1374	HOMO-1 → LUMO+1 HOMO → LUMO	0.119 0.684
287	0.3374	HOMO-1 → LUMO HOMO → LUMO+1	0.588 0.353
277	0.0214	HOMO-1 → LUMO HOMO-1 → LUMO+2 HOMO → LUMO+1 HOMO → LUMO+3 HOMO → LUMO+6	-0.312 -0.152 0.561 0.116 -0.134
254	0.1572	HOMO-9 → LUMO HOMO-5 → LUMO HOMO-4 → LUMO+1 HOMO-2 → LUMO HOMO-1 → LUMO+1 HOMO → LUMO+2	-0.132 -0.236 0.115 -0.307 -0.350 0.387

3 eq (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
359	1.3031	HOMO-1 → LUMO+1 HOMO → LUMO	-0.123 0.685
285	0.2045	HOMO-1 → LUMO HOMO → LUMO+1	0.505 -0.465
276	0.0066	HOMO-2 → LUMO HOMO-1 → LUMO HOMO-1 → LUMO+2 HOMO → LUMO+1 HOMO → LUMO+4 HOMO → LUMO+6	-0.127 0.407 0.130 0.465 0.165 -0.165
255	0.022	HOMO-4 → LUMO HOMO-2 → LUMO	-0.177 0.559

		HOMO-1 → LUMO	0.155
		HOMO → LUMO+4	-0.175

4 ax- $\perp$ (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
379	1.1471	HOMO-1 → LUMO+1	-0.106
		HOMO → LUMO	0.677
		HOMO → LUMO+2	-0.137
314	0.001	HOMO-15 → LUMO	0.272
		HOMO-15 → LUMO+2	0.350
		HOMO-15 → LUMO+9	0.156
		HOMO-14 → LUMO+1	0.412
		HOMO-14 → LUMO+3	0.163
		HOMO-14 → LUMO+5	0.127
		HOMO-14 → LUMO+10	-0.145
314	0	HOMO-15 → LUMO+1	0.407
		HOMO-15 → LUMO+3	0.161
		HOMO-15 → LUMO+5	0.126
		HOMO-15 → LUMO+10	-0.143
		HOMO-14 → LUMO	0.278
		HOMO-14 → LUMO+2	0.355
		HOMO-14 → LUMO+6	0.101
		HOMO-14 → LUMO+9	0.158
296	0.2151	HOMO-1 → LUMO	-0.373
		HOMO → LUMO+1	0.565

4 ax- $\parallel$ (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
367	1.1457	HOMO-1 → LUMO+1	-0.127
		HOMO → LUMO	0.671
		HOMO → LUMO+2	0.147
314	0.0023	HOMO-15 → LUMO	-0.295
		HOMO-15 → LUMO+2	0.344
		HOMO-15 → LUMO+8	-0.179
		HOMO-14 → LUMO+1	0.407
		HOMO-14 → LUMO+3	0.149
		HOMO-14 → LUMO+4	-0.139
		HOMO-14 → LUMO+9	-0.104
		HOMO-14 → LUMO+10	0.115
314	0.0001	HOMO-15 → LUMO+1	0.407
		HOMO-15 → LUMO+3	0.149
		HOMO-15 → LUMO+4	-0.139
		HOMO-15 → LUMO+9	-0.104

		HOMO-15 → LUMO+10	0.115
		HOMO-14 → LUMO	-0.297
		HOMO-14 → LUMO+2	0.347
		HOMO-14 → LUMO+8	-0.180
297	0.3328	HOMO-1 → LUMO	-0.401
		HOMO → LUMO+1	0.549

4 eq (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
363	1.2988	HOMO-1 → LUMO+1	-0.129
		HOMO → LUMO	0.671
		HOMO → LUMO+2	0.146
314	0.001	HOMO-15 → LUMO	0.305
		HOMO-15 → LUMO+2	-0.338
		HOMO-15 → LUMO+9	0.173
		HOMO-14 → LUMO+1	0.412
		HOMO-14 → LUMO+3	0.161
		HOMO-14 → LUMO+6	0.102
		HOMO-14 → LUMO+8	-0.170
313	0.0003	HOMO-15 → LUMO+1	0.411
		HOMO-15 → LUMO+3	0.160
		HOMO-15 → LUMO+6	0.102
		HOMO-15 → LUMO+8	-0.170
		HOMO-14 → LUMO	0.308
		HOMO-14 → LUMO+2	-0.340
		HOMO-14 → LUMO+9	0.174
297	0.1619	HOMO-1 → LUMO	-0.335
		HOMO → LUMO+1	0.590

5 ax- $\perp$ (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
370	0.8519	HOMO → LUMO	0.692
283	0.1139	HOMO-1 → LUMO	0.677
265	0.0871	HOMO → LUMO+1	0.654
		HOMO → LUMO+7	-0.120
255	0.0536	HOMO-8 → LUMO	-0.120
		HOMO-7 → LUMO	0.266
		HOMO-2 → LUMO	0.580
		HOMO → LUMO+1	0.107

5 ax- $\parallel$ (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
356	0.8547	HOMO-1 $\rightarrow$ LUMO+1	0.102
		HOMO $\rightarrow$ LUMO	0.690
280	0.1714	HOMO-1 $\rightarrow$ LUMO	0.674
266	0.093	HOMO-1 $\rightarrow$ LUMO+3	0.119
		HOMO $\rightarrow$ LUMO+1	0.654
		HOMO $\rightarrow$ LUMO+2	-0.115
		HOMO $\rightarrow$ LUMO+7	0.115
249	0.0138	HOMO-6 $\rightarrow$ LUMO	-0.272
		HOMO-5 $\rightarrow$ LUMO	0.102
		HOMO-4 $\rightarrow$ LUMO	-0.160
		HOMO-3 $\rightarrow$ LUMO	0.403
		HOMO $\rightarrow$ LUMO+1	0.124
		HOMO $\rightarrow$ LUMO+2	0.331

5 eq (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
347	1.0025	HOMO-1 $\rightarrow$ LUMO+1	0.109
		HOMO $\rightarrow$ LUMO	0.690
275	0.1035	HOMO-1 $\rightarrow$ LUMO	0.662
		HOMO $\rightarrow$ LUMO+7	0.105
266	0.0636	HOMO-2 $\rightarrow$ LUMO	0.115
		HOMO $\rightarrow$ LUMO+1	0.648
		HOMO $\rightarrow$ LUMO+3	-0.107
		HOMO $\rightarrow$ LUMO+7	-0.117
249	0.0282	HOMO-7 $\rightarrow$ LUMO	-0.112
		HOMO-2 $\rightarrow$ LUMO	0.589
		HOMO-1 $\rightarrow$ LUMO	0.122
		HOMO $\rightarrow$ LUMO+1	-0.145
		HOMO $\rightarrow$ LUMO+3	-0.123

6 ax- $\perp$ (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
408	1.6046	HOMO-2 $\rightarrow$ LUMO	-0.254
		HOMO-1 $\rightarrow$ LUMO+1	0.151
		HOMO $\rightarrow$ LUMO	0.631
342	0.1977	HOMO-3 $\rightarrow$ LUMO	-0.141
		HOMO-1 $\rightarrow$ LUMO	0.631
		HOMO-1 $\rightarrow$ LUMO+2	0.101
		HOMO $\rightarrow$ LUMO+1	0.224
303	0.1697	HOMO-16 $\rightarrow$ LUMO	0.111
		HOMO-2 $\rightarrow$ LUMO	0.539
		HOMO-1 $\rightarrow$ LUMO+1	0.297

289	0.062	HOMO	→	LUMO	0.131
		HOMO	→	LUMO+2	0.227
		HOMO-3	→	LUMO	0.142
		HOMO-2	→	LUMO+1	-0.110
		HOMO-2	→	LUMO+8	0.110
		HOMO-1	→	LUMO	-0.210
		HOMO-1	→	LUMO+2	0.225
		HOMO-1	→	LUMO+7	0.136
		HOMO	→	LUMO+1	0.559

6 ax-|| (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition			Coefficient
390	1.5784	HOMO-2	→	LUMO	-0.256
		HOMO-1	→	LUMO+1	-0.174
		HOMO	→	LUMO	0.621
336	0.33	HOMO-3	→	LUMO	-0.140
		HOMO-1	→	LUMO	0.612
		HOMO-1	→	LUMO+5	-0.125
		HOMO	→	LUMO+1	-0.262
297	0.1055	HOMO-2	→	LUMO	0.520
		HOMO-1	→	LUMO+1	-0.327
		HOMO-1	→	LUMO+9	0.107
		HOMO	→	LUMO+5	-0.254
287	0.0504	HOMO-3	→	LUMO	-0.148
		HOMO-2	→	LUMO+1	-0.150
		HOMO-2	→	LUMO+9	-0.116
		HOMO-1	→	LUMO	0.220
		HOMO-1	→	LUMO+3	0.117
		HOMO-1	→	LUMO+5	0.214
		HOMO	→	LUMO+1	0.520
		HOMO	→	LUMO+3	-0.110

6 eq (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition			Coefficient
383	1.8299	HOMO-2	→	LUMO	-0.237
		HOMO-1	→	LUMO+1	-0.181
		HOMO	→	LUMO	0.627
331	0.1723	HOMO-3	→	LUMO	-0.130
		HOMO-1	→	LUMO	0.604
		HOMO-1	→	LUMO+5	-0.102
		HOMO	→	LUMO+1	-0.277
294	0.0848	HOMO-2	→	LUMO	0.527
		HOMO-1	→	LUMO+1	-0.322

		HOMO-1 → LUMO+8	-0.116
		HOMO → LUMO+5	-0.193
		HOMO → LUMO+7	0.156
286	0.0053	HOMO-1 → LUMO	0.100
		HOMO-1 → LUMO+3	-0.243
		HOMO-1 → LUMO+4	0.322
		HOMO → LUMO+1	0.241
		HOMO → LUMO+3	0.419

8 ax- $\perp$ (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
409	1.2037	HOMO-1 → LUMO	0.339
		HOMO → LUMO	0.546
		HOMO → LUMO+1	-0.237
329	0.1894	HOMO-2 → LUMO	0.189
		HOMO-1 → LUMO	0.549
		HOMO-1 → LUMO+1	-0.103
		HOMO → LUMO	-0.247
		HOMO → LUMO+1	0.199
		HOMO → LUMO+2	-0.170
313	0.0007	HOMO-17 → LUMO	0.390
		HOMO-17 → LUMO+1	0.450
		HOMO-17 → LUMO+2	0.192
		HOMO-17 → LUMO+4	0.166
		HOMO-17 → LUMO+10	0.201
		HOMO-17 → LUMO+15	-0.111
308	0.2156	HOMO-1 → LUMO+1	0.218
		HOMO → LUMO	0.336
		HOMO → LUMO+1	0.463
		HOMO → LUMO+2	-0.298

8 ax- $\parallel$ (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
397	1.176	HOMO-1 → LUMO	0.325
		HOMO → LUMO	0.528
		HOMO → LUMO+1	-0.282
324	0.2769	HOMO-2 → LUMO	0.208
		HOMO-1 → LUMO	0.531
		HOMO → LUMO	-0.176
		HOMO → LUMO+1	0.264
		HOMO → LUMO+2	-0.186
313	0.0012	HOMO-17 → LUMO	0.423
		HOMO-17 → LUMO+1	0.405

		HOMO-17 → LUMO+2	0.227
		HOMO-17 → LUMO+7	-0.133
		HOMO-17 → LUMO+10	-0.179
308	0.273	HOMO-1 → LUMO	-0.129
		HOMO-1 → LUMO+1	0.195
		HOMO → LUMO	0.399
		HOMO → LUMO+1	0.423
		HOMO → LUMO+2	-0.267

8 eq (ground state, M06-2X/6-31G*)

λ_a (nm)	Intensity	Transition	Coefficient
389	1.3542	HOMO-1 → LUMO	-0.323
		HOMO → LUMO	0.524
		HOMO → LUMO+1	-0.291
321	0.1643	HOMO-2 → LUMO	-0.202
		HOMO-1 → LUMO	0.519
		HOMO → LUMO	0.133
		HOMO → LUMO+1	-0.303
		HOMO → LUMO+2	-0.195
313	0.0019	HOMO-17 → LUMO	0.442
		HOMO-17 → LUMO+1	0.390
		HOMO-17 → LUMO+2	-0.216
		HOMO-17 → LUMO+10	-0.220
		HOMO-17 → LUMO+15	-0.111
305	0.289	HOMO-1 → LUMO	0.172
		HOMO-1 → LUMO+1	-0.205
		HOMO → LUMO	0.420
		HOMO → LUMO+1	0.394
		HOMO → LUMO+2	0.245

Cartesian coordinates

2 ax-1 (ground state, B3LYP/6-31G*)

-1829.277402730

S	3.2447020	-2.0401100	-0.5985670
C	3.6845640	-1.2099920	0.8533670
C	2.6354850	-0.5015930	1.3676220
C	1.4423930	-0.6106340	0.5870390
C	1.5933790	-1.4348670	-0.5220630
P	0.0003780	0.3690730	1.0807070
C	0.0019470	1.8854200	0.0561270
C	0.6782690	-1.8869340	-1.5408350
C	-0.6822450	-1.8855440	-1.5408250
C	-1.5964090	-1.4315540	-0.5220700
C	-1.4436880	-0.6076210	0.5870160
C	-2.6365640	-0.4960190	1.3675700
C	-3.6871580	-1.2021370	0.8532690
S	-3.2489890	-2.0333690	-0.5985400
O	0.0007290	0.7073530	2.5448580
H	-2.6838760	0.0920770	2.2766540
H	-4.6923760	-1.2836260	1.2450020
H	-1.1533250	-2.3449200	-2.4072820
H	2.6840230	0.0863920	2.2767130
H	4.6895950	-1.2936270	1.2451230
H	1.1483950	-2.3472420	-2.4073150
C	0.0032770	3.1134710	0.7314730
C	0.0045810	4.3091890	0.0111880
C	0.0045750	4.2844030	-1.3841270
C	0.0032640	3.0621460	-2.0621440
C	0.0019680	1.8656960	-1.3467360
H	0.0033370	3.1135930	1.8172620
H	0.0056450	5.2587520	0.5397770
H	0.0056280	5.2154430	-1.9449980
H	0.0032550	3.0421530	-3.1487600
H	0.0009550	0.9211790	-1.8831600

2 TS1 (ground state, B3LYP/6-31G*)

-1829.27461358

C	0.5308050	1.4755020	0.4370620
C	1.7316590	1.6142010	-0.2503720
C	2.6797730	0.6827590	-0.8013420
C	2.6815850	-0.6756550	-0.8015260

C	1.7359420	-1.6097560	-0.2508100
C	0.5347220	-1.4743660	0.4366360
P	-0.3537440	-0.0006860	1.0028010
S	2.1241860	-3.3164300	-0.4599280
C	0.6932990	-3.8115960	0.3720670
C	-0.0412190	-2.7391990	0.7877670
S	2.1153620	3.3219490	-0.4591220
C	0.6831740	3.8131460	0.3729930
C	-0.0484870	2.7387170	0.7884810
C	-1.9135630	-0.0025120	0.0422620
C	-3.1230380	-0.0054660	0.7490840
C	-4.3370170	-0.0066720	0.0591110
C	-4.3476760	-0.0049600	-1.3366240
C	-3.1434190	-0.0021180	-2.0465500
C	-1.9301610	-0.0009000	-1.3601790
O	-0.6376150	-0.0014010	2.4783120
H	-3.0949380	-0.0067150	1.8348470
H	-5.2731810	-0.0089280	0.6112090
H	-5.2929280	-0.0058610	-1.8731730
H	-3.1515040	-0.0008250	-3.1332770
H	-0.9959850	0.0013620	-1.9168430
H	-0.9754910	2.8276090	1.3436520
H	0.4648410	4.8632190	0.5143390
H	3.5312250	1.1467800	-1.2942780
H	-0.9679980	-2.8306770	1.3428980
H	0.4777370	-4.8622730	0.5131820
H	3.5342570	-1.1372640	-1.2946090

2 TS2 (ground state, B3LYP/6-31G*)

-1829.27576264			
P	-0.0891020	0.2570050	1.1702650
C	1.5638300	-0.2447990	0.6339470
C	1.9121150	-0.7525850	-0.6116450
C	1.1194470	-1.1364650	-1.7558310
C	-0.1887680	-1.5077720	-1.8021750
C	-1.1368560	-1.6218950	-0.7206330
C	-1.1794430	-1.0463480	0.5429630
C	-0.5224490	1.7635750	0.2251010
C	-1.8273440	2.2676460	0.3538320
C	0.4031520	2.4585640	-0.5633870
C	0.0301580	3.6355580	-1.2160080
C	-1.2690420	4.1261540	-1.0870390
C	-2.1981300	3.4405650	-0.2994750
S	3.6552390	-0.9711530	-0.7019320
C	3.8731590	-0.4100260	0.9219550
C	2.6848780	-0.0659460	1.5024030
C	-2.2768600	-1.5082070	1.3330300
C	-3.0735310	-2.4030680	0.6747670
S	-2.4996330	-2.7148260	-0.9282180
O	-0.2051640	0.4317700	2.6580670
H	-2.4447880	-1.1701920	2.3491240
H	-3.9633580	-2.8994840	1.0387920
H	-0.5541580	-1.8321480	-2.7743410
H	2.5827730	0.3109360	2.5134780

H	4.8647800	-0.3668880	1.3526010
H	1.6648670	-1.2041680	-2.6948000
H	-2.5522880	1.7432400	0.9707200
H	-3.2103450	3.8215180	-0.1939470
H	-1.5586190	5.0413630	-1.5966400
H	0.7563700	4.1676000	-1.8247570
H	1.4169990	2.0849410	-0.6671460

2 ax-|| (ground state, B3LYP/6-31G*)

-1829.276017180

P	0.0000450	0.2503970	1.1863720
C	1.4281910	-0.6866050	0.5880450
C	1.5850710	-1.2123950	-0.6880670
C	0.6801350	-1.3096480	-1.8088490
C	-0.6805390	-1.3094930	-1.8088130
C	-1.5853940	-1.2120240	-0.6879860
C	-1.4283340	-0.6862670	0.5881200
C	0.0002310	1.8208520	0.2463810
C	1.2099050	2.4552190	-0.0717790
C	-1.2093130	2.4551930	-0.0723590
C	-1.2083850	3.7007170	-0.6999370
C	0.0004980	4.3244280	-1.0146990
C	1.2092480	3.7007410	-0.6993600
S	3.1924180	-1.9055170	-0.8566970
C	3.6044620	-1.5058420	0.7769720
C	2.5770590	-0.8711950	1.4177010
C	-2.5772160	-0.8705560	1.4178200
C	-3.6047880	-1.5049940	0.7771530
S	-3.1929040	-1.9048020	-0.8565210
O	0.0001210	0.4265140	2.6789200
H	-2.6132560	-0.5290870	2.4459410
H	-4.5799710	-1.7617780	1.1692720
H	-1.1545090	-1.4780140	-2.7735650
H	2.6132150	-0.5297630	2.4458310
H	4.5796030	-1.7628640	1.1690380
H	1.1540130	-1.4782790	-2.7736270
H	2.1542020	1.9744100	0.1681410
H	2.1518960	4.1827650	-0.9442700
H	0.0006140	5.2938010	-1.5060940
H	-2.1509310	4.1827170	-0.9452930

H	-2.1537120	1.9743680	0.1671160
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2 eq (ground state, B3LYP/6-31G*)

-1829.276782530

C	2.0007750	0.0000000	0.1808120
C	3.0817200	-0.0000010	1.0719710
H	2.8801460	-0.0000020	2.1392160
C	4.3908420	-0.0000010	0.5852540
H	5.2260170	-0.0000020	1.2805440
C	4.6252490	0.0000010	-0.7905430
H	5.6442950	0.0000010	-1.1685520
C	3.5502670	0.0000020	-1.6845400
H	3.7322070	0.0000040	-2.7559510
C	2.2422070	0.0000020	-1.2018070
H	1.4090100	0.0000040	-1.9002510
C	-0.4945770	-1.4442970	0.1636090
C	0.2258910	-2.6602140	-0.0729270
H	1.3018320	-2.7410680	0.0282260
C	-0.5736130	-3.7107390	-0.4207050
H	-0.2777620	-4.7267190	-0.6460190
C	-1.8674340	-1.5974500	-0.0150230
C	-2.9712590	-0.6803490	0.0799030
H	-3.9531820	-1.1481740	0.1004550
C	-0.4945770	1.4442960	0.1636080
C	0.2258940	2.6602090	-0.0729420
H	1.3018360	2.7410600	0.0281980
C	-0.5736060	3.7107250	-0.4207570
H	-0.2777510	4.7266970	-0.6461040
C	-1.8674330	1.5974490	-0.0150260
C	-2.9712590	0.6803470	0.0799030
H	-3.9531810	1.1481730	0.1004590
O	0.3479920	0.0000000	2.3976340
P	0.3154240	-0.0000000	0.8953280
S	-2.2413520	-3.2569690	-0.4673930
S	-2.2413540	3.2569780	-0.4673540

3 ax- $\perp$ (ground state, B3LYP/6-31G*)

-2475.883083200

C	6.1599390	-0.6824670	0.8742420
C	5.0530530	-0.8992470	0.0313670
C	5.2751100	-1.5194400	-1.2145740
C	6.5508480	-1.8973260	-1.6079730
C	7.6471400	-1.6750350	-0.7563100

C	7.4384860	-1.0655840	0.4921490
C	3.7004500	-0.4963150	0.4207210
S	3.2442040	-0.2859210	2.0960230
C	1.5949660	0.1537760	1.6757930
C	1.4401290	0.1457400	0.2924760
C	2.6231550	-0.2342720	-0.3975650
C	0.6816350	0.3972630	2.7605670
C	-0.6817980	0.3972290	2.7605980
C	-1.5951590	0.1537960	1.6758300
C	-1.4403910	0.1462290	0.2925130
C	-2.6234440	-0.2336020	-0.3976030
C	-3.7006640	-0.4959920	0.4206640
S	-3.2444620	-0.2857180	2.0959860
P	-0.0000500	0.6398320	-0.6917380
O	-0.0001520	0.0245940	-2.0624770
C	-5.0532370	-0.8990070	0.0312650
C	-5.2751830	-1.5194210	-1.2145840
C	-6.5508940	-1.8973570	-1.6080300
C	-7.6472520	-1.6748990	-0.7564970
C	-7.4387040	-1.0652270	0.4918730
C	-6.1601850	-0.6820530	0.8740080
C	-8.9651640	-2.0683350	-1.1567170
N	-10.0362150	-2.3870600	-1.4812820
C	8.9650800	-2.0684150	-1.1564870
N	10.0361540	-2.3870950	-1.4810190
C	0.0002420	2.4653720	-0.7797860
C	0.0013320	3.0432650	-2.0568380
C	0.0015920	4.4320900	-2.1961630
C	0.0007420	5.2478230	-1.0638790
C	-0.0003790	4.6757920	0.2115170
C	-0.0006340	3.2894860	0.3559340
H	0.0019080	2.3938050	-2.9269050
H	0.0024510	4.8756360	-3.1881080
H	0.0009170	6.3291500	-1.1725880
H	-0.0010770	5.3110570	1.0931670
H	-0.0015170	2.8555770	1.3516940
H	-1.1502000	0.5418670	3.7317030
H	-2.6629870	-0.2814300	-1.4796230
H	-4.4351110	-1.7241440	-1.8700830
H	-6.7066730	-2.3763270	-2.5691950
H	-8.2826760	-0.8882760	1.1505420
H	-6.0213500	-0.1895580	1.8321230
H	1.1500750	0.5419550	3.7316460
H	2.6626460	-0.2823540	-1.4795760
H	4.4351050	-1.7240310	-1.8701990
H	6.7066990	-2.3761220	-2.5692130

H	8.2824000	-0.8887660	1.1509300
H	6.0210450	-0.1901600	1.8324460

3 ax-|| (ground state, B3LYP/6-31G*)

-2475.881570660

S	3.1944620	0.0963310	2.0042760
C	1.5860290	0.5807690	1.4926280
C	1.4270000	0.3338220	0.1329000
C	2.5712260	-0.2561790	-0.4676150
C	3.6277150	-0.4481440	0.3972710
C	0.6816550	1.0934520	2.4896670
C	-0.6816520	1.0934520	2.4896670
C	-1.5860270	0.5807690	1.4926290
C	-1.4269980	0.3338210	0.1329010
C	-2.5712240	-0.2561820	-0.4676140
C	-3.6277130	-0.4481460	0.3972730
S	-3.1944600	0.0963310	2.0042780
P	0.0000010	0.7985350	-0.8814500
C	-0.0000020	2.6250380	-0.9475120
C	1.2101140	3.3301230	-1.0252230
C	1.2089960	4.7165870	-1.1753700
C	-0.0000080	5.4111210	-1.2492210
C	-1.2090100	4.7165770	-1.1754130
C	-1.2101210	3.3301130	-1.0252660
C	-4.9454380	-1.0150050	0.1040650
C	-5.1225630	-1.8544470	-1.0141480
C	-6.3660410	-2.3909010	-1.3160540
C	-7.4737310	-2.1112670	-0.4965980
C	-7.3093200	-1.2829270	0.6260300
C	-6.0636470	-0.7428320	0.9155830
C	-8.7579340	-2.6676510	-0.8016280
N	-9.8017380	-3.1186540	-1.0489080
C	4.9454400	-1.0150030	0.1040630
C	5.1225650	-1.8544440	-1.0141520
C	6.3660430	-2.3908970	-1.3160570
C	7.4737330	-2.1112640	-0.4966010
C	7.3093220	-1.2829260	0.6260280
C	6.0636490	-0.7428310	0.9155820
C	8.7579360	-2.6676480	-0.8016320
N	9.8017400	-3.1186510	-1.0489120
O	-0.0000000	0.1252950	-2.2248320
H	2.1549290	2.7968290	-0.9670810
H	2.1514260	5.2543030	-1.2327300
H	-0.0000110	6.4917350	-1.3636990
H	-2.1514430	5.2542850	-1.2328050

H	-2.1549340	2.7968110	-0.9671550
H	-1.1533670	1.4620810	3.3979800
H	-2.6025760	-0.4939520	-1.5247210
H	-4.2717460	-2.1026400	-1.6401740
H	-6.4868350	-3.0372620	-2.1792640
H	-8.1621530	-1.0615580	1.2593860
H	-5.9611420	-0.0854170	1.7741200
H	1.1533690	1.4620810	3.3979790
H	2.6025780	-0.4939490	-1.5247220
H	4.2717490	-2.1026350	-1.6401780
H	6.4868370	-3.0372570	-2.1792690
H	8.1621540	-1.0615580	1.2593850
H	5.9611440	-0.0854170	1.7741190

3 eq (ground state, B3LYP/6-31G*)

-2475.881978060			
C	6.1840450	-1.2132840	-0.2705400
C	5.0903150	-0.3270920	-0.3054090
C	5.3412770	1.0286810	-0.5970540
C	6.6307320	1.4837350	-0.8320310
C	7.7133250	0.5876300	-0.7946110
C	7.4764620	-0.7682980	-0.5137580
C	3.7239330	-0.7843700	-0.0454260
S	3.2515840	-2.4541250	-0.2585330
C	1.5968060	-2.1307430	0.2369600
C	1.4417810	-0.7805870	0.5510890
C	2.6475210	-0.0409520	0.3843210
C	0.6817200	-3.2360520	0.2227430
C	-0.6817180	-3.2360530	0.2227470
C	-1.5968060	-2.1307450	0.2369700
C	-1.4417810	-0.7805890	0.5510980
C	-2.6475210	-0.0409540	0.3843330
C	-3.7239330	-0.7843710	-0.0454150
S	-3.2515900	-2.4541310	-0.2584970
P	0.0000020	-0.0564790	1.3761640
C	-0.0000010	1.6988930	0.8623260
C	-5.0903140	-0.3270920	-0.3054050
C	-5.3412720	1.0286790	-0.5970620
C	-6.6307270	1.4837330	-0.8320450
C	-7.7133210	0.5876300	-0.7946180
C	-7.4764610	-0.7682950	-0.5137520
C	-6.1840460	-1.2132810	-0.2705290
C	-9.0448450	1.0527680	-1.0444570
N	-10.1261600	1.4313380	-1.2481800
C	9.0448500	1.0527670	-1.0444450

N	10.1261660	1.4313370	-1.2481620
O	0.0000070	-0.2082980	2.8701310
H	-1.1478170	-4.2155630	0.1430050
H	-2.7224930	1.0135580	0.6221300
H	-4.5131350	1.7272330	-0.6591930
H	-6.8086140	2.5303060	-1.0570370
H	-8.3093400	-1.4629570	-0.4794450
H	-6.0233030	-2.2601500	-0.0300340
H	1.1478200	-4.2155620	0.1429960
H	2.7224940	1.0135590	0.6221220
H	4.5131410	1.7272370	-0.6591790
H	6.8086220	2.5303100	-1.0570140
H	8.3093400	-1.4629610	-0.4794550
H	6.0233000	-2.2601540	-0.0300550
C	0.0000010	2.6689590	1.8733800
C	-0.0000020	4.0257670	1.5413950
C	-0.0000070	4.4176390	0.2019660
C	-0.0000100	3.4536630	-0.8110310
C	-0.0000070	2.0983350	-0.4835120
H	0.0000050	2.3459840	2.9103910
H	-0.0000010	4.7745900	2.3286710
H	-0.0000100	5.4734920	-0.0554550
H	-0.0000140	3.7589520	-1.8539710
H	-0.0000080	1.3523600	-1.2744880

4 ax- $\perp$ (ground state, B3LYP/6-31G*)

-2700.399598210			
C	-6.1623460	-0.4259630	1.0291630
C	-5.0621060	-0.7309070	0.2030510
C	-5.2943730	-1.4661090	-0.9780190
C	-6.5748860	-1.8712650	-1.3282920
C	-7.6390660	-1.5507740	-0.4856470
C	-7.4467660	-0.8339050	0.6939090
C	-3.7058500	-0.3000810	0.5450070
S	-3.2471960	0.0969840	2.1851180
C	-1.5959230	0.4747920	1.7174020
C	-1.4414740	0.3081180	0.3438010
C	-2.6270400	-0.1405560	-0.2980320
C	-0.6816910	0.8366640	2.7677170
C	0.6816890	0.8366630	2.7677170
C	1.5959210	0.4747890	1.7174020
S	3.2471910	0.0969710	2.1851200
C	3.7058470	-0.3000850	0.5450080
C	2.6270380	-0.1405610	-0.2980310
C	1.4414720	0.3081130	0.3438020

C	5.0621040	-0.7309100	0.2030530
C	6.1623430	-0.4259670	1.0291660
C	7.4467640	-0.8339080	0.6939120
C	7.6390650	-1.5507740	-0.4856450
C	6.5748850	-1.8712640	-1.3282920
C	5.2943730	-1.4661090	-0.9780180
N	8.9948360	-1.9807520	-0.8483300
O	9.1338600	-2.6080880	-1.8987010
P	-0.0000000	0.6778640	-0.6926420
C	0.0000020	2.4786390	-0.9993870
N	-8.9948370	-1.9807520	-0.8483320
O	-9.1338590	-2.6080930	-1.8987010
O	-0.0000010	-0.0974140	-1.9793880
O	-9.9120960	-1.6876660	-0.0805770
O	9.9120950	-1.6876660	-0.0805750
H	-1.1497030	1.0895400	3.7165510
H	-2.6675370	-0.3123000	-1.3673320
H	-4.4601040	-1.7381540	-1.6159290
H	-6.7613050	-2.4376440	-2.2323590
H	-8.2977460	-0.6002250	1.3215630
H	-6.0142340	0.1546260	1.9349120
H	1.1497010	1.0895370	3.7165510
H	2.6675360	-0.3123050	-1.3673310
H	4.4601030	-1.7381530	-1.6159300
H	6.7613060	-2.4376400	-2.2323600
H	8.2977440	-0.6002290	1.3215670
H	6.0142310	0.1546200	1.9349170
C	0.0000130	2.8975620	-2.3370600
C	0.0000160	4.2593270	-2.6433250
C	0.0000080	5.2060730	-1.6180760
C	-0.0000030	4.7928550	-0.2827650
C	-0.0000060	3.4341570	0.0283440
H	0.0000190	2.1476760	-3.1222130
H	0.0000250	4.5796420	-3.6816180
H	0.0000100	6.2662450	-1.8569670
H	-0.0000100	5.5301600	0.5154510
H	-0.0000150	3.1236150	1.0693330

4 ax-|| (ground state, B3LYP/6-31G*)

P	0.0000140	0.9603420	-0.8962370
C	1.4258970	0.5543540	0.1452640
C	1.5856270	0.8872010	1.4866940
C	0.6816800	1.4659550	2.4474710
C	-0.6816510	1.4659440	2.4474750
C	-1.5855970	0.8871790	1.4867050

C	-1.4258530	0.5543030	0.1452840
C	-0.0000520	2.7796350	-1.0652480
C	-1.2102830	3.4790390	-1.1826700
C	1.2101310	3.4791910	-1.1823360
C	1.2089200	4.8551410	-1.4092710
C	-0.0001590	5.5443620	-1.5217020
C	-1.2091820	4.8549920	-1.4096090
C	-2.5659200	-0.0812070	-0.4140090
C	-3.6205230	-0.2235480	0.4633900
S	-3.1901680	0.4286020	2.0307060
C	2.5659670	-0.0811510	-0.4140310
C	3.6205580	-0.2235190	0.4633760
S	3.1901900	0.4285980	2.0307030
C	-4.9337090	-0.8182300	0.2101770
C	-6.0502650	-0.5093890	1.0127550
C	-7.2927460	-1.0776060	0.7640940
C	-7.4269620	-1.9621680	-0.3044400
C	-6.3453420	-2.2913420	-1.1210910
C	-5.1064370	-1.7237560	-0.8573360
N	-8.7382490	-2.5638960	-0.5745160
O	-9.6729840	-2.2530110	0.1646470
C	4.9337440	-0.8181980	0.2101590
C	6.0502880	-0.5094000	1.0127700
C	7.2927710	-1.0776120	0.7641050
C	7.4270000	-1.9621260	-0.3044670
C	6.3453930	-2.2912590	-1.1211500
C	5.1064860	-1.7236780	-0.8573910
N	8.7382890	-2.5638470	-0.5745480
O	9.6730140	-2.2529960	0.1646430
O	0.0000270	0.2089980	-2.1972430
O	8.8251110	-3.3428150	-1.5241390
O	-8.8250590	-3.3429030	-1.5240770
H	-1.1533210	1.8929330	3.3298500
H	-2.5958870	-0.3880680	-1.4532370
H	-4.2563640	-1.9995130	-1.4723620
H	-6.4850720	-2.9894590	-1.9371740
H	-8.1559000	-0.8425060	1.3743750
H	-5.9497570	0.1978840	1.8307230
H	1.1533500	1.8929510	3.3298420
H	2.5959400	-0.3879820	-1.4532670
H	4.2564230	-1.9994030	-1.4724450
H	6.4851320	-2.9893400	-1.9372610
H	8.1559150	-0.8425440	1.3744120
H	5.9497700	0.1978340	1.8307700
H	-2.1551440	2.9498240	-1.0954790
H	-2.1516050	5.3885780	-1.4971180

H	-0.0002040	6.6168880	-1.6962240
H	2.1513000	5.3888480	-1.4965160
H	2.1550370	2.9501020	-1.0948900

4 eq (ground state, B3LYP/6-31G*)

-2700.398542440

C	6.1786570	-1.2858220	-0.2587630
C	5.0860090	-0.3959170	-0.2464550
C	5.3348250	0.9725230	-0.4807660
C	6.6226860	1.4380650	-0.7062210
C	7.6787390	0.5271470	-0.7114320
C	7.4707460	-0.8333980	-0.4926000
C	3.7215500	-0.8626930	0.0035200
S	3.2503390	-2.5262810	-0.2545060
C	1.5969230	-2.2177580	0.2529030
C	1.4413100	-0.8771280	0.6063110
C	2.6454430	-0.1323740	0.4573960
C	0.6817500	-3.3222480	0.2079200
C	-0.6817460	-3.3222510	0.2079350
C	-1.5969240	-2.2177640	0.2529360
S	-3.2503610	-2.5263040	-0.2543930
C	-3.7215510	-0.8626980	0.0035560
C	-2.6454460	-0.1323820	0.4574380
C	-1.4413100	-0.8771350	0.6063430
P	0.0000070	-0.1783830	1.4546350
C	-0.0000040	1.5918010	0.9969270
C	0.0000060	2.5288920	2.0386210
C	-0.0000020	3.8955580	1.7499400
C	-0.0000210	4.3299890	0.4237010
C	-0.0000310	3.3989570	-0.6196760
C	-0.0000230	2.0338710	-0.3355660
C	-5.0860060	-0.3959180	-0.2464400
C	-5.3348120	0.9725160	-0.4807910
C	-6.6226700	1.4380600	-0.7062620
C	-7.6787290	0.5271490	-0.7114490
C	-7.4707450	-0.8333910	-0.4925760
C	-6.1786590	-1.2858160	-0.2587230
N	-9.0416770	1.0131750	-0.9569690
O	-9.9521610	0.1842080	-0.9619630
N	9.0416900	1.0131720	-0.9569340
O	9.9521680	0.1841960	-0.9619570
O	0.0000240	-0.3793190	2.9426050
O	-9.1926420	2.2210970	-1.1433700
O	9.1926610	2.2210970	-1.1433060
H	0.0000200	2.1728290	3.0647080

H	0.0000050	4.6188850	2.5606670
H	-0.0000270	5.3935010	0.2002550
H	-0.0000460	3.7373760	-1.6522910
H	-0.0000310	1.3135500	-1.1500340
H	-1.1476750	-4.2991300	0.1001700
H	-2.7197310	0.9151940	0.7240320
H	-4.5071180	1.6735540	-0.5058730
H	-6.8220600	2.4867540	-0.8887720
H	-8.3155590	-1.5109150	-0.4994060
H	-6.0181260	-2.3418090	-0.0629030
H	1.1476800	-4.2991240	0.1001400
H	2.7197340	0.9151980	0.7240040
H	4.5071350	1.6735660	-0.5058300
H	6.8220840	2.4867620	-0.8886990
H	8.3155560	-1.5109270	-0.4994490
H	6.0181170	-2.3418200	-0.0629770

5 ax- $\perp$ (ground state, B3LYP/6-31G*)

-2291.397127140

S	3.2504880	-1.0773040	1.7109960
C	1.5941130	-0.5495380	1.4413720
C	1.4452760	-0.1198390	0.1264060
C	2.6342710	-0.2575630	-0.6432750
C	3.7108910	-0.7601980	0.0530960
C	5.0708340	-1.0156590	-0.4344250
C	5.9229890	-1.9352160	0.2036220
C	7.2095080	-2.1688960	-0.2766040
C	7.6720730	-1.4958020	-1.4086700
C	6.8362400	-0.5806430	-2.0528990
C	5.5534540	-0.3375380	-1.5698660
C	0.6772180	-0.6667180	2.5437890
C	-0.6861500	-0.6702720	2.5390850
C	-1.5961040	-0.5625830	1.4300490
S	-3.2473210	-1.1126250	1.6865630
C	-3.7034240	-0.7832500	0.0303290
C	-2.6248000	-0.2791580	-0.6615890
C	-1.4403480	-0.1380350	0.1141430
P	0.0010520	0.6413490	-0.6594480
C	-0.0098810	2.4043000	-0.1671100
C	0.0041840	2.8266690	1.1706410
C	-0.0064890	4.1873700	1.4735280
C	-0.0311310	5.1342820	0.4457830
C	-0.0449240	4.7190490	-0.8864810
C	-0.0342830	3.3574910	-1.1942700
C	-5.0592480	-1.0440020	-0.4648550

C	-5.2750870	-1.2886710	-1.8343390
C	-6.5581710	-1.5228200	-2.3211820
C	-7.6526990	-1.5305640	-1.4531890
C	-7.4514500	-1.2979980	-0.0914800
C	-6.1702670	-1.0537530	0.3977480
O	0.0070230	0.4978420	-2.1555790
H	1.1434070	-0.8360830	3.5121700
H	2.6634340	-0.0097920	-1.6979320
H	5.5683650	-2.4865230	1.0704390
H	7.8486890	-2.8861270	0.2311440
H	8.6745710	-1.6806350	-1.7843340
H	7.1878790	-0.0448460	-2.9304410
H	4.9242100	0.3970550	-2.0628560
H	-1.1581580	-0.8397760	3.5045580
H	-2.6659960	0.0159640	-1.7035660
H	-4.4283090	-1.3144890	-2.5135160
H	-6.7020270	-1.7111330	-3.3816780
H	-8.6524440	-1.7185460	-1.8346280
H	-8.2955220	-1.2978850	0.5928690
H	-6.0317580	-0.8480040	1.4559310
H	0.0238130	2.0985530	1.9763470
H	0.0047910	4.5102120	2.5112100
H	-0.0392590	6.1944260	0.6854790
H	-0.0638420	5.4541240	-1.6867350
H	-0.0440420	3.0167200	-2.2252050

5 ax-|| (ground state, B3LYP/6-31G*)

-2291.395661910			
P	0.0014810	0.6749060	-0.8663890
C	1.4323030	0.0482400	0.0475480
C	1.5841460	0.0411710	1.4295760
C	0.6743680	0.3578790	2.5003380
C	-0.6889160	0.3519370	2.4951070
C	-1.5877810	0.0232080	1.4188720
C	-1.4250600	0.0243090	0.0379670
C	-0.0146440	2.4844040	-0.5919460
C	1.1881700	3.2019130	-0.5177250
C	1.1745510	4.5922060	-0.4072910
C	-0.0403680	5.2791600	-0.3703190
C	-1.2425060	4.5729210	-0.4456590
C	-1.2305980	3.1827290	-0.5560630
C	2.5820310	-0.4198790	-0.6469340
C	3.6356600	-0.7665550	0.1702690
S	3.1991130	-0.5120300	1.8477270
C	-2.5673320	-0.4506580	-0.6635600

C	-3.6253120	-0.7991200	0.1473910
S	-3.1966510	-0.5538510	1.8278930
C	4.9589010	-1.2697740	-0.2152790
C	5.7483120	-2.0255120	0.6703970
C	6.9998330	-2.5000110	0.2842480
C	7.4886960	-2.2373490	-0.9965950
C	6.7148580	-1.4891110	-1.8868330
C	5.4677940	-1.0053640	-1.5010060
C	-4.9425480	-1.3104910	-0.2463020
C	-5.0990940	-1.9847760	-1.4722390
C	-6.3456760	-2.4620610	-1.8675330
C	-7.4613360	-2.2898040	-1.0447510
C	-7.3183150	-1.6311230	0.1778020
C	-6.0745130	-1.1430860	0.5718350
O	0.0097180	0.2727940	-2.3148270
H	1.1419660	0.5560290	3.4626390
H	2.6012690	-0.5080060	-1.7271370
H	5.3701250	-2.2611240	1.6616380
H	7.5903250	-3.0844840	0.9846130
H	8.4636300	-2.6101140	-1.2979370
H	7.0878140	-1.2717050	-2.8840650
H	4.8882780	-0.4018300	-2.1929050
H	-1.1656540	0.5480360	3.4532670
H	-2.5979650	-0.4934460	-1.7462550
H	-4.2332860	-2.1507320	-2.1059640
H	-6.4434770	-2.9808900	-2.8172830
H	-8.4322320	-2.6677410	-1.3526980
H	-8.1795790	-1.4882340	0.8247960
H	-5.9833620	-0.6091580	1.5141320
H	-2.1701880	2.6400500	-0.6119950
H	-2.1900560	5.1041500	-0.4161330
H	-0.0504140	6.3623000	-0.2816030
H	2.1121480	5.1383420	-0.3474730
H	2.1375640	2.6742890	-0.5430030

5 eq (ground state, B3LYP/6-31G*)

-2291.396226470			
O	-0.0085800	0.1968680	2.7357310
C	0.0036450	1.8823150	0.5438710
C	0.0169510	2.1447070	-0.8348870
H	0.0272020	1.3223030	-1.5458840
C	0.0188170	3.4599370	-1.2977000
H	0.0306760	3.6580180	-2.3661790
C	0.0065810	4.5212850	-0.3875970
H	0.0082090	5.5459340	-0.7501950

C	-0.0070940	4.2660580	0.9844150
H	-0.0166840	5.0905950	1.6922430
C	-0.0083230	2.9496530	1.4512080
H	-0.0187530	2.7318960	2.5152390
C	0.6718510	-3.0883600	0.3534230
H	1.1351420	-4.0726410	0.3468900
C	1.5913020	-1.9885420	0.2887390
C	1.4436540	-0.6180540	0.4976560
C	2.6573100	0.1003040	0.2840140
H	2.7248590	1.1771060	0.3850620
C	3.7321140	-0.6777750	-0.0788520
C	5.1067300	-0.2513120	-0.3657230
C	5.9495990	-0.9997760	-1.2070120
H	5.5768400	-1.9090250	-1.6711100
C	7.2497410	-0.5766560	-1.4741100
H	7.8821390	-1.1696410	-2.1292800
C	7.7351280	0.6058380	-0.9130860
H	8.7485990	0.9360070	-1.1232350
C	6.9089310	1.3586070	-0.0752810
H	7.2795180	2.2751290	0.3758520
C	5.6122730	0.9337100	0.2013530
H	4.9908620	1.5094420	0.8805820
C	-0.6913740	-3.0842230	0.3531700
H	-1.1608550	-4.0655200	0.3487710
C	-1.6035590	-1.9789090	0.2819270
C	-1.4464120	-0.6082590	0.4823710
C	-2.6543380	0.1177620	0.2629730
H	-2.7291130	1.1882330	0.4143260
C	-3.7338640	-0.6549000	-0.0976960
C	-5.1041460	-0.2206190	-0.3907170
C	-5.3474840	1.0846180	-0.8582280
H	-4.5109380	1.7547110	-1.0323510
C	-6.6444770	1.5152570	-1.1242000
H	-6.8095610	2.5267440	-1.4855360
C	-7.7264760	0.6506810	-0.9427460
H	-8.7374170	0.9867620	-1.1556740
C	-7.4983100	-0.6495890	-0.4886570
H	-8.3324730	-1.3298100	-0.3397070
C	-6.2028720	-1.0804320	-0.2119590
H	-6.0425100	-2.0861300	0.1673390
P	-0.0025200	0.1859850	1.2329200
S	3.2531800	-2.3577640	-0.1540100
S	-3.2628480	-2.3369100	-0.1789160

6 ax- $\perp$ (ground state, B3LYP/6-31G*)

-3326.296862640

C	11.2784590	-0.8250680	-0.7343830
C	10.1137590	-0.4989830	-0.0220960
C	10.0844380	0.6835490	0.7340650
C	11.1950020	1.5249380	0.7640420
C	12.3552360	1.1947820	0.0602080
C	12.3905060	0.0134070	-0.6836090
N	8.9820350	-1.3622660	-0.0608300
C	9.1735600	-2.7682070	0.0647760
C	8.4998690	-3.6594260	-0.7850930
C	8.6900070	-5.0338110	-0.6533380
C	9.5648280	-5.5401820	0.3103680
C	10.2439430	-4.6547600	1.1499880
C	10.0465480	-3.2797390	1.0375060
C	7.6819650	-0.8303560	-0.2232180
C	6.5787620	-1.4054250	0.4340420
C	5.3019970	-0.8891900	0.2630930
C	5.0669900	0.2366490	-0.5500080
C	6.1778120	0.8097980	-1.1960960
C	7.4553600	0.2861280	-1.0473250
C	3.7152490	0.7746100	-0.7029860
S	3.2550020	1.7336370	-2.0940380
C	1.6026720	1.9324290	-1.5187750
C	1.4504880	1.2827270	-0.2972380
C	2.6353310	0.6294230	0.1409330
P	0.0125340	1.2717410	0.8040420
C	-1.4349010	1.3067410	-0.2843590
C	-1.5872120	1.9581820	-1.5050690
S	-3.2475130	1.7853890	-2.0660390
C	-3.7110460	0.8362290	-0.6697120
C	-2.6264110	0.6737770	0.1651740
C	-0.6724490	2.6651700	-2.3586910
C	0.6921460	2.6541830	-2.3645460
C	-5.0692570	0.3206450	-0.5041030
C	-5.3117990	-0.8091530	0.3014830
C	-6.5926590	-1.3135780	0.4745280
C	-7.6966360	-0.7050560	-0.1509090
C	-7.4646010	0.4236330	-0.9568300
C	-6.1787970	0.9186630	-1.1297700
N	-9.0023970	-1.2168870	0.0255960
C	-9.9372150	-1.1962640	-1.0483010
C	-11.2685630	-0.8138490	-0.8211030
C	-12.1867250	-0.8095930	-1.8695340
C	-11.7921290	-1.1678220	-3.1602490
C	-10.4661570	-1.5411290	-3.3903550
C	-9.5451550	-1.5660900	-2.3447070

O	0.0068550	0.0995400	1.7453810
C	0.0298030	2.8527770	1.7271710
C	0.0356420	4.1074970	1.0994760
C	0.0485720	5.2719430	1.8659270
C	0.0557930	5.1931090	3.2613130
C	0.0500530	3.9473090	3.8903040
C	0.0370820	2.7789100	3.1265790
C	-9.3959850	-1.7590830	1.2829380
C	-10.1080670	-2.9670600	1.3423810
C	-10.5036580	-3.4884400	2.5728500
C	-10.1829690	-2.8268040	3.7600990
C	-9.4680640	-1.6283870	3.7036990
C	-9.0836580	-1.0903230	2.4768800
H	0.0301290	4.1795000	0.0156610
H	0.0530070	6.2417540	1.3753240
H	0.0658520	6.1030220	3.8558670
H	0.0556510	3.8840670	4.9752920
H	0.0323030	1.8012140	3.5989480
H	-1.1398180	3.2457360	-3.1513150
H	-2.6686590	0.1350400	1.1044810
H	-4.4772460	-1.3213330	0.7708800
H	-6.7444370	-2.1966500	1.0862590
H	-8.3016310	0.9186280	-1.4377710
H	-6.0392220	1.8095740	-1.7367290
H	-10.3475100	-3.4902110	0.4219670
H	-11.0541420	-4.4251040	2.6021930
H	-10.4867900	-3.2398090	4.7177330
H	-9.2183290	-1.0986100	4.6192000
H	-8.5403350	-0.1514990	2.4358040
H	-11.5760070	-0.5229810	0.1783770
H	-13.2137360	-0.5109270	-1.6763470
H	-12.5088280	-1.1569450	-3.9764340
H	-10.1464480	-1.8308240	-4.3879200
H	-8.5194620	-1.8719150	-2.5252250
H	1.1620440	3.2271190	-3.1612160
H	2.6756170	0.0875020	1.0785010
H	4.4690330	-1.3709850	0.7660290
H	6.7279530	-2.2677330	1.0752420
H	8.2891070	0.7460740	-1.5671860
H	6.0427780	1.6854570	-1.8256650
H	7.8301500	-3.2688130	-1.5448490
H	8.1606220	-5.7106410	-1.3188110
H	9.7155010	-6.6117060	0.4056110
H	10.9229520	-5.0349390	1.9087090
H	10.5662450	-2.5946840	1.6999430
H	9.1902310	0.9359100	1.2952750

H	11.1562050	2.4365730	1.3545550
H	13.2214200	1.8495120	0.0921510
H	13.2845460	-0.2536710	-1.2409570
H	11.3045460	-1.7360760	-1.3239000

6 ax-|| (ground state, B3LYP/6-31G*)

-3326.295471970

P	0.0222280	1.7838190	0.9245670
O	0.0159350	0.8139380	2.0735530
S	-3.1904620	1.8565150	-2.0199330
C	0.0447990	3.5424190	1.4340780
C	1.2629190	4.1946790	1.6745780
H	2.2006200	3.6808700	1.4817590
C	1.2791660	5.5029600	2.1575520
H	2.2284360	6.0002440	2.3382010
C	0.0790550	6.1725410	2.4043560
H	0.0922800	7.1932040	2.7776450
C	-1.1381150	5.5302350	2.1688110
H	-2.0741570	6.0488610	2.3582780
C	-1.1559850	4.2219610	1.6859120
H	-2.1068350	3.7294860	1.5020520
C	-1.4134830	1.6004480	-0.1612980
C	-1.5694380	2.1784470	-1.4167980
C	-0.6607770	2.9075610	-2.2609660
H	-1.1291810	3.4919300	-3.0502670
C	-2.5680890	0.9029460	0.2866370
H	-2.6028530	0.4162780	1.2544840
C	-3.6324720	0.9442450	-0.5894980
C	-4.9564420	0.3424060	-0.4379030
C	-5.1517680	-0.7425880	0.4392240
H	-4.3035550	-1.1570180	0.9757130
C	-6.3996590	-1.3263440	0.6028590
H	-6.5137920	-2.1721040	1.2726750
C	-7.5172540	-0.8469400	-0.1053310
C	-7.3322910	0.2351340	-0.9841670
H	-8.1812560	0.6308050	-1.5315180
C	-6.0788840	0.8105250	-1.1459590
H	-5.9782070	1.6632000	-1.8126390
N	-8.7898440	-1.4390640	0.0615970
C	-9.1969080	-1.9177150	1.3402680
C	-9.8284880	-3.1651260	1.4614000
H	-9.9939740	-3.7666610	0.5732170
C	-10.2391620	-3.6252180	2.7111680
H	-10.7266600	-4.5935240	2.7883790
C	-10.0126450	-2.8614950	3.8581320

H	-10.3275790	-3.2264960	4.8315310
C	-9.3771490	-1.6233980	3.7409330
H	-9.2011090	-1.0148720	4.6240390
C	-8.9793220	-1.1469540	2.4930530
H	-8.4988240	-0.1777170	2.4036180
C	-9.6778690	-1.5632340	-1.0446750
C	-11.0402830	-1.2596680	-0.8967310
H	-11.4080360	-0.9173530	0.0653790
C	-11.9118200	-1.3990310	-1.9752840
H	-12.9639240	-1.1601640	-1.8438210
C	-11.4399500	-1.8243360	-3.2188680
H	-12.1209070	-1.9256280	-4.0590910
C	-10.0832380	-2.1190450	-3.3706760
H	-9.7031300	-2.4593450	-4.3303520
C	-9.2074180	-2.0003620	-2.2931370
H	-8.1568130	-2.2463600	-2.4111850
S	3.2117240	1.7876920	-2.0453060
C	1.4437740	1.5673570	-0.1736680
C	1.6029130	2.1439620	-1.4293270
C	0.7037500	2.8930650	-2.2661710
H	1.1785420	3.4674230	-3.0589900
C	2.5856280	0.8421500	0.2634110
H	2.6163130	0.3516230	1.2295180
C	3.6437820	0.8615040	-0.6206050
C	4.9560090	0.2299790	-0.4807640
C	5.1324780	-0.8692170	0.3821810
H	4.2822430	-1.2608960	0.9322450
C	6.3724180	-1.4709580	0.5447400
H	6.4777190	-2.3090680	1.2254620
C	7.4940850	-1.0132190	-0.1708120
C	7.3246210	0.0742450	-1.0459180
H	8.1734610	0.4434760	-1.6117450
C	6.0852080	0.6846830	-1.1865490
H	5.9954400	1.5352490	-1.8572840
N	8.7569730	-1.6299350	-0.0150470
C	8.8519400	-3.0376270	0.1802230
C	8.0892410	-3.9196380	-0.6014970
H	7.4246920	-3.5205630	-1.3613710
C	8.1851730	-5.2956810	-0.4023060
H	7.5876560	-5.9652470	-1.0153830
C	9.0525380	-5.8146950	0.5614320
H	9.1295560	-6.8881030	0.7090890
C	9.8198230	-4.9394780	1.3329970
H	10.4941920	-5.3289420	2.0911400
C	9.7172870	-3.5612430	1.1534510
H	10.3055500	-2.8832370	1.7636750

C	9.9469510	-0.8481260	-0.0414120
C	10.0205030	0.3642680	0.6623700
H	9.1610540	0.7028400	1.2324310
C	11.1881410	1.1245290	0.6306620
H	11.2290380	2.0605560	1.1815400
C	12.3037360	0.6826820	-0.0840120
H	13.2146410	1.2742380	-0.1003780
C	12.2362480	-0.5283110	-0.7762020
H	13.0945910	-0.8819430	-1.3414150
C	11.0668140	-1.2864380	-0.7651250
H	11.0132220	-2.2212290	-1.3142090

6 eq (ground state, B3LYP/6-31G*)

-3326.295889390			
C	-11.3655590	-0.2838490	-0.5673120
C	-10.1631400	-0.0738690	0.1257170
C	-10.0525560	-0.5218350	1.4515990
C	-11.1205600	-1.1758270	2.0631090
C	-12.3186020	-1.3767200	1.3741570
C	-12.4345380	-0.9222890	0.0588390
N	-9.0745590	0.5915330	-0.5072250
C	-9.3244980	1.7592250	-1.2828810
C	-8.7060560	1.9326760	-2.5312740
C	-8.9529250	3.0796520	-3.2834950
C	-9.8306860	4.0601190	-2.8159850
C	-10.4549220	3.8847860	-1.5791010
C	-10.2003010	2.7497740	-0.8116250
C	-7.7561510	0.1005960	-0.3607090
C	-6.6649800	0.9815750	-0.2499580
C	-5.3718300	0.4959960	-0.1138630
C	-5.1073540	-0.8859690	-0.0564150
C	-6.2058450	-1.7587630	-0.1634990
C	-7.5001950	-1.2812970	-0.3222910
C	-3.7396960	-1.3771120	0.1150960
S	-3.2608100	-2.9788920	-0.4040410
C	-1.6033250	-2.7515660	0.1436960
C	-1.4529930	-1.4804260	0.6968790
C	-2.6618290	-0.7249420	0.6703880
P	-0.0156310	-0.9074070	1.6362060
C	1.4356560	-1.4859320	0.7220340
C	1.5906430	-2.7579800	0.1719120
S	3.2566100	-2.9918660	-0.3469980
C	3.7323720	-1.3923940	0.1807480
C	2.6477210	-0.7352060	0.7168290
C	0.6755960	-3.8376540	-0.0568200

C	-0.6887860	-3.8349160	-0.0691940
C	5.1036970	-0.9063030	0.0317260
C	5.3702760	0.4744060	-0.0457230
C	6.6649500	0.9562030	-0.1770210
C	7.7592360	0.0731580	-0.2325170
C	7.5026950	-1.3074750	-0.1586370
C	6.2034490	-1.7815490	-0.0343750
N	9.0789340	0.5624220	-0.3616960
C	10.0401550	-0.1509890	-1.1334920
C	11.3431770	-0.3366700	-0.6459710
C	12.2869270	-1.0222850	-1.4085350
C	11.9451950	-1.5474330	-2.6565350
C	10.6470720	-1.3705610	-3.1404000
C	9.7017770	-0.6703330	-2.3930670
C	-0.0102630	0.9105670	1.4120760
O	-0.0292380	-1.2836210	3.0915120
C	9.4652490	1.7689910	0.2896200
C	10.2343650	2.7257600	-0.3907490
C	10.6255150	3.8985080	0.2527030
C	10.2440230	4.1446110	1.5733570
C	9.4719870	3.1975740	2.2497120
C	9.0911600	2.0138330	1.6202840
H	1.1422270	-4.7864090	-0.3128930
H	2.7233020	0.2566050	1.1469160
H	4.5445380	1.1798860	-0.0378280
H	6.8365080	2.0248440	-0.2524400
H	8.3306650	-2.0078780	-0.1853770
H	6.0437080	-2.8533310	0.0499930
H	10.5222600	2.5428150	-1.4212140
H	11.2211770	4.6292780	-0.2880600
H	10.5452470	5.0627160	2.0696240
H	9.1746330	3.3716450	3.2804760
H	8.5040920	1.2733870	2.1544250
H	11.6082860	0.0585500	0.3294960
H	13.2914700	-1.1578360	-1.0164210
H	12.6813490	-2.0874830	-3.2450520
H	10.3691150	-1.7665410	-4.1136260
H	8.6983740	-0.5214190	-2.7794650
H	-1.1546160	-4.7816990	-0.3338490
H	-2.7392160	0.2678250	1.0979210
H	-4.5490750	1.2021970	-0.0542050
H	-6.8370320	2.0523710	-0.2785810
H	-8.3249670	-1.9806820	-0.4096060
H	-6.0471650	-2.8328500	-0.1155850
H	-8.0351930	1.1656270	-2.9052940
H	-8.4664740	3.1983470	-4.2481670

H	-10.0263340	4.9492140	-3.4085890
H	-11.1357650	4.6422500	-1.1996740
H	-10.6776580	2.6226470	0.1548370
H	-9.1286700	-0.3549040	1.9964060
H	-11.0180560	-1.5163750	3.0901020
H	-13.1514080	-1.8804020	1.8564840
H	-13.3586180	-1.0768360	-0.4920510
H	-11.4553840	0.0561080	-1.5942150
C	-0.0194350	1.7044800	2.5660030
C	-0.0156450	3.0971280	2.4590830
C	-0.0026990	3.7012990	1.2010990
C	0.0064120	2.9138200	0.0457170
C	0.0026510	1.5232910	0.1495450
H	-0.0294680	1.2158710	3.5359370
H	-0.0228510	3.7085120	3.3575300
H	0.0002410	4.7850890	1.1181680
H	0.0164690	3.3838280	-0.9341770
H	0.0096890	0.9142230	-0.7509620

8 ax- $\perp$ (ground state, B3LYP/6-31G*)

-3013.348877520

C	-2.9181390	-2.4303880	-1.8377000
C	-3.7426460	-1.4525230	-1.1808110
C	-1.5612820	-2.5714890	-1.8113500
C	-0.5701180	-1.8010700	-1.1128410
C	-0.6407540	-0.8929390	-0.0597250
P	-2.0689260	-0.4667270	0.9695230
C	-3.5085680	-0.5710120	-0.1283970
S	1.0964500	-1.9413650	-1.6623690
C	1.6669680	-0.7513320	-0.5130820
C	0.6122370	-0.3030310	0.2561350
S	-5.3665560	-1.2155880	-1.8109010
C	-5.7058580	0.0737670	-0.6762390
C	-4.6107760	0.2873350	0.1326850
C	-6.9914870	0.7704530	-0.6586360
H	-4.5811660	1.0265830	0.9247050
H	0.7080070	0.4568620	1.0227230
O	-1.9448710	0.8803560	1.6242530
C	-2.2438400	-1.7934900	2.2164850
C	-2.2967600	-1.4042170	3.5618640
C	-2.4322730	-2.3658830	4.5644360
C	-2.5149440	-3.7180480	4.2290650
C	-2.4616630	-4.1110870	2.8888540
C	-2.3263050	-3.1541490	1.8842660
H	-2.2278510	-0.3482510	3.8049270

H	-2.4721800	-2.0587690	5.6060950
H	-2.6197910	-4.4668280	5.0098290
H	-2.5244020	-5.1639950	2.6272310
H	-2.2840050	-3.4706030	0.8460010
H	-1.1620860	-3.3494000	-2.4591220
H	-3.4490490	-3.1109210	-2.4995230
C	-8.1483910	0.1999340	-1.2276410
C	-9.3658730	0.8668870	-1.2026550
C	-9.4361030	2.1200010	-0.5961580
C	-8.3129240	2.7170010	-0.0229520
C	-7.0998030	2.0446710	-0.0620460
H	-8.0985810	-0.7865140	-1.6790470
H	-10.2588490	0.4322890	-1.6345020
N	-10.7195700	2.8278330	-0.5627120
H	-8.4022600	3.6960030	0.4313790
H	-6.2187190	2.5187600	0.3571190
O	-10.7513390	3.9311060	-0.0155390
O	-11.6913220	2.2775890	-1.0833770
C	3.0735600	-0.3606600	-0.4428320
C	3.9632640	-0.5729390	-1.5126610
C	5.2954210	-0.1911320	-1.4372800
C	5.8037560	0.4178930	-0.2753050
C	4.9225360	0.6310860	0.8016980
C	3.5912190	0.2517550	0.7156050
H	3.6000490	-1.0146360	-2.4370390
H	5.9498490	-0.3517840	-2.2873190
N	7.1591290	0.8019340	-0.1906570
H	5.2941320	1.0837130	1.7147770
H	2.9477280	0.4023330	1.5770170
C	7.5324150	1.9762720	0.5257620
C	8.1716930	0.0168020	-0.8142140
C	8.1651030	-1.3817130	-0.6944690
C	9.1588330	-2.1428120	-1.3072240
C	10.1815510	-1.5247130	-2.0300220
C	10.1957530	-0.1327540	-2.1413100
C	9.1962060	0.6354650	-1.5470190
H	7.3807790	-1.8645750	-0.1200610
H	9.1402590	-3.2246360	-1.2047940
H	10.9586690	-2.1206480	-2.4999440
H	10.9825030	0.3612030	-2.7053620
H	9.2032520	1.7164550	-1.6448620
C	8.6308540	1.9536970	1.3987690
C	9.0031860	3.1069410	2.0871740
C	8.2801830	4.2913300	1.9305530
C	7.1824940	4.3139690	1.0674790
C	6.8137440	3.1705350	0.3609990

H	9.1871820	1.0312650	1.5323900
H	9.8561740	3.0736630	2.7598050
H	8.5691030	5.1863960	2.4739130
H	6.6158540	5.2309800	0.9294160
H	5.9695200	3.1959540	-0.3209250

8 ax-|| (ground state, B3LYP/6-31G*)

-3013.347286710

P	-2.1047580	-0.9570960	1.0747200
C	-0.6629280	-1.0868470	-0.0111150
C	-0.5986690	-1.7898490	-1.2101470
C	-1.6038420	-2.4561170	-1.9941060
C	-2.9547440	-2.2663110	-2.0094880
C	-3.7401510	-1.3295600	-1.2495300
C	-3.4915590	-0.6636200	-0.0531820
C	-2.3661640	-2.6312060	1.7645890
C	-1.2725080	-3.4595480	2.0556500
C	-3.6583410	-3.0594390	2.1035290
C	-3.8523800	-4.2944410	2.7212390
C	-2.7580020	-5.1135530	3.0063680
C	-1.4685120	-4.6945290	2.6736160
C	-4.5179420	0.2515720	0.3022840
C	-5.5752240	0.2897050	-0.5821900
S	-5.2879560	-0.8224230	-1.9062830
C	0.5784300	-0.5151160	0.3748380
C	1.6204270	-0.7800430	-0.4916150
S	1.0499760	-1.7672780	-1.8218980
O	-1.9690450	0.1240780	2.1101260
C	3.0155470	-0.3549570	-0.3922150
C	3.8724830	-0.3310290	-1.5084270
C	5.1911940	0.0891320	-1.4042780
C	5.7193660	0.4995510	-0.1664150
C	4.8721110	0.4710030	0.9578400
C	3.5535820	0.0563630	0.8431900
C	-6.7903180	1.0996740	-0.5046830
C	-7.9539300	0.7563100	-1.2229660
C	-9.1044530	1.5290360	-1.1410660
C	-9.1006800	2.6596890	-0.3256920
C	-7.9687800	3.0313810	0.4003770
C	-6.8220380	2.2562470	0.3032860
N	-10.3135120	3.4779140	-0.2310090
O	-11.2947610	3.1261290	-0.8879210
N	7.0594010	0.9264690	-0.0534350
C	8.0771810	0.3366370	-0.8580780
C	8.1428120	-1.0561950	-1.0191970

C	9.1411020	-1.6247170	-1.8083660
C	10.0975720	-0.8199320	-2.4311130
C	10.0406480	0.5651530	-2.2626580
C	9.0352420	1.1438630	-1.4901730
O	-10.2806540	4.4687300	0.5002720
C	7.4126350	1.9592550	0.8638890
C	8.5466350	1.8228950	1.6788780
C	8.9009450	2.8402050	2.5632340
C	8.1247380	3.9969660	2.6611740
C	6.9918850	4.1315600	1.8556810
C	6.6400510	3.1273720	0.9554890
H	-4.4684770	0.8344780	1.2149590
H	0.6751290	0.0921110	1.2673500
H	-0.2664330	-3.1411780	1.7974840
H	-0.6147410	-5.3300190	2.8927440
H	-2.9102500	-6.0769720	3.4855950
H	-4.8574840	-4.6180550	2.9778080
H	-4.5153260	-2.4288820	1.8830150
H	-1.2223510	-3.1616400	-2.7296150
H	-3.5050880	-2.8412690	-2.7508800
H	-7.9640810	-0.1373240	-1.8399730
H	-10.0020310	1.2680170	-1.6878990
H	-7.9989640	3.9211560	1.0170460
H	-5.9321810	2.5588500	0.8449130
H	3.4920490	-0.6123900	-2.4869770
H	5.8182070	0.1149380	-2.2889850
H	5.2600410	0.7641220	1.9274950
H	2.9371060	0.0199300	1.7363070
H	7.4107390	-1.6858870	-0.5233130
H	9.1787910	-2.7048040	-1.9231270
H	10.8786530	-1.2669920	-3.0393380
H	10.7753850	1.2038440	-2.7457170
H	8.9864370	2.2215310	-1.3705260
H	9.1446560	0.9195010	1.6124010
H	9.7820650	2.7201080	3.1879640
H	8.3998520	4.7848410	3.3564540
H	6.3835640	5.0300990	1.9157180
H	5.7676950	3.2420230	0.3197670

8 eq (ground state, B3LYP/6-31G*)

-3013.347904300			
C	6.7353200	2.6157660	-1.0597030
C	7.4842330	1.6794480	-0.3298770
C	8.6009650	2.1160490	0.3991670
C	8.9610170	3.4624270	0.3912590

C	8.2080520	4.3942910	-0.3263140
C	7.0924670	3.9628720	-1.0471660
N	7.1244160	0.3005750	-0.3366310
C	8.1424810	-0.6822990	-0.5067920
C	8.1746240	-1.8243780	0.3085070
C	9.1722820	-2.7819820	0.1346910
C	10.1604140	-2.6085810	-0.8368760
C	10.1363550	-1.4675780	-1.6415390
C	9.1321760	-0.5134240	-1.4871750
C	5.7762140	-0.0866550	-0.1807230
C	5.2619830	-1.2083340	-0.8563490
C	3.9360160	-1.5866080	-0.6956520
C	3.0591450	-0.8646770	0.1352330
C	3.5833520	0.2559480	0.8088270
C	4.9085220	0.6374580	0.6587640
C	1.6576530	-1.2465680	0.3033940
S	1.1030500	-2.8772190	-0.0005640
C	-0.5615640	-2.4763680	0.4052430
C	-0.6524380	-1.1356940	0.7800250
C	0.6005730	-0.4624280	0.7134230
C	-1.5341530	-3.5221190	0.2842550
C	-2.8951400	-3.4504180	0.2222810
C	-3.7481120	-2.2978370	0.2484190
C	-3.5324590	-0.9714450	0.6245610
C	-4.6861750	-0.1583830	0.4342640
C	-5.7824990	-0.8201970	-0.0722580
S	-5.3940630	-2.5067040	-0.3319120
P	-2.0969360	-0.3581000	1.5454880
O	-2.1910220	-0.5494630	3.0327330
C	-7.1069000	-0.2758050	-0.3692890
C	-8.2413840	-1.1073130	-0.4649280
C	-9.4964420	-0.5828360	-0.7434020
C	-9.6275710	0.7931600	-0.9241480
C	-8.5285290	1.6480100	-0.8368230
C	-7.2779980	1.1108240	-0.5673440
N	-10.9497630	1.3546600	-1.2168990
O	-11.8997350	0.5740850	-1.2939490
C	-1.9802230	1.4113860	1.0932320
O	-11.0330920	2.5745010	-1.3688960
H	-4.7106250	0.8892680	0.7100610
H	0.7126400	0.5883550	0.9525300
H	-1.1176890	-4.5208230	0.1704680
H	-3.4072100	-4.3977850	0.0704500
H	-8.1428600	-2.1760410	-0.2997390
H	-10.3718850	-1.2164030	-0.8140150
H	-8.6664660	2.7109650	-0.9916160

H	-6.4171970	1.7699690	-0.5286380
H	3.5665630	-2.4416980	-1.2558330
H	5.9062940	-1.7754500	-1.5195660
H	5.2866510	1.4935430	1.2073230
H	2.9516710	0.8153320	1.4923460
H	7.4174060	-1.9546700	1.0753420
H	9.1840400	-3.6608590	0.7738580
H	10.9406910	-3.3534120	-0.9644950
H	10.8961280	-1.3225700	-2.4049850
H	9.1089030	0.3667290	-2.1220290
H	9.1811190	1.3960460	0.9676690
H	9.8283590	3.7850210	0.9611400
H	8.4878530	5.4438500	-0.3245440
H	6.5025440	4.6755910	-1.6174340
H	5.8769520	2.2814470	-1.6339340
C	-2.0067670	2.3475330	2.1352680
C	-1.9285730	3.7130110	1.8520150
C	-1.8234980	4.1476680	0.5299870
C	-1.7954350	3.2176580	-0.5137540
C	-1.8734200	1.8537940	-0.2345250
H	-2.0885980	1.9904510	3.1577480
H	-1.9498200	4.4354040	2.6634870
H	-1.7628030	5.2103420	0.3103040
H	-1.7120830	3.5558490	-1.5431220
H	-1.8494940	1.1339220	-1.0489240

2 ax- $\perp$ (ground state, CAM-B3LYP/6-31G*)

-1828.871611550			
S	3.7901160	-0.3262390	-0.5980090
C	3.8123130	0.5797190	0.8634660
C	2.5638650	0.7364000	1.3762580
C	1.5508390	0.1216600	0.5787370
C	2.0589760	-0.5196190	-0.5316360
P	-0.1694560	0.3268940	1.0719580
C	-0.8654190	1.6683230	0.0614310
C	1.4384060	-1.3072300	-1.5750940
C	0.2410800	-1.9279670	-1.5753840
C	-0.7604740	-1.9818420	-0.5322210
C	-0.9923590	-1.1977410	0.5785830
C	-2.0785270	-1.6722110	1.3755660
C	-2.6693140	-2.7827700	0.8620150
S	-1.9157360	-3.2855780	-0.5995640
O	-0.3209950	0.6192040	2.5302020
H	-2.3800960	-1.1847100	2.2942440
H	-3.5057330	-3.3372840	1.2640750

H	0.0117620	-2.5184570	-2.4586920
H	2.3384630	1.2638890	2.2946970
H	4.7471400	0.9440690	1.2660600
H	2.0534750	-1.4599920	-2.4581880
C	-1.4297530	2.7466840	0.7426010
C	-1.9812150	3.8081280	0.0332940
C	-1.9703550	3.7952480	-1.3562240
C	-1.4078580	2.7206970	-2.0401350
C	-0.8565200	1.6594200	-1.3353540
H	-1.4276290	2.7369160	1.8276590
H	-2.4194780	4.6456130	0.5672310
H	-2.4007630	4.6238400	-1.9105610
H	-1.3995400	2.7112400	-3.1257030
H	-0.4199840	0.8255100	-1.8760580

2 TS1 (ground state, CAM-B3LYP/6-31G*)

-1828.86801349			
C	0.5306790	1.4667490	0.4345490
C	1.7266590	1.6088240	-0.2386150
C	2.6871490	0.6730280	-0.7736180
C	2.6870510	-0.6734140	-0.7736120
C	1.7264250	-1.6090660	-0.2386000
C	0.5304650	-1.4668140	0.4345620
P	-0.3478560	0.0000340	1.0007970
S	2.1009650	-3.2996330	-0.4598130
C	0.6684220	-3.7938660	0.3492610
C	-0.0599690	-2.7281800	0.7679740
S	2.1014410	3.2993350	-0.4598470
C	0.6689680	3.7937810	0.3492220
C	-0.0595750	2.7282030	0.7679470
C	-1.8967140	0.0001430	0.0452700
C	-3.0999000	0.0002810	0.7493780
C	-4.3091860	0.0003440	0.0617860

C	-4.3183390	0.0002690	-1.3280860
C	-3.1186810	0.0001380	-2.0353700
C	-1.9110640	0.0000770	-1.3509620
O	-0.6310040	0.0000630	2.4680040
H	-3.0693860	0.0003350	1.8344280
H	-5.2448450	0.0004500	0.6124590
H	-5.2623720	0.0003150	-1.8646310
H	-3.1267810	0.0000840	-3.1209390
H	-0.9761550	-0.0000230	-1.9051310
H	-0.9919870	2.8162570	1.3124360
H	0.4443030	4.8433450	0.4773330
H	3.5445950	1.1390120	-1.2518780
H	-0.9923940	-2.8160960	1.3124640
H	0.4436070	-4.8433960	0.4773840
H	3.5444290	-1.1395280	-1.2518660

2 TS2 (ground state, CAM-B3LYP/6-31G*)

-1828.87011515

P	-0.0994060	0.2469990	1.1694910
C	1.5653270	-0.1683460	0.6306570
C	1.9337680	-0.6306780	-0.6148710
C	1.1469550	-0.9954480	-1.7755400
C	-0.1304440	-1.4259290	-1.8243740
C	-1.0539830	-1.6421750	-0.7306580
C	-1.1163240	-1.0963410	0.5334140
C	-0.6050300	1.7268850	0.2412500
C	-1.9199500	2.1752830	0.4019700

C	0.2671030	2.4495420	-0.5711960
C	-0.1692450	3.6012650	-1.2181820
C	-1.4781910	4.0370570	-1.0575570
C	-2.3543890	3.3229470	-0.2447010
S	3.6655130	-0.7946770	-0.7060610
C	3.8664360	-0.2703250	0.9219110
C	2.6757400	0.0235200	1.5072250
C	-2.1687790	-1.6447690	1.3264420
C	-2.9026700	-2.5747080	0.6596820
S	-2.3264070	-2.8124500	-0.9446920
O	-0.2227240	0.3986970	2.6511230
H	-2.3454520	-1.3374270	2.3498560
H	-3.7505940	-3.1385950	1.0229270
H	-0.5011260	-1.7130550	-2.8050460
H	2.5576970	0.3703800	2.5263260
H	4.8545570	-0.2100960	1.3564050
H	1.6835030	-0.9784290	-2.7206930
H	-2.6038330	1.6253750	1.0419500
H	-3.3767710	3.6634810	-0.1140580
H	-1.8177670	4.9356310	-1.5636350
H	0.5172870	4.1584260	-1.8480810
H	1.2917240	2.1170880	-0.6980850

2 ax- $\perp$ (excited state, CAM-B3LYP/6-31G*)

-1828.857987750			
S	3.3359850	-1.8613810	-0.6582390
C	3.7511460	-0.9939660	0.7723290
C	2.6672100	-0.3989510	1.3620090
C	1.4551360	-0.6251960	0.6802690

C	1.6196300	-1.4434590	-0.4725190
P	-0.0001940	0.3023970	1.1595450
C	-0.0022880	1.7505010	0.0481330
C	0.7120750	-1.9705530	-1.3826880
C	-0.7069560	-1.9721460	-1.3827880
C	-1.6157870	-1.4473130	-0.4726000
C	-1.4532190	-0.6289610	0.6804100
C	-2.6658360	-0.4057240	1.3621670
C	-3.7483710	-1.0031000	0.7722890
S	-3.3311710	-1.8691660	-0.6584990
O	-0.0006590	0.7020930	2.6001240
H	-2.7218180	0.1835840	2.2697600
H	-4.7742640	-0.9822050	1.1143200
H	-1.1414300	-2.5341850	-2.2051210
H	2.7217710	0.1907000	2.2694660
H	4.7769750	-0.9706270	1.1143940
H	1.1479170	-2.5317540	-2.2048710
C	-0.0050930	3.0020160	0.6677050
C	-0.0068370	4.1590840	-0.1031060
C	-0.0057940	4.0750730	-1.4904620
C	-0.0029730	2.8277430	-2.1097330
C	-0.0012130	1.6682670	-1.3470470
H	-0.0057960	3.0510140	1.7516670
H	-0.0090010	5.1294090	0.3841950
H	-0.0071500	4.9794000	-2.0912360
H	-0.0021070	2.7585630	-3.1933170
H	0.0010610	0.7022580	-1.8418270

2 ax-|| (ground state, CAM-B3LYP/6-31G*)

-1828.870451520

P	0.0002180	0.2360320	1.1935200
C	1.4178500	-0.6886250	0.5825810
C	1.5764200	-1.1703570	-0.6989390
C	0.6737900	-1.1899870	-1.8319760
C	-0.6751330	-1.1894310	-1.8318200
C	-1.5775010	-1.1690920	-0.6985790
C	-1.4182580	-0.6876000	0.5829480
C	0.0006720	1.8050340	0.2745840
C	1.2056440	2.4365020	-0.0388540
C	-1.2038120	2.4362920	-0.0409540
C	-1.2030170	3.6789490	-0.6618620
C	0.0015740	4.3006330	-0.9722410
C	1.2057400	3.6791250	-0.6597620
S	3.1530220	-1.8872440	-0.8807310
C	3.5640630	-1.5556080	0.7581960

C	2.5540890	-0.9242680	1.4135930
C	-2.5545290	-0.9223580	1.4141740
C	-3.5650370	-1.5531000	0.7590280
S	-3.1546840	-1.8847520	-0.8800770
O	0.0005300	0.3862400	2.6807890
H	-2.5875740	-0.6172560	2.4528440
H	-4.5304030	-1.8452800	1.1483190
H	-1.1546290	-1.2828640	-2.8028280
H	2.5875480	-0.6191900	2.4522560
H	4.5293250	-1.8484170	1.1472730
H	1.1529930	-1.2838130	-2.8030890
H	2.1484580	1.9537330	0.1999420
H	2.1472220	4.1620760	-0.9021710
H	0.0019060	5.2707820	-1.4597520
H	-2.1441470	4.1617610	-0.9059010
H	-2.1469460	1.9533580	0.1962270

2 ax-|| (excited state, CAM-B3LYP/6-31G*)

-1828.855056980

P	0.0000320	0.1833270	1.2250680
C	1.4499590	-0.6990790	0.6558760
C	1.6146770	-1.3406140	-0.6053770
C	0.7092170	-1.7079780	-1.5911400
C	-0.7099780	-1.7077610	-1.5910680
C	-1.6152410	-1.3400960	-0.6052350
C	-1.4502380	-0.6985650	0.6559830
C	0.0003200	1.7059460	0.2034890
C	1.2050390	2.3202010	-0.1513740
C	-1.2041290	2.3200830	-0.1524690
C	-1.2029410	3.5249790	-0.8434880
C	0.0008410	4.1281340	-1.1906570
C	1.2043690	3.5251000	-0.8423760
S	3.3288120	-1.7483380	-0.8359430
C	3.7423070	-1.1039560	0.7093920
C	2.6575390	-0.5909940	1.3729810
C	-2.6577430	-0.5900310	1.3731480
C	-3.7427200	-1.1026630	0.7096470
S	-3.3295240	-1.7472720	-0.8356750
O	0.0001550	0.4256330	2.7007290
H	-2.7085710	-0.1420180	2.3588190
H	-4.7649090	-1.1461490	1.0605580
H	-1.1457180	-2.1320890	-2.4915320
H	2.7085670	-0.1430580	2.3586780
H	4.7645010	-1.1478040	1.0602440
H	1.1447420	-2.1324250	-2.4916520

H	2.1490060	1.8549880	0.1135820
H	2.1464460	3.9922720	-1.1120440
H	0.0010450	5.0679930	-1.7342540
H	-2.1448180	3.9920580	-1.1140170
H	-2.1482910	1.8548020	0.1116640

2 eq (ground state, CAM-B3LYP/6-31G*)

-1828.870644600

C	1.9927360	-0.0000240	0.1990230
C	3.0600200	-0.0000120	1.0959340
H	2.8465310	0.0000030	2.1601690
C	4.3683780	-0.0000200	0.6225990
H	5.1969500	-0.0000100	1.3239430
C	4.6126780	-0.0000420	-0.7454530
H	5.6338490	-0.0000480	-1.1145570
C	3.5498240	-0.0000550	-1.6456670
H	3.7411660	-0.0000720	-2.7142580
C	2.2433710	-0.0000460	-1.1757330
H	1.4158510	-0.0000570	-1.8798800
C	-0.4908810	-1.4309800	0.1578100
C	0.2287320	-2.6290750	-0.1508190
H	1.3068620	-2.7065880	-0.0877290
C	-0.5756990	-3.6602380	-0.5156070
H	-0.2836380	-4.6633290	-0.7934050
C	-1.8559590	-1.5873760	0.0143360
C	-2.9594850	-0.6742940	0.1936490
H	-3.9329620	-1.1482360	0.2877870
C	-0.4908470	1.4309880	0.1578100
C	0.2287930	2.6290710	-0.1508030
H	1.3069230	2.7065620	-0.0876970
C	-0.5756150	3.6602620	-0.5155620
H	-0.2835320	4.6633550	-0.7933280
C	-1.8559220	1.5874180	0.0143360
C	-2.9594700	0.6743630	0.1936480
H	-3.9329360	1.1483270	0.2877790
O	0.3369680	-0.0000050	2.3924780
P	0.3135940	-0.0000060	0.8983400
S	-2.2356220	-3.2118750	-0.4906250
S	-2.2355430	3.2119130	-0.4906720

2 eq (excited state, CAM-B3LYP/6-31G*)

-1828.857972820

C	0.0000150	1.7505070	0.0482020
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C	0.0000410	3.0018910	0.6679840
H	0.0000520	3.0507200	1.7519530
C	0.0000510	4.1591430	-0.1026010
H	0.0000720	5.1293440	0.3849460
C	0.0000350	4.0754090	-1.4899480
H	0.0000430	4.9798190	-2.0905980
C	0.0000080	2.8281660	-2.1094610
H	-0.0000050	2.7592430	-3.1930640
C	-0.0000010	1.6685560	-1.3470330
H	-0.0000230	0.7026470	-1.8419980
C	1.4541380	-0.6272820	0.6803660
C	2.6663540	-0.4032640	1.3625260
H	2.7214800	0.1857750	2.2703550
C	3.7496670	-0.9990970	0.7725480
H	4.7755180	-0.9773610	1.1146530
C	1.6177570	-1.4450950	-0.4729760
C	0.7095120	-1.9702250	-1.3834840
H	1.1445390	-2.5313160	-2.2061730
C	-1.4541490	-0.6272550	0.6803680
C	-2.6663610	-0.4032200	1.3625310
H	-2.7214760	0.1858170	2.2703620
C	-3.7496600	-0.9991640	0.7726390
H	-4.7754960	-0.9774840	1.1147910
C	-1.6177800	-1.4450770	-0.4729660
C	-0.7095450	-1.9702160	-1.3834800
H	-1.1445840	-2.5312980	-2.2061700
O	0.0000050	0.7019340	2.6000760
P	0.0000020	0.3023370	1.1594670
S	3.3335170	-1.8653480	-0.6585100
S	-3.3335600	-1.8652220	-0.6585500

3 ax- $\perp$ (ground state, CAM-B3LYP/6-31G*)

-2475.121440190			
C	6.1201860	-0.6368890	0.8572570
C	5.0102480	-0.9207660	0.0532110
C	5.2073220	-1.6414090	-1.1315220
C	6.4727170	-2.0551190	-1.5080420
C	7.5729920	-1.7656040	-0.6959370
C	7.3883030	-1.0554980	0.4926280
C	3.6626880	-0.4768500	0.4250610
S	3.2106360	-0.2109290	2.0790770
C	1.5873980	0.2474390	1.6460310
C	1.4298270	0.2038490	0.2756270
C	2.6056060	-0.2197770	-0.4030340
C	0.6751170	0.5535690	2.7240840

C	-0.6751420	0.5535810	2.7240780
C	-1.5874220	0.2474560	1.6460200
C	-1.4298440	0.2038460	0.2756170
C	-2.6056200	-0.2197920	-0.4030420
C	-3.6627110	-0.4768350	0.4250500
S	-3.2106670	-0.2108810	2.0790640
P	-0.0000080	0.6800190	-0.7128660
O	-0.0000050	0.0416690	-2.0644460
C	-5.0102730	-0.9207450	0.0532010
C	-5.2073420	-1.6414420	-1.1314990
C	-6.4727380	-2.0551460	-1.5080190
C	-7.5730200	-1.7655730	-0.6959440
C	-7.3883370	-1.0554130	0.4925910
C	-6.1202180	-0.6368090	0.8572180
C	-8.8860360	-2.1977830	-1.0796530
N	-9.9452280	-2.5454970	-1.3882510
C	8.8860060	-2.1978190	-1.0796490
N	9.9451990	-2.5455350	-1.3882410
C	0.0000120	2.4915040	-0.8362880
C	0.0000510	3.0380450	-2.1197030
C	0.0001020	4.4182670	-2.2888850
C	0.0001210	5.2540340	-1.1787220
C	0.0000810	4.7122340	0.1040470
C	0.0000260	3.3351200	0.2772620
H	0.0000400	2.3683080	-2.9734170
H	0.0001260	4.8401840	-3.2889900
H	0.0001680	6.3317530	-1.3104640
H	0.0000940	5.3661550	0.9705280
H	-0.0000120	2.9212880	1.2807770
H	-1.1495380	0.7566680	3.6806000
H	-2.6459250	-0.3022360	-1.4822970
H	-4.3557360	-1.8944890	-1.7532300
H	-6.6151370	-2.6136590	-2.4264050
H	-8.2421670	-0.8278460	1.1209070
H	-5.9934680	-0.0649910	1.7709220
H	1.1495070	0.7566430	3.6806120
H	2.6459160	-0.3022000	-1.4822910
H	4.3557220	-1.8944120	-1.7532790
H	6.6151190	-2.6135890	-2.4264540
H	8.2421270	-0.8279770	1.1209690
H	5.9934340	-0.0651120	1.7709870

3 ax- $\perp$ (excited state, CAM-B3LYP/6-31G*)

-2475.108588090			
C	6.1654500	-0.9276200	0.8257310

C	5.1045000	-0.7978590	-0.0924010
C	5.4058510	-0.9019380	-1.4662160
C	6.6975630	-1.1183340	-1.8980230
C	7.7402450	-1.2411270	-0.9700930
C	7.4596560	-1.1435380	0.3976260
C	3.7505030	-0.5642910	0.3501110
S	3.3116820	-0.5758710	2.0395940
C	1.6115870	-0.2581150	1.6780470
C	1.4479500	-0.1196430	0.2732890
C	2.6320260	-0.3040630	-0.4351450
C	0.7044180	-0.2405580	2.7318830
C	-0.7044180	-0.2405590	2.7318830
C	-1.6115870	-0.2581150	1.6780470
C	-1.4479500	-0.1196430	0.2732890
C	-2.6320260	-0.3040630	-0.4351450
C	-3.7505020	-0.5642910	0.3501110
S	-3.3116810	-0.5758720	2.0395940
P	0.0000000	0.4578260	-0.6202590
O	0.0000000	0.0532320	-2.0591490
C	-5.1045000	-0.7978600	-0.0924010
C	-5.4058510	-0.9019370	-1.4662160
C	-6.6975630	-1.1183330	-1.8980230
C	-7.7402450	-1.2411260	-0.9700930
C	-7.4596560	-1.1435390	0.3976260
C	-6.1654500	-0.9276210	0.8257310
C	-9.0813610	-1.4663380	-1.4166550
N	-10.1662980	-1.6477830	-1.7771300
C	9.0813610	-1.4663380	-1.4166550
N	10.1662980	-1.6477840	-1.7771300
C	-0.0000000	2.2672450	-0.4218970
C	0.0000000	3.0232580	-1.5949470
C	-0.0000000	4.4119690	-1.5266960
C	-0.0000000	5.0487210	-0.2914060
C	-0.0000000	4.2963900	0.8803020
C	-0.0000000	2.9097830	0.8188190
H	0.0000000	2.5096740	-2.5507970
H	0.0000000	4.9964940	-2.4414530
H	-0.0000000	6.1330780	-0.2387280
H	-0.0000000	4.7931780	1.8455180
H	-0.0000000	2.3328340	1.7382410
H	-1.1431000	-0.3106600	3.7236300
H	-2.6597010	-0.2349900	-1.5156460
H	-4.6141170	-0.8210010	-2.2015280
H	-6.9119620	-1.1979740	-2.9579650
H	-8.2647740	-1.2377930	1.1178280
H	-5.9723740	-0.8499560	1.8907680

H	1.1431000	-0.3106600	3.7236300
H	2.6597010	-0.2349900	-1.5156460
H	4.6141160	-0.8210030	-2.2015280
H	6.9119610	-1.1979760	-2.9579650
H	8.2647750	-1.2377910	1.1178280
H	5.9723750	-0.8499530	1.8907670

3 ax-|| (ground state, CAM-B3LYP/6-31G*)

-2475.120122380

S	3.1525760	0.1443570	1.9654540
C	1.5767090	0.6592620	1.4382330
C	1.4160670	0.3989570	0.0935080
C	2.5480390	-0.2297170	-0.4922740
C	3.5799250	-0.4318680	0.3828430
C	0.6751890	1.2271130	2.4168510
C	-0.6751840	1.2271110	2.4168520
C	-1.5767040	0.6592590	1.4382360
C	-1.4160620	0.3989520	0.0935100
C	-2.5480330	-0.2297240	-0.4922690
C	-3.5799190	-0.4318730	0.3828480
S	-3.1525690	0.1443520	1.9654580
P	0.0000010	0.8658100	-0.9158870
C	-0.0000050	2.6810030	-0.9663620
C	1.2051730	3.3827810	-1.0331010
C	1.2045510	4.7657330	-1.1626960
C	-0.0000230	5.4577540	-1.2264270
C	-1.2045890	4.7657080	-1.1627970
C	-1.2051930	3.3827570	-1.0332020
C	-4.8855910	-1.0426140	0.1114100
C	-5.0253920	-1.9574170	-0.9400220
C	-6.2514780	-2.5331900	-1.2216740
C	-7.3685550	-2.2139540	-0.4444240
C	-7.2404290	-1.3099770	0.6126640
C	-6.0122010	-0.7307690	0.8813790
C	-8.6403770	-2.8135590	-0.7288820
N	-9.6664550	-3.2961080	-0.9576270
C	4.8855970	-1.0426080	0.1114040
C	5.0253980	-1.9574090	-0.9400290
C	6.2514840	-2.5331810	-1.2216830
C	7.3685600	-2.2139480	-0.4444320
C	7.2404350	-1.3099730	0.6126580
C	6.0122070	-0.7307650	0.8813740
C	8.6403830	-2.8135520	-0.7288910
N	9.6664610	-3.2961010	-0.9576360
O	-0.0000010	0.1980750	-2.2530810

H	2.1486180	2.8477260	-0.9816760
H	2.1456870	5.3041920	-1.2123570
H	-0.0000310	6.5388610	-1.3254840
H	-2.1457320	5.3041470	-1.2125370
H	-2.1486310	2.8476820	-0.9818550
H	-1.1533880	1.6470780	3.2978620
H	-2.5803260	-0.4863550	-1.5442830
H	-4.1585540	-2.2324860	-1.5305370
H	-6.3490000	-3.2409390	-2.0372930
H	-8.1073460	-1.0596600	1.2138460
H	-5.9316510	-0.0126570	1.6911650
H	1.1533950	1.6470800	3.2978610
H	2.5803310	-0.4863470	-1.5442880
H	4.1585600	-2.2324760	-1.5305460
H	6.3490060	-3.2409300	-2.0373030
H	8.1073510	-1.0596580	1.2138410
H	5.9316570	-0.0126550	1.6911620

3 ax-|| (excited state, CAM-B3LYP/6-31G*)

-2475.106074960

S	3.2996790	-0.0265650	2.0517500
C	1.6089110	0.2409490	1.6155570
C	1.4420140	0.0094740	0.2230780
C	2.6136760	-0.3920150	-0.4108130
C	3.7294990	-0.4734820	0.4187840
C	0.7044190	0.5684690	2.6190310
C	-0.7044180	0.5684690	2.6190310
C	-1.6089100	0.2409500	1.6155580
C	-1.4420130	0.0094740	0.2230780
C	-2.6136740	-0.3920170	-0.4108120
C	-3.7294980	-0.4734820	0.4187850
S	-3.2996780	-0.0265620	2.0517500
P	0.0000000	0.4179020	-0.7662440
C	-0.0000010	2.2419370	-0.8261640
C	1.2048450	2.9467960	-0.8951840
C	1.2039450	4.3288210	-1.0326890
C	-0.0000050	5.0211870	-1.1000620
C	-1.2039530	4.3288150	-1.0327180
C	-1.2048490	2.9467900	-0.8952140
C	-5.0718840	-0.8600830	0.0575910
C	-5.3657190	-1.3154370	-1.2449070
C	-6.6473580	-1.6795390	-1.6003990
C	-7.6876390	-1.6044480	-0.6645180
C	-7.4143670	-1.1582820	0.6337530
C	-6.1303770	-0.7951710	0.9859350

C	-9.0183000	-1.9821320	-1.0320070
N	-10.0950340	-2.2864020	-1.3288180
C	5.0718850	-0.8600820	0.0575900
C	5.3657210	-1.3154320	-1.2449100
C	6.6473600	-1.6795340	-1.6004020
C	7.6876400	-1.6044460	-0.6645200
C	7.4143680	-1.1582850	0.6337520
C	6.1303780	-0.7951730	0.9859350
C	9.0183020	-1.9821300	-1.0320090
N	10.0950360	-2.2864000	-1.3288200
O	-0.0000000	-0.2570220	-2.0999780
H	2.1492140	2.4147700	-0.8410510
H	2.1456560	4.8660080	-1.0848570
H	-0.0000060	6.1017620	-1.2043420
H	-2.1456650	4.8659970	-1.0849100
H	-2.1492170	2.4147590	-0.8411030
H	-1.1429440	0.7752880	3.5915590
H	-2.6354310	-0.6073010	-1.4722730
H	-4.5758490	-1.3916550	-1.9828130
H	-6.8556960	-2.0290130	-2.6055280
H	-8.2173030	-1.0995410	1.3601590
H	-5.9431470	-0.4486630	1.9971200
H	1.1429450	0.7752870	3.5915590
H	2.6354330	-0.6072970	-1.4722740
H	4.5758510	-1.3916480	-1.9828170
H	6.8556990	-2.0290050	-2.6055320
H	8.2173030	-1.0995460	1.3601590
H	5.9431470	-0.4486690	1.9971210

3 eq (ground state, CAM-B3LYP/6-31G*)

-2475.119994870			
C	6.1316560	-1.1714870	-0.3005670
C	5.0300810	-0.3101260	-0.3615980
C	5.2446270	1.0267040	-0.7201570
C	6.5176810	1.4925220	-0.9964330
C	7.6091860	0.6217610	-0.9326700
C	7.4075430	-0.7160780	-0.5853290
C	3.6747600	-0.7796070	-0.0551240
S	3.2096540	-2.4371660	-0.2679080
C	1.5871440	-2.1336510	0.2856150
C	1.4291850	-0.8011830	0.6182050
C	2.6222770	-0.0479020	0.4178690
C	0.6751080	-3.2498970	0.3037690
C	-0.6750240	-3.2499330	0.3038950
C	-1.5870920	-2.1337100	0.2858010

C	-1.4291180	-0.8012130	0.6182620
C	-2.6222090	-0.0479380	0.4178740
C	-3.6746870	-0.7796800	-0.0550680
S	-3.2096860	-2.4373100	-0.2674460
P	0.0000450	-0.1087520	1.4698470
C	-0.0000440	1.6514040	1.0159290
C	-5.0299970	-0.3101950	-0.3616110
C	-5.2444530	1.0265130	-0.7206720
C	-6.5174930	1.4923400	-0.9970130
C	-7.6090680	0.6217000	-0.9328080
C	-7.4075130	-0.7160220	-0.5849610
C	-6.1316410	-1.1714360	-0.3001390
C	-8.9294020	1.0995390	-1.2266650
N	-9.9935530	1.4856040	-1.4644330
C	8.9295340	1.0995980	-1.2264660
N	9.9936970	1.4856640	-1.4641800
O	0.0001240	-0.3058280	2.9500680
H	-1.1479630	-4.2270640	0.2552120
H	-2.6989440	1.0045840	0.6607930
H	-4.3999390	1.7020260	-0.8013600
H	-6.6731720	2.5288060	-1.2748460
H	-8.2544220	-1.3908660	-0.5311410
H	-5.9919320	-2.2069770	-0.0071050
H	1.1480880	-4.2270030	0.2549520
H	2.6990180	1.0045920	0.6609030
H	4.4001690	1.7023290	-0.8005000
H	6.6734280	2.5290840	-1.2738710
H	8.2543950	-1.3910210	-0.5318550
H	5.9918900	-2.2071330	-0.0079290
C	-0.0002750	2.5818020	2.0543120
C	-0.0004760	3.9438380	1.7690770
C	-0.0004100	4.3776620	0.4488720
C	-0.0001460	3.4519050	-0.5922090
C	0.0000400	2.0923460	-0.3105120
H	-0.0003180	2.2217130	3.0783090
H	-0.0006950	4.6656280	2.5797200
H	-0.0005740	5.4404970	0.2270370
H	-0.0000830	3.7918230	-1.6232080
H	0.0002470	1.3721890	-1.1242930

3 eq (excited state, CAM-B3LYP/6-31G*)

-2475.107224190			
C	6.1975770	-1.2719530	-0.3336160
C	5.1497370	-0.3542600	-0.1130810
C	5.4846750	1.0130180	-0.0111130

C	6.7917990	1.4372170	-0.1203720
C	7.8196340	0.5096560	-0.3388790
C	7.5067560	-0.8510820	-0.4438830
C	3.7816050	-0.7926130	0.0041620
S	3.3111660	-2.4509450	-0.2517880
C	1.6091120	-2.0991010	0.0644260
C	1.4554270	-0.7162970	0.3616080
C	2.6640500	-0.0244730	0.3233370
C	0.7029090	-3.1454780	-0.0410710
C	-0.7029080	-3.1454790	-0.0410680
C	-1.6091120	-2.0991030	0.0644310
C	-1.4554250	-0.7162980	0.3616070
C	-2.6640480	-0.0244730	0.3233340
C	-3.7816040	-0.7926140	0.0041640
S	-3.3111660	-2.4509480	-0.2517780
P	0.0000000	0.0811790	1.0658820
C	0.0000000	1.7532380	0.3572980
C	-5.1497360	-0.3542610	-0.1130800
C	-5.4846740	1.0130170	-0.0111110
C	-6.7917980	1.4372160	-0.1203720
C	-7.8196330	0.5096560	-0.3388820
C	-7.5067540	-0.8510830	-0.4438870
C	-6.1975760	-1.2719540	-0.3336190
C	-9.1759060	0.9500560	-0.4558760
N	-10.2729510	1.3073750	-0.5516020
C	9.1759070	0.9500570	-0.4558710
N	10.2729530	1.3073760	-0.5515960
O	-0.0000010	0.1108030	2.5628530
H	-1.1424850	-4.1244360	-0.2116410
H	-2.7314740	1.0324140	0.5495740
H	-4.7072020	1.7508910	0.1480640
H	-7.0312710	2.4918160	-0.0406600
H	-8.2997560	-1.5716060	-0.6106870
H	-5.9804190	-2.3323530	-0.4107880
H	1.1424870	-4.1244340	-0.2116480
H	2.7314760	1.0324130	0.5495820
H	4.7072020	1.7508930	0.1480580
H	7.0312720	2.4918170	-0.0406620
H	8.2997580	-1.5716050	-0.6106800
H	5.9804200	-2.3323530	-0.4107830
C	-0.0000130	2.8305350	1.2424700
C	-0.0000150	4.1332100	0.7520810
C	-0.0000050	4.3594910	-0.6188670
C	0.0000080	3.2853020	-1.5065950
C	0.0000110	1.9853570	-1.0209380
H	-0.0000200	2.6316370	2.3096840

H	-0.0000250	4.9706000	1.4427370
H	-0.0000070	5.3757850	-1.0008480
H	0.0000160	3.4639520	-2.5772310
H	0.0000210	1.1484620	-1.7141190

4 ax- $\perp$ (ground state, CAM-B3LYP/6-31G*)

-2699.593672280

C	-6.1204000	-0.3784230	0.9897130
C	-5.0138210	-0.7450390	0.2132600
C	-5.2142510	-1.5803080	-0.8941900
C	-6.4812790	-2.0273500	-1.2263930
C	-7.5535890	-1.6439530	-0.4341700
C	-7.3918930	-0.8268080	0.6739200
C	-3.6646180	-0.2692440	0.5358710
S	-3.2119350	0.1724770	2.1514550
C	-1.5879060	0.5769880	1.6715910
C	-1.4302980	0.3855550	0.3138170
C	-2.6069640	-0.1059500	-0.3152090
C	-0.6750970	0.9963480	2.7105300
C	0.6750890	0.9963950	2.7105170
C	1.5878940	0.5770370	1.6715740
S	3.2119440	0.1725880	2.1514240
C	3.6645770	-0.2692820	0.5358650
C	2.6068780	-0.1061340	-0.3151860
C	1.4302440	0.3854670	0.3138260
C	5.0137850	-0.7450700	0.2132610
C	6.1203860	-0.3783060	0.9896130
C	7.3918790	-0.8267010	0.6738310
C	7.5535510	-1.6440030	-0.4341470
C	6.4812180	-2.0275440	-1.2262700
C	5.2141920	-1.5804910	-0.8940780
N	8.8963860	-2.1184830	-0.7766930
O	9.0103520	-2.8368690	-1.7583350
P	-0.0000130	0.7489570	-0.7212500
C	0.0000270	2.5351350	-1.0436720
N	-8.8964250	-2.1184180	-0.7767300
O	-9.0104100	-2.8366740	-1.7584640
O	-0.0000100	-0.0347130	-1.9939230
O	-9.8216050	-1.7668120	-0.0600250
O	9.8215830	-1.7667660	-0.0600660
H	-1.1492810	1.3009540	3.6398000
H	-2.6472640	-0.3045010	-1.3792400
H	-4.3649590	-1.8966610	-1.4891780
H	-6.6504640	-2.6735620	-2.0778890
H	-8.2560260	-0.5485450	1.2629770

H	-5.9891040	0.2811520	1.8413080
H	1.1492700	1.3010540	3.6397710
H	2.6471350	-0.3047830	-1.3792000
H	4.3648820	-1.8969490	-1.4889840
H	6.6503880	-2.6738700	-2.0776820
H	8.2560290	-0.5483260	1.2628100
H	5.9891070	0.2813940	1.8411130
C	0.0001740	2.9363260	-2.3796540
C	0.0002380	4.2894500	-2.7001410
C	0.0001610	5.2427500	-1.6891120
C	0.0000110	4.8462180	-0.3542730
C	-0.0000560	3.4966430	-0.0300550
H	0.0002280	2.1763440	-3.1540960
H	0.0003450	4.5984180	-3.7406910
H	0.0002160	6.2992760	-1.9392350
H	-0.0000560	5.5918500	0.4346310
H	-0.0001890	3.1960870	1.0131090

4 ax- $\perp$ (excited state, CAM-B3LYP/6-31G*)

-2699.581038430			
C	-6.1603290	-0.6222570	1.0828170
C	-5.1014790	-0.6789090	0.1530520
C	-5.4018670	-1.0610150	-1.1720850
C	-6.6927960	-1.3657360	-1.5505510
C	-7.7089010	-1.2939360	-0.6032100
C	-7.4549580	-0.9248730	0.7122690
C	-3.7484200	-0.3561410	0.5370450
S	-3.3088610	-0.0198170	2.1914740
C	-1.6111590	0.2220440	1.7706480
C	-1.4477260	0.0706480	0.3677080
C	-2.6304590	-0.2588900	-0.2869620
C	-0.7037900	0.4564770	2.7987300
C	0.7037890	0.4564750	2.7987300
C	1.6111580	0.2220430	1.7706480
S	3.3088600	-0.0198200	2.1914740
C	3.7484200	-0.3561390	0.5370450
C	2.6304590	-0.2588860	-0.2869620
C	1.4477260	0.0706510	0.3677070
C	5.1014790	-0.6789070	0.1530520
C	6.1603260	-0.6222750	1.0828230
C	7.4549540	-0.9248910	0.7122750
C	7.7089040	-1.2939330	-0.6032090
C	6.6928010	-1.3657110	-1.5505550
C	5.4018710	-1.0609910	-1.1720900
N	9.0740440	-1.6153010	-0.9993440

O	9.2673660	-1.9364960	-2.1644450
P	-0.0000010	0.4509560	-0.6284540
C	-0.0000020	2.2613640	-0.8110060
N	-9.0740400	-1.6153050	-0.9993450
O	-9.2673540	-1.9365200	-2.1644420
O	-0.0000000	-0.2466370	-1.9497140
O	-9.9464570	-1.5441220	-0.1435820
O	9.9464590	-1.5441430	-0.1435790
H	-1.1426890	0.5908930	3.7837230
H	-2.6592710	-0.4134140	-1.3584770
H	-4.6109490	-1.1281590	-1.9094440
H	-6.9313890	-1.6616460	-2.5638580
H	-8.2732520	-0.8805780	1.4191600
H	-5.9654570	-0.3291310	2.1091970
H	1.1426890	0.5908890	3.7837230
H	2.6592720	-0.4134090	-1.3584770
H	4.6109570	-1.1281180	-1.9094540
H	6.9313970	-1.6616040	-2.5638670
H	8.2732450	-0.8806120	1.4191700
H	5.9654500	-0.3291670	2.1092070
C	-0.0000040	2.7564890	-2.1157300
C	-0.0000050	4.1291030	-2.3376210
C	-0.0000040	5.0085660	-1.2616000
C	-0.0000030	4.5166040	0.0410520
C	-0.0000020	3.1475430	0.2691580
H	-0.0000040	2.0555840	-2.9440780
H	-0.0000060	4.5106850	-3.3538390
H	-0.0000050	6.0801460	-1.4355000
H	-0.0000020	5.2033280	0.8817450
H	-0.0000000	2.7746260	1.2885730

4 ax-|| (ground state, CAM-B3LYP/6-31G*)

-2699.592346230			
P	0.0000160	1.0279580	-0.9254470
C	1.4154180	0.6134120	0.1078540
C	1.5764510	0.9465410	1.4364720
C	0.6751800	1.5693030	2.3816050
C	-0.6751310	1.5692880	2.3816140
C	-1.5764040	0.9465170	1.4364920
C	-1.4153630	0.6133680	0.1078810
C	-0.0000530	2.8378860	-1.0682820
C	-1.2053330	3.5351530	-1.1711300
C	1.2051310	3.5354320	-1.1703120
C	1.2044040	4.9100480	-1.3696640
C	-0.0002400	5.5978020	-1.4686070

C	-1.2047940	4.9097660	-1.3704870
C	-2.5450280	-0.0508930	-0.4412920
C	-3.5756310	-0.2078740	0.4448050
S	-3.1499680	0.4572540	1.9925640
C	2.5450840	-0.0508470	-0.4413220
C	3.5756820	-0.2078400	0.4447760
S	3.1500080	0.4572530	1.9925470
C	-4.8793730	-0.8365560	0.2081230
C	-6.0047500	-0.4889620	0.9662600
C	-7.2327270	-1.0847750	0.7327790
C	-7.3325890	-2.0316760	-0.2747560
C	-6.2403430	-2.4004580	-1.0463690
C	-5.0164430	-1.8046090	-0.7961780
N	-8.6294360	-2.6631850	-0.5297130
O	-9.5735680	-2.3192910	0.1657330
C	4.8794270	-0.8365120	0.2080840
C	6.0048020	-0.4889250	0.9662270
C	7.2327810	-1.0847310	0.7327380
C	7.3326450	-2.0316170	-0.2748110
C	6.2404020	-2.4003930	-1.0464290
C	5.0165000	-1.8045520	-0.7962290
N	8.6294950	-2.6631170	-0.5297770
O	9.5736220	-2.3192390	0.1656840
O	0.0000050	0.2910180	-2.2255840
O	8.6889270	-3.4950970	-1.4224570
O	-8.6888600	-3.4951890	-1.4223700
H	-1.1533980	2.0379970	3.2376370
H	-2.5766380	-0.3656860	-1.4774330
H	-4.1498650	-2.1058110	-1.3738100
H	-6.3600360	-3.1502010	-1.8176220
H	-8.1107410	-0.8235880	1.3089880
H	-5.9242100	0.2697970	1.7378280
H	1.1534520	2.0380220	3.2376180
H	2.5767000	-0.3656140	-1.4774710
H	4.1499220	-2.1057500	-1.3738640
H	6.3600970	-3.1501250	-1.8176930
H	8.1107940	-0.8235510	1.3089510
H	5.9242590	0.2698210	1.7378070
H	-2.1487960	3.0033390	-1.0933530
H	-2.1459520	5.4448780	-1.4478140
H	-0.0003140	6.6724890	-1.6222670
H	2.1454890	5.4453810	-1.4463460
H	2.1486680	3.0038440	-1.0919020

4 ax-|| (excited state, CAM-B3LYP/6-31G*)

-2699.578571170

P	0.0000040	0.4895630	-0.7590580
C	1.4412600	0.1961810	0.2735020
C	1.6083560	0.5866310	1.6293600
C	0.7038100	1.0327950	2.5869150
C	-0.7037980	1.0328010	2.5869150
C	-1.6083460	0.5866400	1.6293620
C	-1.4412500	0.1961790	0.2735070
C	-0.0000070	2.2931200	-1.0293200
C	-1.2051010	2.9846890	-1.1806300
C	1.2050710	2.9847730	-1.1803660
C	1.2040320	4.3411640	-1.4784940
C	-0.0000380	5.0206940	-1.6265960
C	-1.2040930	4.3410790	-1.4787590
C	-2.6106090	-0.2816870	-0.3078860
C	-3.7255470	-0.2711210	0.5284570
S	-3.2960080	0.3632610	2.0968680
C	2.6106200	-0.2816780	-0.3078960
C	3.7255560	-0.2711210	0.5284480
S	3.2960170	0.3632440	2.0968650
C	-5.0661080	-0.7024590	0.2159090
C	-6.1271780	-0.5173720	1.1267610
C	-7.4103930	-0.9241690	0.8226210
C	-7.6510840	-1.5289440	-0.4053730
C	-6.6323320	-1.7335420	-1.3304790
C	-5.3527130	-1.3238630	-1.0189670
N	-9.0039280	-1.9611460	-0.7305550
O	-9.8783520	-1.7710610	0.1049650
C	5.0661180	-0.7024580	0.2158970
C	6.1271840	-0.5173910	1.1267580
C	7.4103990	-0.9241880	0.8226170
C	7.6510910	-1.5289400	-0.4053870
C	6.6323450	-1.7335170	-1.3305040
C	5.3527260	-1.3238390	-1.0189890
N	9.0039330	-1.9611450	-0.7305680
O	9.8783510	-1.7710570	0.1049570
O	-0.0000020	-0.3379230	-2.0032820
O	9.1861920	-2.4879450	-1.8202990
O	-9.1861870	-2.4879820	-1.8202680
H	-1.1426360	1.3531210	3.5280200
H	-2.6334140	-0.6172160	-1.3375810
H	-4.5593000	-1.4949670	-1.7366670
H	-6.8600800	-2.2124440	-2.2739260
H	-8.2302810	-0.7831190	1.5148290
H	-5.9428660	-0.0406590	2.0839280
H	1.1426510	1.3531090	3.5280200

H	2.6334250	-0.6171940	-1.3375950
H	4.5593160	-1.4949260	-1.7366970
H	6.8600960	-2.2124030	-2.2739580
H	8.2302850	-0.7831550	1.5148320
H	5.9428690	-0.0406970	2.0839330
H	-2.1496940	2.4627580	-1.0658800
H	-2.1457250	4.8683800	-1.5940250
H	-0.0000500	6.0814810	-1.8571490
H	2.1456530	4.8685310	-1.5935530
H	2.1496760	2.4629080	-1.0654150

4 eq (ground state, CAM-B3LYP/6-31G*)

-2699.592280180

C	6.1276720	-1.2431980	-0.2767480
C	5.0267240	-0.3775130	-0.2937940
C	5.2384800	0.9757150	-0.5910290
C	6.5100970	1.4559740	-0.8509000
C	7.5763420	0.5689910	-0.8259460
C	7.4039390	-0.7775710	-0.5452020
C	3.6725450	-0.8602620	-0.0041940
S	3.2085210	-2.5087100	-0.2795840
C	1.5871060	-2.2274530	0.2874330
C	1.4287220	-0.9091010	0.6724750
C	2.6206390	-0.1479210	0.4992360
C	0.6750490	-3.3437250	0.2626880
C	-0.6750480	-3.3437270	0.2626970
C	-1.5871080	-2.2274580	0.2874540
S	-3.2085380	-2.5087250	-0.2795170
C	-3.6725480	-0.8602660	-0.0041690
C	-2.6206420	-0.1479260	0.4992620
C	-1.4287230	-0.9091050	0.6724950
P	0.0000040	-0.2524700	1.5531760
C	-0.0000020	1.5252130	1.1758260
C	0.0000060	2.4087910	2.2543030
C	0.0000030	3.7820140	2.0293070
C	-0.0000090	4.2736110	0.7294850
C	-0.0000180	3.3947480	-0.3515020
C	-0.0000140	2.0240900	-0.1300360
C	-5.0267230	-0.3775140	-0.2937810
C	-5.2384730	0.9757100	-0.5910380
C	-6.5100860	1.4559720	-0.8509180
C	-7.5763360	0.5689950	-0.8259520
C	-7.4039400	-0.7775630	-0.5451860
C	-6.1276760	-1.2431930	-0.2767230
N	-8.9235460	1.0698400	-1.1084500

O	-9.8435070	0.2662160	-1.0848530
N	8.9235540	1.0698350	-1.1084340
O	9.8435140	0.2662080	-1.0848370
O	0.0000150	-0.5137750	3.0233230
O	-9.0455330	2.2612540	-1.3508410
O	9.0455490	2.2612530	-1.3507960
H	0.0000160	2.0036660	3.2612890
H	0.0000090	4.4674270	2.8709110
H	-0.0000120	5.3451670	0.5547590
H	-0.0000270	3.7798280	-1.3664650
H	-0.0000210	1.3405600	-0.9748730
H	-1.1479700	-4.3182240	0.1761190
H	-2.6969750	0.8944450	0.7825800
H	-4.3936840	1.6538050	-0.6367930
H	-6.6883980	2.4979140	-1.0827800
H	-8.2635980	-1.4348420	-0.5319300
H	-5.9879220	-2.2908980	-0.0315330
H	1.1479720	-4.3182200	0.1761000
H	2.6969760	0.8944480	0.7825630
H	4.3936950	1.6538140	-0.6367740
H	6.6884140	2.4979190	-1.0827450
H	8.2635940	-1.4348530	-0.5319550
H	5.9879130	-2.2909060	-0.0315760

4 eq (excited state, CAM-B3LYP/6-31G*)

-2699.579866670

C	6.1893460	-1.3406760	-0.3168270
C	5.1390000	-0.4216730	-0.1061960
C	5.4650710	0.9507740	-0.0329270
C	6.7684370	1.3819280	-0.1600120
C	7.7745050	0.4426640	-0.3661270
C	7.4960020	-0.9173670	-0.4453670
C	3.7744150	-0.8643170	0.0293730
S	3.3066910	-2.5245490	-0.2098040
C	1.6086180	-2.1754210	0.1220260
C	1.4531700	-0.7924200	0.4135280
C	2.6576980	-0.0963400	0.3570520
C	0.7021800	-3.2240660	0.0296090
C	-0.7021790	-3.2240670	0.0296090
C	-1.6086170	-2.1754210	0.1220260
S	-3.3066900	-2.5245490	-0.2098030
C	-3.7744140	-0.8643170	0.0293730
C	-2.6576970	-0.0963410	0.3570520
C	-1.4531690	-0.7924200	0.4135280
P	0.0000000	-0.0085130	1.1399720

C	0.0000000	1.6807550	0.4778030
C	-0.0000000	2.7326070	1.3933310
C	-0.0000000	4.0483410	0.9396450
C	0.0000000	4.3128320	-0.4245200
C	0.0000010	3.2642890	-1.3423140
C	0.0000010	1.9510880	-0.8936080
C	-5.1389990	-0.4216740	-0.1061960
C	-5.4650700	0.9507740	-0.0329300
C	-6.7684360	1.3819270	-0.1600140
C	-7.7745050	0.4426640	-0.3661270
C	-7.4960010	-0.9173680	-0.4453640
C	-6.1893450	-1.3406770	-0.3168250
N	-9.1508680	0.8950600	-0.5044030
O	-10.0140250	0.0458830	-0.6876770
N	9.1508660	0.8950610	-0.5044040
O	10.0140210	0.0458810	-0.6876780
O	0.0000000	-0.0269080	2.6364460
O	-9.3647010	2.0986650	-0.4298350
O	9.3646960	2.0986660	-0.4298320
H	-0.0000010	2.5042630	2.4546090
H	-0.0000010	4.8660110	1.6534050
H	0.0000000	5.3394150	-0.7777640
H	0.0000020	3.4731540	-2.4074190
H	0.0000020	1.1344270	-1.6105290
H	-1.1420430	-4.2041790	-0.1334100
H	-2.7253530	0.9614030	0.5783660
H	-4.6839390	1.6866920	0.1160870
H	-7.0261940	2.4316700	-0.1067470
H	-8.3066390	-1.6166970	-0.6037540
H	-5.9764300	-2.4032990	-0.3703060
H	1.1420440	-4.2041790	-0.1334110
H	2.7253540	0.9614030	0.5783670
H	4.6839410	1.6866930	0.1160910
H	7.0261960	2.4316710	-0.1067430
H	8.3066400	-1.6166950	-0.6037590
H	5.9764310	-2.4032980	-0.3703100

5 ax- $\perp$ (ground state, CAM-B3LYP/6-31G*)

-2290.718957050

S	3.2147140	-0.9880540	1.7410940
C	1.5849080	-0.4410150	1.4557560
C	1.4340970	-0.0721120	0.1348180
C	2.6155060	-0.2699650	-0.6342590
C	3.6715640	-0.7591950	0.0822860
C	5.0257920	-1.0683300	-0.3954560

C	5.8167700	-2.0381740	0.2289800
C	7.0919500	-2.3223200	-0.2403330
C	7.5975700	-1.6486010	-1.3461730
C	6.8192770	-0.6828690	-1.9758160
C	5.5484200	-0.3901720	-1.5023630
C	0.6681150	-0.4753480	2.5718780
C	-0.6822320	-0.4785350	2.5665480
C	-1.5904280	-0.4520930	1.4433300
S	-3.2159770	-1.0184640	1.7146730
C	-3.6658550	-0.7790310	0.0556610
C	-2.6060650	-0.2889560	-0.6546820
C	-1.4303280	-0.0885690	0.1219400
P	0.0012920	0.6617400	-0.6734000
C	-0.0087280	2.4297410	-0.2493270
C	0.0011480	2.9009290	1.0655720
C	-0.0083540	4.2666250	1.3140370
C	-0.0276800	5.1685310	0.2534010
C	-0.0373480	4.7039810	-1.0562330
C	-0.0278160	3.3364810	-1.3088950
C	-5.0143330	-1.0962530	-0.4320870
C	-5.2036680	-1.4747160	-1.7659840
C	-6.4736210	-1.7614590	-2.2455300
C	-7.5761600	-1.6881650	-1.4004970
C	-7.3983410	-1.3217890	-0.0713100
C	-6.1299340	-1.0247870	0.4083100
O	0.0079770	0.4646330	-2.1556020
H	1.1392860	-0.5671840	3.5471510
H	2.6458000	-0.0738630	-1.6990310
H	5.4232120	-2.5891250	1.0779640
H	7.6892980	-3.0805360	0.2563360
H	8.5935170	-1.8731770	-1.7146040
H	7.2073830	-0.1458510	-2.8357000
H	4.9582230	0.3834930	-1.9821770
H	-1.1606550	-0.5710940	3.5381620
H	-2.6460090	-0.0472010	-1.7096570
H	-4.3449260	-1.5613750	-2.4235600
H	-6.6008520	-2.0542500	-3.2830710
H	-8.5683740	-1.9177350	-1.7758770
H	-8.2523610	-1.2582050	0.5957930
H	-6.0061600	-0.7155590	1.4419770
H	0.0164860	2.2041750	1.8978030
H	-0.0003840	4.6300540	2.3370030
H	-0.0350090	6.2362210	0.4510930
H	-0.0523180	5.4066250	-1.8836660
H	-0.0344920	2.9527000	-2.3238450

5 ax- $\perp$ (excited state, CAM-B3LYP/6-31G*)

-2290.706130660

S	3.3169730	-1.2794830	1.5521390
C	1.6123230	-0.8799770	1.3008680
C	1.4499080	-0.3150180	0.0070830
C	2.6409190	-0.2584050	-0.7174850
C	3.7591340	-0.7379910	-0.0491670
C	5.1215110	-0.8123350	-0.5339750
C	6.1771710	-1.2163140	0.3032900
C	7.4783280	-1.2762670	-0.1677790
C	7.7652920	-0.9384930	-1.4869020
C	6.7315650	-0.5395570	-2.3314480
C	5.4297560	-0.4773620	-1.8664870
C	0.7051140	-1.1947900	2.3062760
C	-0.7051710	-1.1948050	2.3062570
C	-1.6123670	-0.8799920	1.3008320
S	-3.3170120	-1.2795440	1.5520790
C	-3.7591870	-0.7379410	-0.0491800
C	-2.6409860	-0.2583010	-0.7174740
C	-1.4499670	-0.3149610	0.0070840
P	-0.0000160	0.5041100	-0.6612230
C	0.0000390	2.1627910	0.0932270
C	-0.0001790	2.3862430	1.4727450
C	-0.0000960	3.6840710	1.9649000
C	0.0002020	4.7658080	1.0880610
C	0.0004140	4.5465230	-0.2843790
C	0.0003340	3.2488230	-0.7834390
C	-5.1215690	-0.8122620	-0.5339870
C	-5.4297820	-0.4774290	-1.8665400
C	-6.7315910	-0.5396010	-2.3315040
C	-7.7653470	-0.9383770	-1.4869190
C	-7.4784140	-1.2760130	-0.1677540
C	-6.1772560	-1.2160790	0.3033180
O	-0.0000000	0.5758690	-2.1552960
H	1.1440550	-1.5690510	3.2273480
H	2.6705130	0.1427410	-1.7231010
H	5.9756960	-1.4791590	1.3372910
H	8.2751500	-1.5887100	0.4999930
H	8.7849890	-0.9874500	-1.8552880
H	6.9428190	-0.2776370	-3.3635450
H	4.6387970	-0.1741520	-2.5430700
H	-1.1441290	-1.5690900	3.2273110
H	-2.6705930	0.1429170	-1.7230610
H	-4.6387940	-0.1743620	-2.5431560
H	-6.9428210	-0.2777940	-3.3636350

H	-8.7850440	-0.9873190	-1.8553080
H	-8.2752600	-1.5883260	0.5000500
H	-5.9758060	-1.4787950	1.3373570
H	-0.0004190	1.5501410	2.1649370
H	-0.0002690	3.8534030	3.0373380
H	0.0002640	5.7794180	1.4772710
H	0.0006400	5.3878130	-0.9707800
H	0.0004830	3.0593220	-1.8518750

5 ax-|| (ground state, CAM-B3LYP/6-31G*)

-2290.717738960

P	0.0017960	0.7060440	-0.8934690
C	1.4216220	0.0924410	0.0257590
C	1.5744930	0.1226860	1.3955210
C	0.6660330	0.5115740	2.4517070
C	-0.6844400	0.5043060	2.4459090
C	-1.5801010	0.1036940	1.3833050
C	-1.4149770	0.0691830	0.0149400
C	-0.0145000	2.5056850	-0.6338160
C	1.1829800	3.2187820	-0.5542830
C	1.1690760	4.6037360	-0.4462710
C	-0.0416490	5.2870740	-0.4169660
C	-1.2389540	4.5841430	-0.4973760
C	-1.2258550	3.1993640	-0.6052540
C	2.5609810	-0.4224180	-0.6528520
C	3.5918840	-0.7632100	0.1783930
S	3.1592230	-0.4507460	1.8325950
C	-2.5462390	-0.4515760	-0.6721160
C	-3.5819220	-0.7963450	0.1516490
S	-3.1587430	-0.4937540	1.8098730
C	4.9061090	-1.3100730	-0.1847810
C	5.6350490	-2.1102670	0.7009190
C	6.8722590	-2.6245000	0.3373730
C	7.4009520	-2.3555130	-0.9198030
C	6.6841960	-1.5619170	-1.8093500
C	5.4521860	-1.0386570	-1.4444220
C	-4.8885320	-1.3541590	-0.2208630
C	-5.0151750	-2.1166330	-1.3875530
C	-6.2460250	-2.6354400	-1.7626870
C	-7.3705960	-2.4143540	-0.9743480
C	-7.2544850	-1.6662040	0.1915880
C	-6.0260210	-1.1373150	0.5634790
O	0.0107110	0.2853190	-2.3281290
H	1.1389240	0.7799420	3.3929820
H	2.5813950	-0.5446170	-1.7290090

H	5.2214450	-2.3488390	1.6762320
H	7.4210690	-3.2458830	1.0381630
H	8.3668790	-2.7603860	-1.2046120
H	7.0907300	-1.3399150	-2.7911220
H	4.9118850	-0.3990880	-2.1345280
H	-1.1681800	0.7687930	3.3827050
H	-2.5773160	-0.5294120	-1.7521430
H	-4.1369990	-2.3165920	-1.9925660
H	-6.3245500	-3.2249460	-2.6708200
H	-8.3318240	-2.8253080	-1.2663280
H	-8.1263560	-1.4852670	0.8124910
H	-5.9522500	-0.5339130	1.4634230
H	-2.1636200	2.6551780	-0.6646560
H	-2.1853980	5.1152610	-0.4738140
H	-0.0522840	6.3692950	-0.3300450
H	2.1049620	5.1500360	-0.3823730
H	2.1310760	2.6899440	-0.5732000

5 ax-|| (excited state, CAM-B3LYP/6-31G*)

-2290.703744290			
P	0.0000560	0.3596300	-0.8140940
C	1.4442980	-0.2575350	0.0511990
C	1.6102760	-0.3490400	1.4603770
C	0.7055420	-0.2687960	2.5118960
C	-0.7052170	-0.2687910	2.5119590
C	-1.6100260	-0.3490350	1.4605050
C	-1.4441050	-0.2576210	0.0513250
C	-0.0001680	2.1528180	-0.4557350
C	1.2038930	2.8557690	-0.3605800
C	1.2028890	4.2333590	-0.1822910
C	-0.0008470	4.9236750	-0.0946180
C	-1.2042710	4.2334720	-0.1876790
C	-1.2045950	2.8559040	-0.3659200
C	2.6247050	-0.4823200	-0.6562630
C	3.7420770	-0.7334550	0.1309010
S	3.3083980	-0.6862180	1.8236340
C	-2.6245300	-0.4825760	-0.6560670
C	-3.7418430	-0.7336570	0.1311800
S	-3.3081080	-0.6862770	1.8238680
C	5.0948090	-1.0050370	-0.3068370
C	6.1613030	-1.0816060	0.6074590
C	7.4532310	-1.3342440	0.1765840
C	7.7202250	-1.5205730	-1.1764880
C	6.6755660	-1.4517940	-2.0957490
C	5.3827050	-1.1998820	-1.6716340

C	-5.0945930	-1.0053370	-0.3064970
C	-5.3824280	-1.2006750	-1.6712270
C	-6.6752910	-1.4526660	-2.0952990
C	-7.7199850	-1.5210320	-1.1760460
C	-7.4530430	-1.3342080	0.1769660
C	-6.1611150	-1.0814860	0.6077940
O	-0.0000890	0.0191930	-2.2708320
H	1.1442760	-0.2906270	3.5059320
H	2.6495920	-0.4431790	-1.7386270
H	5.9755310	-0.9314160	1.6666380
H	8.2587790	-1.3853190	0.9025320
H	8.7326860	-1.7203610	-1.5124770
H	6.8708890	-1.6008540	-3.1531640
H	4.5819870	-1.1647920	-2.4018140
H	-1.1438710	-0.2906240	3.5060300
H	-2.6494830	-0.4436060	-1.7384380
H	-4.5816590	-1.1659340	-2.4013700
H	-6.8705940	-1.6021180	-3.1526620
H	-8.7324450	-1.7208870	-1.5120020
H	-8.2586310	-1.3849550	0.9028930
H	-5.9753630	-0.9308710	1.6669160
H	-2.1486760	2.3248760	-0.4339750
H	-2.1464870	4.7681520	-0.1183510
H	-0.0011150	6.0000210	0.0480330
H	2.1448430	4.7679430	-0.1087680
H	2.1482170	2.3246850	-0.4245720

5 eq (ground state, CAM-B3LYP/6-31G*)

-2290.717851370			
O	-0.0068360	0.1624410	2.8167250
C	0.0027700	1.8728840	0.6657990
C	0.0167750	2.1581940	-0.7022160
H	0.0297820	1.3488190	-1.4270010
C	0.0161180	3.4761190	-1.1390310
H	0.0287960	3.6943540	-2.2023950
C	0.0005710	4.5159500	-0.2123430
H	0.0001610	5.5461080	-0.5556480
C	-0.0137710	4.2372230	1.1490510
H	-0.0259810	5.0478300	1.8710020
C	-0.0124130	2.9172580	1.5891960
H	-0.0233640	2.6769140	2.6476640
C	0.6641910	-3.0796110	0.5261030
H	1.1341740	-4.0577030	0.5869020
C	1.5803330	-1.9757440	0.3848970
C	1.4297410	-0.6143480	0.5686600

C	2.6275920	0.1072080	0.2856060
H	2.6950400	1.1856720	0.3566230
C	3.6772230	-0.6754470	-0.1023960
C	5.0376940	-0.2519380	-0.4607150
C	5.8119560	-0.9794860	-1.3701840
H	5.4009050	-1.8711580	-1.8340500
C	7.0926790	-0.5606710	-1.7044090
H	7.6772760	-1.1377400	-2.4140860
C	7.6205970	0.5957220	-1.1417560
H	8.6212320	0.9238080	-1.4047740
C	6.8595340	1.3269080	-0.2356900
H	7.2663560	2.2257990	0.2170370
C	5.5830330	0.9048550	0.1072580
H	5.0076120	1.4629800	0.8385120
C	-0.6859550	-3.0751950	0.5250550
H	-1.1626600	-4.0499390	0.5863540
C	-1.5938960	-1.9654770	0.3785980
C	-1.4323400	-0.6045700	0.5559880
C	-2.6237810	0.1256790	0.2692200
H	-2.6987610	1.1993140	0.3891850
C	-3.6787770	-0.6499520	-0.1184250
C	-5.0330910	-0.2159770	-0.4854880
C	-5.2335600	1.0486480	-1.0499610
H	-4.3785010	1.6885060	-1.2423360
C	-6.5090840	1.4791320	-1.3859300
H	-6.6450490	2.4633580	-1.8233440
C	-7.6065870	0.6505170	-1.1770670
H	-8.6033860	0.9862050	-1.4449880
C	-7.4179510	-0.6115880	-0.6254370
H	-8.2681290	-1.2645940	-0.4548070
C	-6.1438290	-1.0403640	-0.2792450
H	-6.0110260	-2.0180060	0.1743880
P	-0.0019350	0.1763350	1.3223980
S	3.2071470	-2.3455140	-0.1171470
S	-3.2181100	-2.3226520	-0.1406540

5 eq (excited state, CAM-B3LYP/6-31G*)

-2290.704701000			
O	-0.0001420	0.3847640	2.4372320
C	0.0000270	1.8629400	0.1268130
C	0.0001490	2.0036250	-1.2633650
H	0.0002040	1.1217860	-1.8983150
C	0.0002010	3.2678120	-1.8351210
H	0.0002990	3.3739770	-2.9155030
C	0.0001300	4.3996950	-1.0219750

H	0.0001730	5.3882190	-1.4712980
C	0.0000060	4.2649570	0.3606800
H	-0.0000500	5.1466010	0.9942620
C	-0.0000460	2.9974300	0.9366840
H	-0.0001430	2.8690880	2.0147030
C	0.7037340	-2.9970580	-0.2216480
H	1.1438570	-3.9671770	-0.4361030
C	1.6099610	-1.9599440	-0.0535330
C	1.4613900	-0.5888270	0.2965550
C	2.6817830	0.0899200	0.3264990
H	2.7524280	1.1360340	0.5985880
C	3.7994690	-0.6722640	0.0104240
C	5.1805560	-0.2462870	-0.0445790
C	6.2240300	-1.1696000	-0.2433380
H	5.9961260	-2.2257940	-0.3495990
C	7.5443710	-0.7548780	-0.2921760
H	8.3300820	-1.4885610	-0.4434100
C	7.8655560	0.5914070	-0.1453850
H	8.9007290	0.9151070	-0.1839060
C	6.8455420	1.5201690	0.0506560
H	7.0836900	2.5733220	0.1635820
C	5.5243500	1.1124070	0.0992740
H	4.7462570	1.8540900	0.2410880
C	-0.7037940	-2.9970970	-0.2214920
H	-1.1439160	-3.9672640	-0.4357360
C	-1.6100260	-1.9599800	-0.0534050
C	-1.4614100	-0.5887800	0.2963450
C	-2.6817870	0.0900180	0.3260940
H	-2.7524620	1.1361640	0.5980610
C	-3.7994830	-0.6722330	0.0102470
C	-5.1805640	-0.2462320	-0.0447530
C	-5.5241160	1.1127540	0.0968390
H	-4.7458240	1.8546070	0.2366810
C	-6.8452990	1.5205640	0.0482860
H	-7.0832720	2.5739470	0.1594190
C	-7.8655190	0.5915540	-0.1454810
H	-8.9006820	0.9152900	-0.1839720
C	-7.5445610	-0.7550260	-0.2900660
H	-8.3304400	-1.4888980	-0.4395000
C	-6.2242350	-1.1697980	-0.2412600
H	-5.9964840	-2.2262150	-0.3456330
P	-0.0000440	0.2375130	0.9457360
S	3.3203170	-2.3130480	-0.3374430
S	-3.3203950	-2.3131160	-0.3371960

6 ax- $\perp$ (ground state, CAM-B3LYP/6-31G*)

-3325.034108140

C	11.1935060	-0.8995600	-0.6779290
C	10.0293030	-0.5689900	0.0195650
C	10.0039490	0.5984240	0.7867270
C	11.1197350	1.4228010	0.8421530
C	12.2805720	1.0880030	0.1531600
C	12.3113200	-0.0795400	-0.6017020
N	8.8916700	-1.4146900	-0.0453820
C	9.0640880	-2.8202120	0.0541350
C	8.3861970	-3.6819640	-0.8114280
C	8.5568490	-5.0558130	-0.7051400
C	9.4175370	-5.5888510	0.2484540
C	10.1014880	-4.7316750	1.1037110
C	9.9219130	-3.3576680	1.0164760
C	7.6032800	-0.8655980	-0.2107340
C	6.4930100	-1.4398590	0.4189820
C	5.2279180	-0.9070080	0.2440740
C	5.0211200	0.2328870	-0.5411330
C	6.1365240	0.8062270	-1.1598290
C	7.4021270	0.2646720	-1.0097630
C	3.6754750	0.7940460	-0.6940420
S	3.2185540	1.6995080	-2.1038250
C	1.5949640	1.9526020	-1.5205330
C	1.4407570	1.3610840	-0.2833540
C	2.6178790	0.7009070	0.1677280
P	0.0146320	1.4086600	0.8155580
C	-1.4230070	1.3845630	-0.2690890
C	-1.5798900	1.9784970	-1.5048620
S	-3.2132620	1.7519990	-2.0717890
C	-3.6707390	0.8549240	-0.6570930
C	-2.6062480	0.7442290	0.1942240
C	-0.6664170	2.6814230	-2.3743110
C	0.6845410	2.6704330	-2.3809700
C	-5.0233030	0.3163110	-0.4902410
C	-5.2390350	-0.8232820	0.2932500
C	-6.5084220	-1.3447420	0.4694500
C	-7.6186180	-0.7399300	-0.1314100
C	-7.4109410	0.3990730	-0.9162600
C	-6.1364390	0.9106140	-1.0932200
N	-8.9135140	-1.2678810	0.0487420
C	-9.8540350	-1.2397300	-1.0134460
C	-11.1808640	-0.8770360	-0.7702680
C	-12.1039820	-0.8649090	-1.8073270
C	-11.7168240	-1.1950240	-3.1015570
C	-10.3943050	-1.5485480	-3.3470840
C	-9.4692260	-1.5816610	-2.3122800

O	0.0104850	0.2892280	1.8071380
C	0.0317930	3.0221010	1.6543040
C	0.0356230	4.2399310	0.9701940
C	0.0487290	5.4340510	1.6780320
C	0.0580850	5.4199120	3.0702930
C	0.0543350	4.2105400	3.7547580
C	0.0411950	3.0124380	3.0488890
C	-9.2885070	-1.8319830	1.2961820
C	-9.9981130	-3.0342150	1.3410960
C	-10.3762040	-3.5775750	2.5615850
C	-10.0384590	-2.9431280	3.7521240
C	-9.3250530	-1.7500280	3.7094920
C	-8.9596220	-1.1902130	2.4925990
H	0.0283760	4.2594080	-0.1150970
H	0.0516090	6.3791360	1.1437160
H	0.0682830	6.3558080	3.6209080
H	0.0616140	4.1985780	4.8403120
H	0.0378810	2.0572460	3.5637570
H	-1.1402640	3.2541140	-3.1674380
H	-2.6483150	0.2386210	1.1510420
H	-4.3923110	-1.3285290	0.7463910
H	-6.6458010	-2.2380640	1.0681600
H	-8.2587690	0.8893960	-1.3810190
H	-6.0107180	1.8108020	-1.6878490
H	-10.2516790	-3.5368250	0.4139600
H	-10.9283050	-4.5123050	2.5801010
H	-10.3287870	-3.3743740	4.7046900
H	-9.0603520	-1.2402660	4.6308520
H	-8.4150260	-0.2526520	2.4615390
H	-11.4822620	-0.6079300	0.2363020
H	-13.1318880	-0.5820500	-1.6016360
H	-12.4391010	-1.1777550	-3.9112910
H	-10.0793390	-1.8160830	-4.3511420
H	-8.4418700	-1.8719120	-2.5042150
H	1.1598400	3.2353380	-3.1787940
H	2.6602670	0.1932410	1.1234570
H	4.3814030	-1.3871820	0.7238600
H	6.6262950	-2.3172220	1.0416320
H	8.2476740	0.7239060	-1.5090720
H	6.0166620	1.6969490	-1.7695980
H	7.7247530	-3.2677930	-1.5648120
H	8.0215280	-5.7128420	-1.3838030
H	9.5540700	-6.6627610	0.3241780
H	10.7724310	-5.1343160	1.8564340
H	10.4467630	-2.6909400	1.6921390
H	9.1049530	0.8545230	1.3369990

H	11.0838480	2.3272530	1.4418200
H	13.1534800	1.7306650	0.2050560
H	13.2091010	-0.3511620	-1.1486220
H	11.2154870	-1.8035610	-1.2768860

6 ax- $\perp$ (excited state, CAM-B3LYP/6-31G*)

-3325.022123260

C	11.2555830	-0.5706280	-1.3025770
C	10.1776280	-0.2495700	-0.4746340
C	10.2056900	0.9413910	0.2550450
C	11.2909230	1.8000790	0.1458600
C	12.3666360	1.4769990	-0.6748080
C	12.3440940	0.2862740	-1.3932580
N	9.0702910	-1.1329360	-0.3684030
C	9.3135930	-2.5243910	-0.2186150
C	8.5837380	-3.4554720	-0.9616630
C	8.8264990	-4.8136460	-0.8081900
C	9.8079230	-5.2604120	0.0705410
C	10.5421740	-4.3333810	0.8026830
C	10.2946740	-2.9740990	0.6679220
C	7.7592290	-0.6384150	-0.4071040
C	6.7318160	-1.2547250	0.3283670
C	5.4443550	-0.7682270	0.2881440
C	5.1030730	0.3654090	-0.4805790
C	6.1441210	0.9729800	-1.2117370
C	7.4338620	0.4869410	-1.1807910
C	3.7572830	0.8714350	-0.5074080
S	3.3210100	2.3088360	-1.4069510
C	1.6195440	2.1823840	-0.9421370
C	1.4534450	1.0654300	-0.0842380
C	2.6347240	0.3553950	0.1297070
P	0.0057810	0.6247980	0.8795900
C	-1.4423780	1.0866370	-0.0728440
C	-1.5988700	2.2076520	-0.9270750
S	-3.3010870	2.3575580	-1.3813480
C	-3.7521080	0.9280560	-0.4769980
C	-2.6326090	0.3940560	0.1498360
C	-0.6871160	3.1099930	-1.4707900
C	0.7171240	3.0983860	-1.4782260
C	-5.1053830	0.4422640	-0.4386360
C	-5.4296870	-0.7700630	0.2074110
C	-6.7218660	-1.2442230	0.2496470
C	-7.7727840	-0.5281670	-0.3490340
C	-7.4658380	0.6805260	-0.9933310
C	-6.1687840	1.1456980	-1.0398200

N	-9.0893680	-1.0091400	-0.3063420
C	-9.9770050	-0.7751550	-1.3900900
C	-11.2917970	-0.3708990	-1.1476600
C	-12.1625120	-0.1581640	-2.2077610
C	-11.7327670	-0.3292560	-3.5194760
C	-10.4217410	-0.7259140	-3.7620790
C	-9.5490440	-0.9569290	-2.7075860
O	-0.0032280	-0.8087500	1.3100320
C	0.0209870	1.7477230	2.3148400
C	0.0324450	3.1406310	2.2017560
C	0.0437990	3.9296890	3.3438610
C	0.0438980	3.3377880	4.6042240
C	0.0326060	1.9527660	4.7202900
C	0.0211790	1.1579020	3.5795310
C	-9.5546900	-1.7380340	0.8202310
C	-10.3164470	-2.8953030	0.6430800
C	-10.7828920	-3.5982510	1.7455020
C	-10.4851640	-3.1686050	3.0344550
C	-9.7216020	-2.0195440	3.2117440
C	-9.2650010	-1.3010750	2.1152140
H	0.0326130	3.6113180	1.2236960
H	0.0526600	5.0115230	3.2512580
H	0.0528610	3.9587160	5.4950550
H	0.0327470	1.4882000	5.7017860
H	0.0123890	0.0750670	3.6505100
H	-1.1256870	3.9206700	-2.0468400
H	-2.6621280	-0.4873710	0.7786590
H	-4.6447830	-1.3617910	0.6649440
H	-6.9315270	-2.1877780	0.7403270
H	-8.2606850	1.2574230	-1.4520040
H	-5.9746490	2.0912330	-1.5368100
H	-10.5390720	-3.2373830	-0.3617740
H	-11.3736540	-4.4963510	1.5935750
H	-10.8458240	-3.7243170	3.8939280
H	-9.4886990	-1.6689790	4.2124820
H	-8.6819100	-0.3971440	2.2543870
H	-11.6243240	-0.2265530	-0.1254320
H	-13.1818480	0.1557540	-2.0050480
H	-12.4141930	-0.1559290	-4.3460480
H	-10.0760040	-0.8711600	-4.7809080
H	-8.5312900	-1.2804900	-2.8973180
H	1.1628990	3.9014530	-2.0593810
H	2.6528210	-0.5328000	0.7493980
H	4.6838890	-1.2647160	0.8802390
H	6.9600010	-2.1180330	0.9427600
H	8.2051580	0.9718920	-1.7680160

H	5.9308100	1.8367070	-1.8339250
H	7.8279560	-3.1075030	-1.6575380
H	8.2515220	-5.5264990	-1.3911380
H	9.9992220	-6.3226110	0.1833130
H	11.3074340	-4.6693820	1.4956000
H	10.8591670	-2.2521270	1.2479810
H	9.3736310	1.1867200	0.9061730
H	11.3000750	2.7224230	0.7184270
H	13.2162910	2.1475230	-0.7529150
H	13.1754210	0.0249000	-2.0407440
H	11.2332160	-1.4939740	-1.8712230

6 ax-|| (ground state, CAM-B3LYP/6-31G*)

-3325.032924530

P	0.0250630	1.9052320	0.9550770
O	0.0203290	0.9795020	2.1294350
S	-3.1510350	1.8622270	-1.9854100
C	0.0471600	3.6716220	1.3881590
C	1.2604220	4.3307720	1.5941970
H	2.1966670	3.8078080	1.4239890
C	1.2770910	5.6553090	2.0125130
H	2.2250660	6.1608760	2.1681340
C	0.0813730	6.3319110	2.2279790
H	0.0946430	7.3680350	2.5523470
C	-1.1313860	5.6819440	2.0261560
H	-2.0661010	6.2083740	2.1924470
C	-1.1488270	4.3574100	1.6078560
H	-2.0983070	3.8553270	1.4483630
C	-1.4012180	1.6824770	-0.1186810
C	-1.5602410	2.2264100	-1.3756930
C	-0.6538760	2.9744130	-2.2171530
H	-1.1289800	3.5746920	-2.9888610
C	-2.5459680	0.9698890	0.3330600
H	-2.5819780	0.4995700	1.3081920
C	-3.5877070	0.9765440	-0.5540820
C	-4.9037890	0.3483030	-0.4097220
C	-5.0666900	-0.7694970	0.4169040
H	-4.2035150	-1.1919410	0.9208680
C	-6.3013670	-1.3735640	0.5746160
H	-6.3966030	-2.2477400	1.2086960
C	-7.4292500	-0.8774780	-0.0896690
C	-7.2743630	0.2386900	-0.9184220
H	-8.1371150	0.6454400	-1.4335980
C	-6.0338810	0.8335230	-1.0756550
H	-5.9511690	1.7136480	-1.7067830

N	-8.6890220	-1.4895140	0.0715130
C	-9.0674370	-2.0275950	1.3295120
C	-9.6913450	-3.2750100	1.4031030
H	-9.8749930	-3.8320600	0.4907400
C	-10.0742040	-3.7936590	2.6328170
H	-10.5591080	-4.7642640	2.6736320
C	-9.8256970	-3.0881320	3.8051750
H	-10.1192530	-3.4996790	4.7654250
C	-9.1971330	-1.8495280	3.7344100
H	-9.0026100	-1.2846440	4.6409890
C	-8.8282830	-1.3152300	2.5070910
H	-8.3505270	-0.3428700	2.4534400
C	-9.5908310	-1.5733470	-1.0209790
C	-10.9476020	-1.2966480	-0.8373830
H	-11.3025750	-1.0072800	0.1458140
C	-11.8319590	-1.3950670	-1.9032230
H	-12.8838640	-1.1782930	-1.7438260
C	-11.3769120	-1.7514270	-3.1680710
H	-12.0694850	-1.8206840	-4.0006580
C	-10.0249390	-2.0192540	-3.3546020
H	-9.6565820	-2.3060640	-4.3348840
C	-9.1371210	-1.9418280	-2.2899570
H	-8.0857950	-2.1658820	-2.4352190
S	3.1718740	1.7949700	-2.0147130
C	1.4354250	1.6506120	-0.1325070
C	1.5949950	2.1926770	-1.3902060
C	0.6971960	2.9602800	-2.2231970
H	1.1779180	3.5505350	-2.9991400
C	2.5681560	0.9116630	0.3075020
H	2.6022230	0.4380830	1.2811790
C	3.6016290	0.8970200	-0.5888420
C	4.9054440	0.2394550	-0.4577620
C	5.0482070	-0.8934480	0.3515030
H	4.1816910	-1.2962030	0.8656040
C	6.2745080	-1.5154450	0.5079200
H	6.3595940	-2.3848850	1.1498540
C	7.4065260	-1.0414430	-0.1648170
C	7.2683730	0.0808840	-0.9879740
H	8.1320320	0.4627800	-1.5204190
C	6.0429400	0.7121910	-1.1199260
H	5.9726510	1.5939520	-1.7501270
N	8.6551780	-1.6806660	-0.0177640
C	8.7267330	-3.0927910	0.1061390
C	7.9614750	-3.9174330	-0.7221450
H	7.3106410	-3.4691410	-1.4651220
C	8.0326790	-5.2979430	-0.5923760

H	7.4302070	-5.9254720	-1.2420620
C	8.8792590	-5.8762440	0.3473310
H	8.9379030	-6.9557700	0.4413330
C	9.6500020	-5.0569200	1.1650650
H	10.3111960	-5.4946280	1.9067580
C	9.5704460	-3.6751460	1.0547920
H	10.1629780	-3.0373720	1.7017770
C	9.8513150	-0.9176960	0.0106790
C	9.9244130	0.2603660	0.7581010
H	9.0571250	0.5884510	1.3208950
C	11.0970640	1.0034640	0.7789210
H	11.1377660	1.9173080	1.3638680
C	12.2171960	0.5756880	0.0742190
H	13.1346540	1.1547590	0.0990440
C	12.1495260	-0.6024750	-0.6615020
H	13.0145880	-0.9460970	-1.2205130
C	10.9747630	-1.3414430	-0.7030560
H	10.9201770	-2.2540150	-1.2867770

6 ax-|| (excited state, CAM-B3LYP/6-31G*)

-3325.019718750

P	0.0076310	1.0078950	0.8774710
O	-0.0013130	-0.2378170	1.7075930
S	-3.2835680	2.0642540	-1.7694320
C	0.0225530	2.5540490	1.8537390
C	1.2320910	3.1047410	2.2844210
H	2.1707180	2.6556180	1.9756030
C	1.2437160	4.2275220	3.1022280
H	2.1902740	4.6473290	3.4285760
C	0.0464400	4.8143020	3.4968240
H	0.0557850	5.6942880	4.1329460
C	-1.1625680	4.2745010	3.0725850
H	-2.0998060	4.7310200	3.3757220
C	-1.1747240	3.1513870	2.2549100
H	-2.1222810	2.7385960	1.9236570
C	-1.4332790	1.1601110	-0.1770500
C	-1.5918160	2.0670980	-1.2560100
C	-0.6812330	2.8592420	-1.9508960
H	-1.1181770	3.5391200	-2.6776620
C	-2.6105510	0.4974290	0.1668220
H	-2.6351680	-0.2246830	0.9741810
C	-3.7264000	0.8513960	-0.5853220
C	-5.0673520	0.3449760	-0.4726410
C	-5.3788770	-0.7096220	0.4127000
H	-4.5918870	-1.1650770	1.0032760

C	-6.6592070	-1.2028790	0.5285450
H	-6.8582050	-2.0251000	1.2062330
C	-7.7110720	-0.6652350	-0.2333370
C	-7.4171380	0.3854550	-1.1165610
H	-8.2134740	0.8247410	-1.7063890
C	-6.1315700	0.8696000	-1.2343940
H	-5.9475920	1.6913250	-1.9197060
N	-9.0152430	-1.1669860	-0.1160420
C	-9.4897110	-1.6556310	1.1303650
C	-10.2035110	-2.8547210	1.1895630
H	-10.3817890	-3.4136660	0.2773200
C	-10.6785790	-3.3236280	2.4067430
H	-11.2316040	-4.2573220	2.4388080
C	-10.4368110	-2.6151730	3.5790190
H	-10.8037820	-2.9880740	4.5297390
C	-9.7208620	-1.4239080	3.5217570
H	-9.5319700	-0.8575800	4.4285160
C	-9.2561620	-0.9392620	2.3067660
H	-8.7098200	-0.0033580	2.2606640
C	-9.8809380	-1.1971800	-1.2413890
C	-11.2118980	-0.7929040	-1.1148820
H	-11.5733430	-0.4451240	-0.1532230
C	-12.0614690	-0.8382140	-2.2118610
H	-13.0937080	-0.5210750	-2.0996780
C	-11.5947910	-1.2706660	-3.4486910
H	-12.2600190	-1.2990090	-4.3055960
C	-10.2678180	-1.6677980	-3.5770130
H	-9.8932170	-2.0153720	-4.5348840
C	-9.4155200	-1.6412480	-2.4816500
H	-8.3849260	-1.9651340	-2.5788970
S	3.3152950	2.0199750	-1.7662080
C	1.4500510	1.1375710	-0.1787460
C	1.6226180	2.0439850	-1.2561800
C	0.7236940	2.8493470	-1.9507500
H	1.1703180	3.5233960	-2.6770560
C	2.6162690	0.4548370	0.1625670
H	2.6264980	-0.2761270	0.9621710
C	3.7380440	0.7932540	-0.5886270
C	5.0701600	0.2637830	-0.4803060
C	5.3867100	-0.7357230	0.4654630
H	4.6167590	-1.1086240	1.1314880
C	6.6603800	-1.2459260	0.5805280
H	6.8695600	-2.0036270	1.3268850
C	7.6977950	-0.7911220	-0.2520720
C	7.3977760	0.2002230	-1.1995520
H	8.1776970	0.5587680	-1.8614380

C	6.1218810	0.7115120	-1.3061010
H	5.9281880	1.4681220	-2.0602000
N	8.9937750	-1.3145820	-0.1398860
C	9.1932640	-2.6745950	0.2180730
C	8.4255890	-3.6819170	-0.3716120
H	7.6748650	-3.4173950	-1.1084720
C	8.6252310	-5.0087390	-0.0156670
H	8.0213940	-5.7816090	-0.4811120
C	9.6002890	-5.3505460	0.9156140
H	9.7577570	-6.3893560	1.1870210
C	10.3720240	-4.3489920	1.4953190
H	11.1327560	-4.6023520	2.2272660
C	10.1680490	-3.0180600	1.1575530
H	10.7619710	-2.2361130	1.6182050
C	10.1266310	-0.4956450	-0.3904960
C	10.1967540	0.7965320	0.1362150
H	9.3776070	1.1700800	0.7411680
C	11.3068750	1.5916850	-0.1133050
H	11.3484170	2.5938040	0.3022570
C	12.3661530	1.1065630	-0.8733270
H	13.2353540	1.7285710	-1.0609430
C	12.3015210	-0.1833940	-1.3894260
H	13.1194470	-0.5720790	-1.9882480
C	11.1880760	-0.9797090	-1.1585620
H	11.1334050	-1.9814840	-1.5706130

6 eq (ground state, CAM-B3LYP/6-31G*)

-3325.032956840			
C	-11.2421280	-0.1259640	-0.6897070
C	-10.0508770	0.0469620	0.0187900
C	-9.9712310	-0.4072690	1.3375410
C	-11.0607210	-1.0329790	1.9284930
C	-12.2486780	-1.1971060	1.2242460
C	-12.3332350	-0.7354390	-0.0848390
N	-8.9395320	0.6832640	-0.5932400
C	-9.1459410	1.8548430	-1.3667360
C	-8.5006890	2.0172760	-2.5952410
C	-8.7043140	3.1678170	-3.3452840
C	-9.5661480	4.1618270	-2.8942890
C	-10.2175540	3.9968610	-1.6766870
C	-10.0047920	2.8580390	-0.9115570
C	-7.6404150	0.1591170	-0.4278040
C	-6.5352610	1.0079530	-0.3000740
C	-5.2610970	0.4892580	-0.1473780
C	-5.0399770	-0.8911620	-0.0884820

C	-6.1502010	-1.7328210	-0.2107650
C	-7.4250350	-1.2223020	-0.3881300
C	-3.6859830	-1.4199720	0.1033360
S	-3.2155210	-2.9727720	-0.5149540
C	-1.5945400	-2.8210140	0.1076580
C	-1.4410730	-1.6124750	0.7602750
C	-2.6347400	-0.8315000	0.7475640
P	-0.0192830	-1.1569000	1.7663640
C	1.4194030	-1.6195560	0.7879000
C	1.5792770	-2.8288090	0.1379990
S	3.2110630	-2.9881580	-0.4540450
C	3.6771330	-1.4380030	0.1735890
C	2.6167500	-0.8443630	0.7981330
C	0.6675760	-3.9110740	-0.1313190
C	-0.6831920	-3.9077770	-0.1443530
C	5.0359490	-0.9151510	0.0060460
C	5.2630580	0.4646050	-0.0494840
C	6.5393890	0.9784240	-0.1968720
C	7.6457660	0.1259180	-0.2898650
C	7.4264600	-1.2546500	-0.2368480
C	6.1452160	-1.7605960	-0.0969070
N	8.9474140	0.6469540	-0.4359530
C	9.9052720	-0.0294720	-1.2358120
C	11.2155790	-0.1910170	-0.7799830
C	12.1555520	-0.8397830	-1.5695140
C	11.8009250	-1.3517550	-2.8129130
C	10.4945570	-1.1988390	-3.2649980
C	9.5534670	-0.5344510	-2.4899250
C	-0.0148720	0.6628060	1.7616440
O	-0.0341450	-1.7050280	3.1566960
C	9.3178400	1.8463060	0.2266770
C	10.0577940	2.8219020	-0.4453610
C	10.4336250	3.9879950	0.2079080
C	10.0635440	4.2073170	1.5303880
C	9.3197400	3.2406010	2.1985420
C	8.9561000	2.0633430	1.5584600
H	1.1412670	-4.8462550	-0.4180640
H	2.6929080	0.1136520	1.2972880
H	4.4198220	1.1466480	-0.0083440
H	6.6859770	2.0511260	-0.2531690
H	8.2703360	-1.9325720	-0.2950850
H	6.0098580	-2.8362540	-0.0326120
H	10.3373420	2.6577520	-1.4804560
H	11.0101150	4.7361250	-0.3276830
H	10.3528690	5.1228660	2.0360660
H	9.0301070	3.3948940	3.2335100

H	8.3884640	1.3048070	2.0866320
H	11.4907290	0.1968420	0.1948220
H	13.1703870	-0.9565820	-1.2016500
H	12.5360080	-1.8649040	-3.4244500
H	10.2054590	-1.5871740	-4.2368470
H	8.5389780	-0.4036900	-2.8509760
H	-1.1559110	-4.8405910	-0.4402490
H	-2.7149360	0.1274830	1.2442540
H	-4.4184380	1.1692480	-0.0751270
H	-6.6804240	2.0818800	-0.3305110
H	-8.2673980	-1.8973390	-0.4881610
H	-6.0179620	-2.8095440	-0.1607970
H	-7.8394200	1.2369010	-2.9563260
H	-8.1946820	3.2794720	-4.2975150
H	-9.7292160	5.0563050	-3.4867160
H	-10.8893360	4.7668670	-1.3096750
H	-10.5049320	2.7366690	0.0431880
H	-9.0507790	-0.2682580	1.8943360
H	-10.9823010	-1.3818780	2.9536520
H	-13.1008550	-1.6798190	1.6915890
H	-13.2526820	-0.8612620	-0.6484740
H	-11.3063350	0.2226360	-1.7148050
C	-0.0260230	1.3083780	2.9970390
C	-0.0236380	2.6986020	3.0575630
C	-0.0102020	3.4454280	1.8857210
C	0.0009520	2.8051920	0.6486350
C	-0.0013550	1.4181440	0.5859710
H	-0.0365750	0.7054750	3.8996100
H	-0.0324240	3.1977700	4.0215320
H	-0.0084140	4.5302630	1.9332650
H	0.0114630	3.3890070	-0.2666470
H	0.0074020	0.9208170	-0.3800490

6 eq (excited state, CAM-B3LYP/6-31G*)

-3325.020768920			
C	-11.3816070	-0.5157730	-0.7270260
C	-10.2604500	-0.4286400	0.1014720
C	-10.2015900	-1.2097950	1.2582870
C	-11.2445340	-2.0707080	1.5713730
C	-12.3634940	-2.1524040	0.7489280
C	-12.4270990	-1.3675280	-0.3975760
N	-9.1966620	0.4536560	-0.2262780
C	-9.5036110	1.7707590	-0.6585430
C	-8.8386640	2.3306690	-1.7524280
C	-9.1436480	3.6194370	-2.1683760

C	-10.1232090	4.3593060	-1.5140840
C	-10.7925400	3.7987800	-0.4312570
C	-10.4828940	2.5168130	0.0016710
C	-7.8642700	0.0293040	-0.1237260
C	-6.8463620	0.9252840	0.2477310
C	-5.5384320	0.5073270	0.3469510
C	-5.1643060	-0.8301630	0.0899230
C	-6.1976890	-1.7174150	-0.2778900
C	-7.5077270	-1.3031440	-0.3860510
C	-3.7984290	-1.2612350	0.2015730
S	-3.3231240	-2.9267740	-0.0385610
C	-1.6166600	-2.5712500	0.2568610
C	-1.4643520	-1.1872130	0.5349420
C	-2.6770470	-0.4947470	0.4998440
P	-0.0051780	-0.3509480	1.1733380
C	1.4519070	-1.1958650	0.5420210
C	1.5978420	-2.5818850	0.2708010
S	3.3036100	-2.9481300	-0.0149290
C	3.7878040	-1.2856500	0.2274640
C	2.6691340	-0.5108390	0.5131470
C	0.6880840	-3.6286430	0.1681830
C	-0.7129570	-3.6237460	0.1603360
C	5.1580140	-0.8643380	0.1321200
C	5.5174950	0.4984220	0.2235540
C	6.8287050	0.9086030	0.1345320
C	7.8656280	-0.0232840	-0.0467290
C	7.5242560	-1.3819940	-0.1388810
C	6.2091810	-1.7860950	-0.0562950
N	9.2018890	0.3932890	-0.1341190
C	10.1184340	-0.2997110	-0.9683920
C	11.3999010	-0.6058400	-0.5044800
C	12.2985370	-1.2711400	-1.3272490
C	11.9297630	-1.6525410	-2.6130590
C	10.6517850	-1.3533410	-3.0737330
C	9.7520870	-0.6742880	-2.2636760
C	0.0023280	1.2579640	0.3170060
O	-0.0089360	-0.1629960	2.6602330
C	9.6593650	1.5080770	0.6169890
C	10.4910750	2.4615390	0.0248050
C	10.9486770	3.5431010	0.7648820
C	10.5733390	3.6978860	2.0952670
C	9.7401770	2.7522140	2.6839480
C	9.2909720	1.6587660	1.9563450
H	1.1288360	-4.6099380	0.0135690
H	2.7378370	0.5497710	0.7229410
H	4.7463730	1.2509310	0.3452010

H	7.0665140	1.9645390	0.1940250
H	8.3070510	-2.1210840	-0.2654400
H	5.9881940	-2.8474070	-0.1144150
H	10.7747380	2.3479740	-1.0158580
H	11.5944470	4.2767900	0.2922410
H	10.9279040	4.5480300	2.6689660
H	9.4462310	2.8567100	3.7237890
H	8.6535570	0.9141100	2.4206540
H	11.6842230	-0.3187190	0.5020230
H	13.2911870	-1.5032990	-0.9538700
H	12.6327720	-2.1780280	-3.2512050
H	10.3539790	-1.6383340	-4.0781020
H	8.7606100	-0.4288710	-2.6287170
H	-1.1587050	-4.6017620	-0.0006450
H	-2.7379040	0.5685710	0.6977260
H	-4.7871290	1.2267820	0.6526660
H	-7.0989620	1.9557200	0.4700080
H	-8.2722180	-2.0106690	-0.6860410
H	-5.9617340	-2.7530440	-0.5022860
H	-8.0851940	1.7488170	-2.2722170
H	-8.6194350	4.0420820	-3.0199960
H	-10.3634390	5.3641820	-1.8459110
H	-11.5554740	4.3676190	0.0912530
H	-10.9971250	2.0848680	0.8532910
H	-9.3356940	-1.1360330	1.9073390
H	-11.1860910	-2.6718990	2.4734500
H	-13.1797510	-2.8218700	1.0002000
H	-13.2926910	-1.4258580	-1.0502800
H	-11.4266710	0.0874680	-1.6273240
C	0.0057080	2.4108840	1.1001520
C	0.0124520	3.6653040	0.4961420
C	0.0158770	3.7690560	-0.8892620
C	0.0124770	2.6190340	-1.6762550
C	0.0057250	1.3679610	-1.0757760
H	0.0030720	2.3055770	2.1806590
H	0.0150940	4.5611090	1.1097120
H	0.0212430	4.7472730	-1.3608350
H	0.0151520	2.7005700	-2.7588900
H	0.0030690	0.4717370	-1.6900160

8 ax- $\perp$ (ground state, CAM-B3LYP/6-31G*)

-3012.314275460			
C	-2.9130790	-2.3615250	-1.9381330
C	-3.7247650	-1.3974060	-1.2316390
C	-1.5723860	-2.5234560	-1.9115090

C	-0.5747160	-1.7933490	-1.1655920
C	-0.6479990	-0.9822750	-0.0511000
P	-2.0709910	-0.6422660	0.9984240
C	-3.4869170	-0.6184420	-0.1175210
S	1.0702970	-1.8719700	-1.7370690
C	1.6391380	-0.7833850	-0.5108850
C	0.6037510	-0.4066600	0.3009530
S	-5.3054690	-1.0556670	-1.8782810
C	-5.6302280	0.1432010	-0.6650840
C	-4.5656150	0.2578650	0.1846150
C	-6.8933810	0.8863370	-0.6292500
H	-4.5335350	0.9319020	1.0318760
H	0.7033700	0.2918180	1.1226380
O	-1.9384550	0.6301040	1.7721710
C	-2.2786170	-2.0663810	2.1075210
C	-2.3289230	-1.8005900	3.4758990
C	-2.4888780	-2.8424450	4.3828790
C	-2.5986620	-4.1502060	3.9260110
C	-2.5481990	-4.4198600	2.5608660
C	-2.3882870	-3.3825340	1.6524190
H	-2.2391340	-0.7727340	3.8118780
H	-2.5270150	-2.6317900	5.4471120
H	-2.7231880	-4.9641160	4.6338520
H	-2.6327130	-5.4419460	2.2049180
H	-2.3486540	-3.6013170	0.5899440
H	-1.1746700	-3.2763540	-2.5874220
H	-3.4566480	-2.9999990	-2.6294060
C	-8.0679960	0.3562580	-1.1786690
C	-9.2578620	1.0630010	-1.1340060
C	-9.2703890	2.3092080	-0.5265780
C	-8.1270350	2.8661260	0.0281220
C	-6.9422070	2.1537880	-0.0321440
H	-8.0558460	-0.6299330	-1.6311200
H	-10.1727850	0.6633960	-1.5516140
N	-10.5258070	3.0602120	-0.4718590
H	-8.1781460	3.8458180	0.4851130
H	-6.0366360	2.5915090	0.3723260
O	-10.5091470	4.1545870	0.0716900
O	-11.5160230	2.5478450	-0.9727580
C	3.0464990	-0.3843220	-0.4269300
C	3.8840510	-0.3827570	-1.5469880
C	5.2069890	0.0150480	-1.4574890
C	5.7484550	0.4204090	-0.2325000
C	4.9183230	0.4121380	0.8952210
C	3.5955770	0.0201000	0.7953770
H	3.4874220	-0.6654840	-2.5177500

H	5.8279530	0.0247180	-2.3458790
N	7.0935320	0.8252780	-0.1343670
H	5.3218680	0.7055870	1.8575470
H	2.9830010	-0.0020150	1.6907790
C	7.4668090	1.8635720	0.7601130
C	8.0909650	0.2088540	-0.9350420
C	8.1240490	-1.1797160	-1.0841210
C	9.1015880	-1.7750440	-1.8701800
C	10.0694070	-1.0003750	-2.5006490
C	10.0445410	0.3811750	-2.3438130
C	9.0589930	0.9858140	-1.5750190
H	7.3793010	-1.7871460	-0.5810800
H	9.1136550	-2.8554230	-1.9774170
H	10.8367940	-1.4694010	-3.1079020
H	10.7911540	0.9985640	-2.8339160
H	9.0342790	2.0643440	-1.4628200
C	8.6057490	1.7292500	1.5569310
C	8.9796800	2.7512800	2.4192140
C	8.2167670	3.9102710	2.5129160
C	7.0780360	4.0423280	1.7255100
C	6.7079440	3.0330360	0.8467240
H	9.1950580	0.8209210	1.4925300
H	9.8684460	2.6331480	3.0315270
H	8.5074540	4.7041900	3.1932170
H	6.4772590	4.9448060	1.7833500
H	5.8275020	3.1444320	0.2230070

8 ax- $\perp$ (excited state, CAM-B3LYP/6-31G*)

-3012.302768670			
C	-2.9179390	-2.2420010	-1.9696490
C	-3.7430040	-1.3426130	-1.2900430
C	-1.5255090	-2.4006490	-1.9607160
C	-0.5442990	-1.6875630	-1.2723690
C	-0.6211220	-0.7156150	-0.2410070
P	-2.0371500	-0.2891760	0.7831260
C	-3.4973460	-0.4168190	-0.2486630
S	1.1425860	-1.9085750	-1.7457800
C	1.6982900	-0.6852010	-0.6221300
C	0.6147110	-0.1681620	0.0879160
S	-5.4292150	-1.2143130	-1.7939880
C	-5.7561870	0.0713530	-0.6562910
C	-4.6133910	0.3563760	0.0766900
C	-7.0550200	0.6926770	-0.5506380
H	-4.5715550	1.1090610	0.8544420
H	0.7053350	0.6002970	0.8457380

O	-1.8843710	1.0425600	1.4472040
C	-2.1733560	-1.6328140	2.0043740
C	-2.0899020	-1.2719190	3.3496750
C	-2.1845940	-2.2442460	4.3390350
C	-2.3621210	-3.5777850	3.9899050
C	-2.4468910	-3.9409730	2.6483990
C	-2.3539280	-2.9741050	1.6566550
H	-1.9539900	-0.2254920	3.6026470
H	-2.1212760	-1.9583330	5.3845230
H	-2.4368930	-4.3369600	4.7625780
H	-2.5882650	-4.9820640	2.3747960
H	-2.4255600	-3.2666340	0.6138090
H	-1.1560890	-3.1445590	-2.6611830
H	-3.4291510	-2.8867300	-2.6800710
C	-8.1635750	0.2085950	-1.2758200
C	-9.4054430	0.8009300	-1.1696150
C	-9.5611570	1.8982990	-0.3300480
C	-8.4916980	2.4083350	0.4011000
C	-7.2545380	1.8104620	0.2881730
H	-8.0486530	-0.6515740	-1.9272170
H	-10.2591670	0.4307770	-1.7223430
N	-10.8653980	2.5263950	-0.2152370
H	-8.6489930	3.2665190	1.0414870
H	-6.4230180	2.2184050	0.8505270
O	-10.9727000	3.4907600	0.5338400
O	-11.7875970	2.0576660	-0.8731280
C	3.0782180	-0.3239700	-0.5076300
C	4.0805860	-0.9367330	-1.2929530
C	5.4067020	-0.5911780	-1.1762590
C	5.8154820	0.3990580	-0.2621970
C	4.8259930	1.0214790	0.5262860
C	3.5036570	0.6697700	0.4051920
H	3.8042010	-1.6915340	-2.0225260
H	6.1447820	-1.0728840	-1.8063460
N	7.1560090	0.7548190	-0.1411140
H	5.1158840	1.7764430	1.2472460
H	2.7762840	1.1623090	1.0401690
C	7.5279080	2.0700200	0.2570950
C	8.1881940	-0.1865220	-0.4130890
C	8.1279360	-1.4748950	0.1224240
C	9.1421300	-2.3848700	-0.1429320
C	10.2303120	-2.0175150	-0.9278280
C	10.2948550	-0.7305640	-1.4518190
C	9.2784500	0.1816410	-1.2032310
H	7.2870080	-1.7547430	0.7479640
H	9.0866960	-3.3834110	0.2790260

H	11.0243470	-2.7293990	-1.1281680
H	11.1378920	-0.4349780	-2.0683330
H	9.3221290	1.1827150	-1.6183620
C	8.5047980	2.2525520	1.2372630
C	8.8801380	3.5353400	1.6121440
C	8.2800780	4.6447570	1.0254640
C	7.3044020	4.4621790	0.0508780
C	6.9329420	3.1830810	-0.3404570
H	8.9640510	1.3860000	1.7005320
H	9.6396810	3.6671930	2.3762590
H	8.5721370	5.6459870	1.3248300
H	6.8363080	5.3210190	-0.4196630
H	6.1836850	3.0388850	-1.1115390

8 ax-|| (ground state, CAM-B3LYP/6-31G*)

-3012.312946670			
P	-2.1145160	-1.0725230	1.0994360
C	-0.6773310	-1.1417770	0.0196780
C	-0.6096700	-1.7898670	-1.1959240
C	-1.6193770	-2.4599660	-1.9841200
C	-2.9553100	-2.2613070	-1.9973950
C	-3.7286950	-1.3114990	-1.2283360
C	-3.4805460	-0.7044890	-0.0151910
C	-2.3885110	-2.7762440	1.6699140
C	-1.3066520	-3.6266260	1.9045040
C	-3.6803740	-3.2157190	1.9661130
C	-3.8867860	-4.4863980	2.4873550
C	-2.8037380	-5.3282890	2.7168240
C	-1.5140610	-4.8975210	2.4260130
C	-4.4853140	0.2296510	0.3564700
C	-5.5095930	0.3258390	-0.5450340
S	-5.2313790	-0.7381250	-1.8915400
C	0.5588420	-0.5620220	0.4154600
C	1.5798070	-0.7778750	-0.4708310
S	1.0136640	-1.7136630	-1.8215170
O	-1.9823240	-0.0611620	2.1923760
C	2.9744630	-0.3382530	-0.3738350
C	3.7706490	-0.1475320	-1.5078690
C	5.0837940	0.2777330	-1.4036430
C	5.6579540	0.5207200	-0.1508400
C	4.8683590	0.3274660	0.9893270
C	3.5545070	-0.0907130	0.8756180
C	-6.7020680	1.1749150	-0.4667220
C	-7.8835080	0.8372420	-1.1398110
C	-9.0067450	1.6424150	-1.0566640

C	-8.9463000	2.7928140	-0.2851800
C	-7.7943840	3.1589790	0.3960920
C	-6.6755270	2.3508100	0.2962190
N	-10.1315780	3.6466270	-0.1890600
O	-11.1304690	3.3019400	-0.8033870
N	6.9958450	0.9453570	-0.0400770
C	7.9776260	0.4719280	-0.9502760
C	8.0357330	-0.8812460	-1.2920720
C	8.9976810	-1.3361190	-2.1840210
C	9.9254040	-0.4561460	-2.7310320
C	9.8760200	0.8893090	-2.3827590
C	8.9053590	1.3554550	-1.5061480
O	-10.0519950	4.6527630	0.4999250
C	7.3826180	1.8443870	0.9891290
C	8.5511560	1.6163150	1.7189700
C	8.9379160	2.5038160	2.7142460
C	8.1591170	3.6177760	3.0082040
C	6.9910010	3.8421740	2.2874560
C	6.6073400	2.9699100	1.2775180
H	-4.4377520	0.7788210	1.2892200
H	0.6582290	0.0129270	1.3280700
H	-0.2979300	-3.2962720	1.6762980
H	-0.6674140	-5.5532510	2.6034820
H	-2.9655690	-6.3224200	3.1221190
H	-4.8944940	-4.8209060	2.7129990
H	-4.5298680	-2.5636110	1.7863220
H	-1.2382010	-3.1748450	-2.7090970
H	-3.5188670	-2.8352640	-2.7281390
H	-7.9309220	-0.0765190	-1.7231150
H	-9.9259630	1.3910960	-1.5695360
H	-7.7866920	4.0696540	0.9807870
H	-5.7615610	2.6422180	0.8011880
H	3.3480440	-0.3025140	-2.4963030
H	5.6721510	0.4341680	-2.3004600
H	5.2968200	0.4954050	1.9707590
H	2.9752330	-0.2591230	1.7776660
H	7.3223950	-1.5718560	-0.8551670
H	9.0295930	-2.3905410	-2.4409910
H	10.6809460	-0.8160300	-3.4218850
H	10.5912980	1.5880130	-2.8058320
H	8.8609570	2.4070060	-1.2439170
H	9.1534990	0.7415000	1.4989400
H	9.8497290	2.3140310	3.2722570
H	8.4600370	4.3057120	3.7916470
H	6.3772380	4.7117920	2.5014600
H	5.7035560	3.1547750	0.7068180

8 ax-|| (excited state, CAM-B3LYP/6-31G*)

-3012.300423790

P	-2.0480190	-0.4963010	0.8831530
C	-0.6245870	-0.7692620	-0.1798100
C	-0.5489790	-1.6570260	-1.2842820
C	-1.5356370	-2.3301690	-2.0038320
C	-2.9258410	-2.1499010	-2.0111920
C	-3.7372620	-1.2648120	-1.2990330
C	-3.4837830	-0.4280350	-0.1857940
C	-2.2284870	-2.0638180	1.8020160
C	-1.0968940	-2.7529270	2.2458670
C	-3.4942080	-2.5430320	2.1477370
C	-3.6251450	-3.6876190	2.9241430
C	-2.4931930	-4.3659950	3.3615310
C	-1.2287870	-3.8968540	3.0223170
C	-4.5738140	0.3661430	0.1707160
C	-5.7081660	0.1850820	-0.6105290
S	-5.4009000	-1.0250220	-1.8354240
C	0.6055650	-0.2289000	0.1777020
C	1.6876190	-0.6707660	-0.5864250
S	1.1334320	-1.8104160	-1.7968110
O	-1.8895930	0.7137360	1.7484240
C	3.0628700	-0.2950160	-0.4648750
C	4.0578530	-0.8042050	-1.3297960
C	5.3793320	-0.4428000	-1.2088940
C	5.7913900	0.4588670	-0.2085250
C	4.8095100	0.9757410	0.6617690
C	3.4914650	0.6102400	0.5346580
C	-6.9828690	0.8496480	-0.4898860
C	-8.0914200	0.4638610	-1.2728140
C	-9.3115610	1.0964040	-1.1513440
C	-9.4463420	2.1363830	-0.2378230
C	-8.3761730	2.5494060	0.5517400
C	-7.1604510	1.9124270	0.4231090
N	-10.7274520	2.8057700	-0.1065390
O	-11.6502600	2.4231730	-0.8176450
N	7.1268490	0.8311280	-0.0827840
C	8.1715530	-0.0493660	-0.4816730
C	8.1548010	-1.3893400	-0.0888480
C	9.1810030	-2.2395140	-0.4777800
C	10.2385250	-1.7619770	-1.2450810
C	10.2601930	-0.4243620	-1.6262210
C	9.2312530	0.4297330	-1.2535980
O	-10.8170640	3.7168980	0.7089500

C	7.4821330	2.1047340	0.4455180
C	8.4788150	2.2029050	1.4176780
C	8.8384200	3.4461960	1.9195260
C	8.2029630	4.5985240	1.4684970
C	7.2077480	4.4997480	0.5016100
C	6.8515890	3.2618840	-0.0162440
H	-4.5230510	1.0513650	1.0082160
H	0.6931480	0.4769660	0.9948050
H	-0.1064740	-2.3957620	1.9814570
H	-0.3425560	-4.4250440	3.3601500
H	-2.5963020	-5.2622020	3.9656920
H	-4.6139350	-4.0512700	3.1856270
H	-4.3826080	-2.0208950	1.8073520
H	-1.1731220	-3.0373450	-2.7447650
H	-3.4416000	-2.7451350	-2.7604770
H	-7.9934730	-0.3514130	-1.9821880
H	-10.1648390	0.8013970	-1.7482360
H	-8.5163630	3.3653460	1.2488370
H	-6.3280440	2.2464380	1.0312200
H	3.7781170	-1.4858950	-2.1269220
H	6.1104520	-0.8413800	-1.9019950
H	5.1023770	1.6589880	1.4498570
H	2.7706860	1.0191960	1.2334070
H	7.3378390	-1.7561150	0.5233380
H	9.1594070	-3.2790990	-0.1662910
H	11.0421160	-2.4278530	-1.5421390
H	11.0791340	-0.0424040	-2.2275560
H	9.2415730	1.4709020	-1.5572800
H	8.9658430	1.3019590	1.7748260
H	9.6136520	3.5122500	2.6763620
H	8.4827090	5.5682220	1.8669870
H	6.7119020	5.3934850	0.1362510
H	6.0867370	3.1847120	-0.7816480

8 eq (ground state, CAM-B3LYP/6-31G*)

-3012.313029700			
C	6.6340670	2.6576260	-0.9531570
C	7.4136550	1.6744220	-0.3390940
C	8.5718760	2.0518450	0.3440610
C	8.9434430	3.3882920	0.4046820
C	8.1600430	4.3671650	-0.1969620
C	7.0025480	3.9937890	-0.8715260
N	7.0416140	0.3064850	-0.4154240
C	8.0373300	-0.6691820	-0.6871950
C	8.0911770	-1.8528330	0.0524080

C	9.0657190	-2.8034040	-0.2205990
C	10.0097860	-2.5803390	-1.2172520
C	9.9643580	-1.3971680	-1.9466650
C	8.9812220	-0.4500500	-1.6927770
C	5.7023210	-0.0810490	-0.2167170
C	5.1515280	-1.1505700	-0.9312940
C	3.8365310	-1.5324990	-0.7276950
C	3.0162400	-0.8615840	0.1850340
C	3.5741720	0.2065000	0.8968800
C	4.8893820	0.5903930	0.7046610
C	1.6185320	-1.2476880	0.3988510
S	1.0714930	-2.8733170	0.1368410
C	-0.5674310	-2.4814110	0.5799880
C	-0.6639700	-1.1488170	0.9349000
C	0.5814750	-0.4643420	0.8234280
C	-1.5419100	-3.5403150	0.5138880
C	-2.8879260	-3.4657980	0.4332990
C	-3.7307610	-2.2978540	0.3823850
C	-3.5143740	-0.9816460	0.7457700
C	-4.6454980	-0.1552820	0.4828940
C	-5.7082690	-0.8150650	-0.0662850
S	-5.3308540	-2.4962310	-0.2753050
P	-2.1045750	-0.3854770	1.6979680
O	-2.2192160	-0.5970550	3.1724480
C	-7.0099650	-0.2593200	-0.4478570
C	-8.1593310	-1.0590530	-0.4925570
C	-9.3859410	-0.5249580	-0.8496340
C	-9.4611930	0.8247900	-1.1574560
C	-8.3449100	1.6479430	-1.1229160
C	-7.1233200	1.0992280	-0.7747390
N	-10.7548080	1.3973940	-1.5341280
O	-11.7204000	0.6488570	-1.5621740
C	-1.9826730	1.3792660	1.2763640
O	-10.7917770	2.5901220	-1.7984280
H	-4.6727770	0.8971100	0.7368200
H	0.6944300	0.5903680	1.0407480
H	-1.1227530	-4.5421770	0.4686290
H	-3.4110500	-4.4129830	0.3341870
H	-8.0971830	-2.1091410	-0.2265990
H	-10.2815960	-1.1313710	-0.8849670
H	-8.4459350	2.6946810	-1.3785440
H	-6.2390930	1.7265670	-0.7737020
H	3.4319910	-2.3510150	-1.3158880
H	5.7597820	-1.6777230	-1.6573150
H	5.3016030	1.4095160	1.2827290
H	2.9773190	0.7236250	1.6411840

H	7.3653090	-2.0221480	0.8405350
H	9.0944160	-3.7192080	0.3618660
H	10.7749940	-3.3218010	-1.4229510
H	10.6924290	-1.2121360	-2.7305450
H	8.9395270	0.4674320	-2.2699030
H	9.1780260	1.2910140	0.8237440
H	9.8471380	3.6659120	0.9385790
H	8.4493960	5.4115800	-0.1414970
H	6.3856390	4.7466410	-1.3526770
H	5.7390090	2.3674080	-1.4928240
C	-2.0303510	2.2934480	2.3279400
C	-1.9495950	3.6581890	2.0690830
C	-1.8207720	4.1112050	0.7615870
C	-1.7717550	3.2018130	-0.2924490
C	-1.8525820	1.8394630	-0.0368380
H	-2.1305840	1.9175870	3.3412930
H	-1.9870910	4.3672840	2.8901130
H	-1.7574270	5.1762520	0.5600710
H	-1.6690590	3.5563710	-1.3133330
H	-1.8118340	1.1318200	-0.8604020

8 eq (excited state, CAM-B3LYP/6-31G*)

-3012.301269740

C	6.9578830	2.3873960	-1.3678890
C	7.5415540	1.6331650	-0.3476640
C	8.5151410	2.2122150	0.4681890
C	8.8979470	3.5305080	0.2624330
C	8.3093320	4.2859650	-0.7465850
C	7.3374090	3.7091270	-1.5576150
N	7.1610680	0.2763840	-0.1488840
C	8.1856260	-0.6961560	0.0249610
C	8.1021350	-1.6315080	1.0586430
C	9.1069910	-2.5748770	1.2235220
C	10.2085530	-2.5860670	0.3740130
C	10.2963660	-1.6466580	-0.6482050
C	9.2897320	-0.7080790	-0.8291310
C	5.8185440	-0.0910140	-0.1216370
C	5.4091870	-1.3755570	-0.5299310
C	4.0827510	-1.7354800	-0.4965450
C	3.0778530	-0.8438370	-0.0551270
C	3.5041910	0.4443520	0.3481930
C	4.8274280	0.8111600	0.3173890
C	1.6993860	-1.2213620	-0.0114750
S	1.1481320	-2.8109910	-0.4870780
C	-0.5375020	-2.4189330	-0.1380250

C	-0.6294320	-1.0842970	0.3400110
C	0.6100960	-0.4506740	0.3982960
C	-1.4954080	-3.3973350	-0.3909350
C	-2.8912340	-3.3121560	-0.4088110
C	-3.7462940	-2.2381460	-0.1664850
C	-3.5330090	-0.9304030	0.3353250
C	-4.7058090	-0.1720270	0.3806210
C	-5.8498880	-0.8176820	-0.0694230
S	-5.4524250	-2.4443400	-0.5634710
P	-2.0497830	-0.3163190	1.1441090
O	-2.0451950	-0.4711740	2.6335140
C	-7.1911930	-0.2956150	-0.1456280
C	-8.2761780	-1.1099190	-0.5362390
C	-9.5598160	-0.6106830	-0.6089430
C	-9.7866350	0.7245850	-0.2902840
C	-8.7435220	1.5616310	0.0996090
C	-7.4640310	1.0547450	0.1681980
N	-11.1333980	1.2553750	-0.3676390
O	-12.0310290	0.4959430	-0.7174480
C	-1.9533100	1.4347560	0.6589050
O	-11.3024060	2.4358500	-0.0795420
H	-4.7220540	0.8417470	0.7613310
H	0.7206650	0.5661000	0.7542950
H	-1.1029320	-4.3668610	-0.6847550
H	-3.3843240	-4.2293720	-0.7202760
H	-8.1069810	-2.1537960	-0.7793820
H	-10.3939510	-1.2330240	-0.9060480
H	-8.9563380	2.5955100	0.3386640
H	-6.6566860	1.7143300	0.4637640
H	3.8072690	-2.7297800	-0.8337620
H	6.1486300	-2.0820450	-0.8876620
H	5.1177310	1.8001070	0.6513630
H	2.7771930	1.1621200	0.7104540
H	7.2504170	-1.6112680	1.7301050
H	9.0334760	-3.2969180	2.0306070
H	10.9951210	-3.3211710	0.5093440
H	11.1502220	-1.6489860	-1.3183410
H	9.3515530	0.0192890	-1.6313270
H	8.9654420	1.6242380	1.2605670
H	9.6546040	3.9724830	0.9029430
H	8.6077920	5.3176420	-0.9013350
H	6.8790120	4.2867930	-2.3540930
H	6.2118030	1.9308640	-2.0094710
C	-1.8941560	2.3867760	1.6755850
C	-1.8241640	3.7406540	1.3593630
C	-1.8133940	4.1437000	0.0297180

C	-1.8724770	3.1954510	-0.9895650
C	-1.9423970	1.8451190	-0.6767900
H	-1.9065210	2.0497070	2.7074780
H	-1.7804720	4.4797800	2.1532960
H	-1.7610880	5.1998590	-0.2169610
H	-1.8665470	3.5116320	-2.0280640
H	-1.9918030	1.1067720	-1.4723790

2 ax- $\perp$ (ground state, M06-2X/6-31G*)

-1828.891967840

S	3.2294770	-1.9867610	-0.6109650
C	3.6589910	-1.2153170	0.8620710
C	2.6154460	-0.5165020	1.3896800
C	1.4359700	-0.5950000	0.5887390
C	1.5998340	-1.3780390	-0.5374020
P	-0.0029990	0.3657060	1.0903810
C	-0.0168040	1.8695080	0.0728800
C	0.6916800	-1.7859670	-1.5905650
C	-0.6593980	-1.7981120	-1.5903460
C	-1.5744710	-1.4068430	-0.5368120
C	-1.4246910	-0.6208330	0.5892290
C	-2.6053340	-0.5635170	1.3902840
C	-3.6362630	-1.2807780	0.8626420
S	-3.1930310	-2.0444700	-0.6104930
O	-0.0057030	0.6959750	2.5483060
H	-2.6516330	-0.0050340	2.3179120
H	-4.6333670	-1.4058690	1.2615540
H	-1.1328170	-2.2074630	-2.4799390
H	2.6518260	0.0430060	2.3171340
H	4.6581130	-1.3226990	1.2610750
H	1.1723520	-2.1865880	-2.4802480
C	-0.0276130	3.0924910	0.7450110
C	-0.0386920	4.2817850	0.0195990
C	-0.0390430	4.2472560	-1.3718350
C	-0.0284000	3.0251630	-2.0439010
C	-0.0173630	1.8356720	-1.3245340
H	-0.0269640	3.0912470	1.8313820
H	-0.0472610	5.2340420	0.5409910
H	-0.0478750	5.1741970	-1.9374620
H	-0.0289360	3.0017290	-3.1292930
H	-0.0090670	0.8839540	-1.8503900

2 TS1 (ground state, M06-2X/6-31G*)

	-1828.8878634		
C	0.5308020	1.4639550	0.4515950
C	1.7265070	1.6068410	-0.2253220
C	2.6968920	0.6726650	-0.7506680
C	2.6960250	-0.6760120	-0.7506960
C	1.7244650	-1.6089670	-0.2253530
C	0.5289760	-1.4645810	0.4516290
P	-0.3451700	0.0002380	1.0279820
S	2.0785380	-3.2981590	-0.4727430
C	0.6410580	-3.7902330	0.3246990
C	-0.0796050	-2.7226500	0.7625930
S	2.0826940	3.2955840	-0.4727190
C	0.6457700	3.7894660	0.3246100
C	-0.0762410	2.7227860	0.7624870
C	-1.8818090	0.0011720	0.0551260
C	-3.0946300	0.0019040	0.7441000
C	-4.2938850	0.0026040	0.0342030
C	-4.2777350	0.0025720	-1.3577940
C	-3.0649070	0.0018450	-2.0473190
C	-1.8670260	0.0011450	-1.3422260
O	-0.6413160	0.0004420	2.4919460
H	-3.0779570	0.0019120	1.8308020
H	-5.2395410	0.0031770	0.5676830
H	-5.2123880	0.0031170	-1.9106490
H	-3.0564540	0.0018240	-3.1329100
H	-0.9180120	0.0005650	-1.8755360
H	-1.0132890	2.8075650	1.3019860

H	0.4134820	4.8398610	0.4323160
H	3.5576380	1.1400130	-1.2230640
H	-1.0167130	-2.8062560	1.3021720
H	0.4074700	-4.8403360	0.4324410
H	3.5561650	-1.1444430	-1.2231220

2 TS2 (ground state, M06-2X/6-31G*)

-1828.89101871			
P	-0.0919270	0.2260290	1.1969150
C	1.5772070	-0.1516090	0.6480010
C	1.9415290	-0.5581400	-0.6199590
C	1.1470290	-0.8751880	-1.7920950
C	-0.1257740	-1.3265030	-1.8455450
C	-1.0252320	-1.6182980	-0.7465650
C	-1.0823160	-1.1266530	0.5415320
C	-0.6292210	1.6936230	0.2679420
C	-1.9363850	2.1391750	0.4965540
C	0.1941820	2.3911150	-0.6162790
C	-0.2875680	3.5244580	-1.2686010
C	-1.5886880	3.9609040	-1.0409630
C	-2.4144770	3.2683090	-0.1560520
S	3.6731590	-0.6887840	-0.7309120
C	3.8808210	-0.2267170	0.9126460
C	2.6896570	0.0264750	1.5237930
C	-2.1097320	-1.7294390	1.3273190
C	-2.8284180	-2.6529300	0.6284120
S	-2.2679510	-2.8112820	-0.9895150

O	-0.2245570	0.3637710	2.6788540
H	-2.2828420	-1.4640530	2.3639710
H	-3.6579550	-3.2541970	0.9744760
H	-0.5089580	-1.5675750	-2.8345080
H	2.5750600	0.3354040	2.5562970
H	4.8736530	-0.1670670	1.3367440
H	1.6703540	-0.7965810	-2.7422970
H	-2.5732310	1.6018360	1.1955750
H	-3.4281390	3.6116760	0.0257310
H	-1.9610710	4.8447170	-1.5503210
H	0.3565720	4.0677760	-1.9531810
H	1.2128790	2.0570200	-0.7910580

2 ax-|| (ground state, M06-2X/6-31G*)

-1828.891566240

P	-0.0001780	0.1731020	1.2473620
C	1.4147410	-0.7250140	0.5968640
C	1.5769870	-1.0843090	-0.7253740
C	0.6771220	-0.9784840	-1.8587850
C	-0.6749880	-0.9794200	-1.8590320
C	-1.5750570	-1.0864510	-0.7259240
C	-1.4136200	-0.7270300	0.5963730
C	-0.0012740	1.7501810	0.3428700
C	1.2064230	2.3782620	0.0286690
C	-1.2102030	2.3775080	0.0318020
C	-1.2104570	3.6236320	-0.5866940
C	-0.0037140	4.2463120	-0.8972510
C	1.2042260	3.6244030	-0.5898180
S	3.1504130	-1.7880190	-0.9646880
C	3.5555170	-1.6105700	0.6975800
C	2.5446960	-1.0369170	1.4096260
C	-2.5431620	-1.0409400	1.4089510
C	-3.5529220	-1.6161360	0.6966530
S	-3.1472610	-1.7927620	-0.9655670
O	-0.0006980	0.2827690	2.7374440
H	-2.5758080	-0.8259040	2.4707540

H	-4.5160550	-1.9507640	1.0565090
H	-1.1557830	-0.9631950	-2.8345690
H	2.5768160	-0.8216290	2.4713890
H	4.5191480	-1.9435530	1.0576300
H	1.1582640	-0.9615950	-2.8341380
H	2.1484160	1.8880970	0.2634170
H	2.1441920	4.1094790	-0.8341250
H	-0.0046490	5.2179070	-1.3822890
H	-2.1513570	4.1081030	-0.8285640
H	-2.1512400	1.8866970	0.2690290

2 eq (ground state, M06-2X/6-31G*)

-1828.890993500

C	2.0017990	-0.0000010	0.2273990
C	3.0531360	-0.0000030	1.1439260
H	2.8198500	-0.0000050	2.2052410
C	4.3700810	-0.0000030	0.6876960
H	5.1900440	-0.0000050	1.3991900
C	4.6326770	0.0000000	-0.6792160
H	5.6590360	0.0000010	-1.0338620
C	3.5821400	0.0000030	-1.5976780
H	3.7904640	0.0000060	-2.6631440
C	2.2669460	0.0000030	-1.1463810
H	1.4440210	0.0000050	-1.8586260
C	-0.4814280	-1.4197980	0.1279020
C	0.2311530	-2.5927840	-0.2765800
H	1.3127950	-2.6634610	-0.2764940
C	-0.5920320	-3.6128500	-0.6449840
H	-0.3140590	-4.6005370	-0.9859520
C	-1.8527270	-1.5809440	0.0518740
C	-2.9455840	-0.6757200	0.3335240
H	-3.9064540	-1.1539580	0.5083240
C	-0.4814230	1.4197930	0.1278970
C	0.2311640	2.5927580	-0.2766380
H	1.3128080	2.6634150	-0.2765970
C	-0.5920150	3.6127880	-0.6451500
H	-0.3140370	4.6004370	-0.9862250
C	-1.8527210	1.5809410	0.0518660
C	-2.9455810	0.6757220	0.3335240
H	-3.9064450	1.1539660	0.5083380
O	0.3023060	0.0000020	2.3921470
P	0.3140270	-0.0000010	0.8992260
S	-2.2490820	-3.1814680	-0.5025500
S	-2.2490680	3.1815120	-0.5024280

3 ax- $\perp$ (ground state, M06-2X/6-31G*)

-2475.248436010

C	6.1311370	-0.5814150	0.8526740
C	5.0323820	-0.9046320	0.0449210
C	5.2484820	-1.6284500	-1.1362510
C	6.5282040	-2.0087270	-1.5080720
C	7.6168130	-1.6793020	-0.6925330
C	7.4133710	-0.9663490	0.4928950
C	3.6727800	-0.4931960	0.4117820
S	3.2190440	-0.2368050	2.0629890
C	1.5886820	0.1948950	1.6328200
C	1.4301070	0.1461220	0.2600770
C	2.6109750	-0.2569450	-0.4221150
C	0.6763010	0.4870890	2.7167820
C	-0.6765380	0.4872620	2.7167800
C	-1.5889520	0.1951760	1.6328100
C	-1.4303140	0.1463870	0.2600780
C	-2.6111730	-0.2566500	-0.4221640
C	-3.6730050	-0.4928770	0.4116990
S	-3.2193240	-0.2364790	2.0629280
P	-0.0000660	0.6173120	-0.7306920
O	-0.0001910	-0.0129230	-2.0857250
C	-5.0326030	-0.9043220	0.0448290
C	-5.2486510	-1.6283800	-1.1362040
C	-6.5283630	-2.0087020	-1.5080170
C	-7.6170070	-1.6790810	-0.6926050
C	-7.4136170	-0.9658760	0.4926800
C	-6.1313930	-0.5808960	0.8524510
C	-8.9467970	-2.0749250	-1.0723800
N	-10.0179010	-2.3909610	-1.3758330
C	8.9466170	-2.0750850	-1.0723230
N	10.0177230	-2.3910800	-1.3758130
C	0.0002530	2.4278600	-0.8294820
C	0.0004020	3.0006370	-2.1021490
C	0.0007480	4.3870960	-2.2365000
C	0.0009320	5.1955450	-1.1033910
C	0.0007720	4.6230920	0.1686530
C	0.0004300	3.2403990	0.3084370
H	0.0002640	2.3486930	-2.9709150
H	0.0008820	4.8349820	-3.2253960
H	0.0012270	6.2762120	-1.2091230
H	0.0009200	5.2565980	1.0501150
H	0.0002790	2.7965120	1.3012450
H	-1.1518470	0.6807420	3.6755800
H	-2.6551430	-0.3348260	-1.5032840

H	-4.4022460	-1.9099420	-1.7543520
H	-6.6930890	-2.5689670	-2.4221610
H	-8.2623270	-0.7098330	1.1176160
H	-5.9823920	-0.0048200	1.7613990
H	1.1516450	0.6804550	3.6755890
H	2.6549880	-0.3351050	-1.5032340
H	4.4021110	-1.9098750	-1.7545080
H	6.6929660	-2.5687990	-2.4223260
H	8.2620510	-0.7104550	1.1179320
H	5.9821080	-0.0055420	1.7617460

3 ax-|| (ground state, M06-2X/6-31G*)

-2475.247862580

S	3.1474500	0.2302100	1.8955580
C	1.5763070	0.7240060	1.3419010
C	1.4131560	0.3876860	0.0123780
C	2.5398370	-0.2746990	-0.5433620
C	3.5707350	-0.4309100	0.3480050
C	0.6767200	1.3637020	2.2804260
C	-0.6767130	1.3636990	2.2804270
C	-1.5763000	0.7239990	1.3419040
C	-1.4131490	0.3876780	0.0123810
C	-2.5398290	-0.2747090	-0.5433580
C	-3.5707260	-0.4309210	0.3480100
S	-3.1474420	0.2302030	1.8955620
P	0.0000010	0.8506420	-1.0017960
C	-0.0000080	2.6662580	-0.9961270
C	1.2088180	3.3663650	-1.0289190
C	1.2075380	4.7560570	-1.0948680
C	-0.0000300	5.4497240	-1.1265600
C	-1.2075870	4.7560360	-1.0949090
C	-1.2088450	3.3663440	-1.0289590
C	-4.8776540	-1.0559940	0.1172750
C	-5.0232150	-2.0208860	-0.8900460
C	-6.2528450	-2.6126660	-1.1310620
C	-7.3612350	-2.2563530	-0.3543460
C	-7.2277070	-1.3020160	0.6590520
C	-5.9964280	-0.7072140	0.8864090
C	-8.6381790	-2.8735630	-0.5943640
N	-9.6670850	-3.3680920	-0.7843330
C	4.8776630	-1.0559830	0.1172690
C	5.0232230	-2.0208750	-0.8900510
C	6.2528520	-2.6126570	-1.1310670
C	7.3612420	-2.2563450	-0.3543500
C	7.2277150	-1.3020080	0.6590480

C	5.9964360	-0.7072050	0.8864040
C	8.6381860	-2.8735570	-0.5943680
N	9.6670910	-3.3680870	-0.7843360
O	0.0000010	0.1965820	-2.3448370
H	2.1509680	2.8240920	-0.9976590
H	2.1477480	5.2980220	-1.1185240
H	-0.0000380	6.5344110	-1.1748430
H	-2.1478050	5.2979850	-1.1185960
H	-2.1509860	2.8240550	-0.9977320
H	-1.1565640	1.8471790	3.1280310
H	-2.5748300	-0.5803010	-1.5837560
H	-4.1590440	-2.3212410	-1.4737120
H	-6.3615710	-3.3601290	-1.9094630
H	-8.0912410	-1.0273980	1.2551140
H	-5.9052020	0.0507780	1.6591660
H	1.1565700	1.8471840	3.1280290
H	2.5748370	-0.5802900	-1.5837600
H	4.1590510	-2.3212300	-1.4737180
H	6.3615790	-3.3601190	-1.9094680
H	8.0912480	-1.0273910	1.2551100
H	5.9052110	0.0507870	1.6591610

3 eq (ground state, M06-2X/6-31G*)

-2475.247157500

C	6.0871370	-1.1443580	-0.4142280
C	4.9762850	-0.2901690	-0.4141290
C	5.1587530	1.0579110	-0.7546400
C	6.4164120	1.5438860	-1.0732230
C	7.5172250	0.6800440	-1.0700070
C	7.3474300	-0.6687320	-0.7421810
C	3.6381030	-0.7780850	-0.0622180
S	3.1888250	-2.4371160	-0.2740440
C	1.5828470	-2.1595270	0.3342920
C	1.4208880	-0.8310380	0.6870620
C	2.5946630	-0.0577110	0.4556650
C	0.6765020	-3.2837970	0.3677640
C	-0.6765200	-3.2837910	0.3677660
C	-1.5828580	-2.1595210	0.3343100
C	-1.4209190	-0.8310460	0.6871420
C	-2.5946930	-0.0577200	0.4557430
C	-3.6381120	-0.7780800	-0.0622030
S	-3.1887860	-2.4370730	-0.2741950
P	0.0000050	-0.1763910	1.5813280
C	0.0000030	1.5948900	1.1769300
C	-4.9763010	-0.2901680	-0.4140970

C	-5.1587900	1.0579340	-0.7545080
C	-6.4164520	1.5439050	-1.0730830
C	-7.5172460	0.6800390	-1.0699560
C	-7.3474300	-0.6687590	-0.7422290
C	-6.0871330	-1.1443820	-0.4142850
C	-8.8231430	1.1791400	-1.4084510
N	-9.8733550	1.5815520	-1.6811210
C	8.8231200	1.1791460	-1.4085080
N	9.8733230	1.5815750	-1.6811860
O	0.0000560	-0.4273360	3.0519410
H	-1.1526600	-4.2604720	0.3247940
H	-2.6684040	0.9943820	0.7094850
H	-4.3014640	1.7226970	-0.7873410
H	-6.5542390	2.5871230	-1.3365290
H	-8.2055410	-1.3320780	-0.7381610
H	-5.9662620	-2.1873310	-0.1354040
H	1.1526340	-4.2604810	0.3248010
H	2.6683480	0.9944110	0.7093580
H	4.3014150	1.7226540	-0.7875420
H	6.5541790	2.5870870	-1.3367450
H	8.2055550	-1.3320340	-0.7380430
H	5.9662850	-2.1872880	-0.1352690
C	-0.0000480	2.5000770	2.2377700
C	-0.0000440	3.8702260	1.9782920
C	0.0000250	4.3298270	0.6647140
C	0.0000810	3.4248220	-0.3979440
C	0.0000710	2.0578940	-0.1434860
H	-0.0000870	2.1153400	3.2540930
H	-0.0000860	4.5767330	2.8023930
H	0.0000350	5.3969980	0.4642740
H	0.0001380	3.7867610	-1.4214670
H	0.0000990	1.3480540	-0.9686170

4 ax- $\perp$ (ground state, M06-2X/6-31G*)

-2699.671898430			
C	-6.1154150	-0.3519430	0.9813930
C	-5.0104700	-0.7443940	0.2121580
C	-5.2087410	-1.6098230	-0.8740200
C	-6.4785850	-2.0644790	-1.1946480
C	-7.5484800	-1.6546720	-0.4093530
C	-7.3900400	-0.8067430	0.6778780
C	-3.6596910	-0.2639140	0.5234310
S	-3.2108500	0.2024690	2.1301620
C	-1.5874220	0.6014630	1.6472110
C	-1.4278920	0.3864280	0.2907140

C	-2.6014840	-0.1152400	-0.3349960
C	-0.6764460	1.0367570	2.6840220
C	0.6764460	1.0367600	2.6840210
C	1.5874230	0.6014660	1.6472100
S	3.2108510	0.2024730	2.1301610
C	3.6596920	-0.2639100	0.5234300
C	2.6014850	-0.1152370	-0.3349980
C	1.4278920	0.3864300	0.2907130
C	5.0104720	-0.7443900	0.2121570
C	6.1154160	-0.3519360	0.9813900
C	7.3900420	-0.8067360	0.6778760
C	7.5484810	-1.6546700	-0.4093530
C	6.4785850	-2.0644790	-1.1946460
C	5.2087420	-1.6098220	-0.8740190
N	8.8960390	-2.1388470	-0.7397660
O	9.0065390	-2.8815790	-1.6976100
P	-0.0000000	0.7439070	-0.7490500
C	-0.0000030	2.5287620	-1.0621050
N	-8.8960380	-2.1388490	-0.7397670
O	-9.0065390	-2.8815670	-1.6976220
O	0.0000010	-0.0404020	-2.0208270
O	-9.8154820	-1.7663750	-0.0343410
O	9.8154820	-1.7663750	-0.0343370
H	-1.1524080	1.3551580	3.6086380
H	-2.6419760	-0.3276900	-1.3980430
H	-4.3565320	-1.9428200	-1.4573190
H	-6.6515740	-2.7354320	-2.0272010
H	-8.2559150	-0.5119180	1.2578440
H	-5.9787600	0.3333640	1.8129300
H	1.1524090	1.3551620	3.6086360
H	2.6419770	-0.3276880	-1.3980440
H	4.3565320	-1.9428220	-1.4573160
H	6.6515740	-2.7354350	-2.0271960
H	8.2559160	-0.5119090	1.2578400
H	5.9787610	0.3333740	1.8129250
C	0.0000240	2.9374640	-2.3966800
C	0.0000250	4.2961940	-2.7036680
C	-0.0000010	5.2398990	-1.6808320
C	-0.0000280	4.8316500	-0.3469260
C	-0.0000290	3.4770090	-0.0347090
H	0.0000430	2.1813720	-3.1768410
H	0.0000450	4.6169700	-3.7407000
H	-0.0000010	6.2989300	-1.9206220
H	-0.0000500	5.5708230	0.4482340
H	-0.0000500	3.1597750	1.0055450

4 ax-|| (ground state, M06-2X/6-31G*)

-2699.671305870

P	0.0000040	1.0567090	-1.0137170
C	1.4110880	0.6301810	0.0194730
C	1.5746230	1.0213800	1.3338600
C	0.6766770	1.7073410	2.2413660
C	-0.6766980	1.7073660	2.2413560
C	-1.5746570	1.0214330	1.3338410
C	-1.4111140	0.6302250	0.0194580
C	0.0000290	2.8706860	-1.0771680
C	-1.2088270	3.5688500	-1.1380960
C	1.2089120	3.5688070	-1.1380590
C	1.2076340	4.9547500	-1.2597220
C	0.0000790	5.6466360	-1.3191060
C	-1.2075010	4.9547930	-1.2597610
C	-2.5309580	-0.0688800	-0.5031740
C	-3.5571080	-0.1991550	0.3980210
S	-3.1389580	0.5363220	1.9129360
C	2.5309270	-0.0689320	-0.5031540
C	3.5570780	-0.1992070	0.3980430
S	3.1388950	0.5362060	1.9129800
C	-4.8552940	-0.8522990	0.1979900
C	-5.9712730	-0.5058010	0.9737060
C	-7.1948930	-1.1288460	0.7781270
C	-7.2938140	-2.0975500	-0.2108020
C	-6.2123830	-2.4654960	-1.0010430
C	-4.9923390	-1.8433910	-0.7860630
N	-8.5876980	-2.7592920	-0.4277090
O	-9.5140570	-2.4306220	0.2903950
C	4.8552720	-0.8523330	0.1980070
C	5.9712340	-0.5058670	0.9737630
C	7.1948610	-1.1288950	0.7781770
C	7.2938070	-2.0975500	-0.2107980
C	6.2123940	-2.4654650	-1.0010770
C	4.9923420	-1.8433780	-0.7860890
N	8.5877010	-2.7592700	-0.4277160
O	9.5140430	-2.4306340	0.2904260
O	0.0000020	0.3509700	-2.3300150
O	8.6507170	-3.5936000	-1.3115970
O	-8.6506910	-3.5936660	-1.3115500
H	-1.1574550	2.2287980	3.0656070
H	-2.5641170	-0.4206080	-1.5289240
H	-4.1294330	-2.1406000	-1.3726820
H	-6.3372110	-3.2323390	-1.7555100
H	-8.0673460	-0.8727960	1.3664780

H	-5.8853970	0.2712600	1.7276600
H	1.1574450	2.2287530	3.0656220
H	2.5640920	-0.4206500	-1.5289070
H	4.1294490	-2.1405670	-1.3727370
H	6.3372410	-3.2322720	-1.7555760
H	8.0673010	-0.8728670	1.3665570
H	5.8853410	0.2711540	1.7277560
H	-2.1510890	3.0284170	-1.0859710
H	-2.1477900	5.4951990	-1.3055110
H	0.0000890	6.7284640	-1.4111680
H	2.1479450	5.4951200	-1.3054380
H	2.1511670	3.0283660	-1.0859110

4 eq (ground state, M06-2X/6-31G*)

-2699.670787340

C	6.0784740	-1.2096830	-0.3831030
C	4.9664380	-0.3561500	-0.3527170
C	5.1434100	1.0040450	-0.6482700
C	6.3988740	1.5058900	-0.9536640
C	7.4763350	0.6298100	-0.9744520
C	7.3387840	-0.7233440	-0.6975900
C	3.6304050	-0.8590040	-0.0143440
S	3.1840060	-2.5100770	-0.2871220
C	1.5820360	-2.2590700	0.3413350
C	1.4192360	-0.9455960	0.7466160
C	2.5889850	-0.1606360	0.5372150
C	0.6765260	-3.3848030	0.3386690
C	-0.6765260	-3.3848030	0.3386700
C	-1.5820360	-2.2590700	0.3413360
S	-3.1840060	-2.5100780	-0.2871210
C	-3.6304050	-0.8590050	-0.0143460
C	-2.5889850	-0.1606360	0.5372140
C	-1.4192370	-0.9455960	0.7466160
P	-0.0000000	-0.3463060	1.6820700
C	-0.0000000	1.4474100	1.4029790
C	0.0000000	2.2700730	2.5294620
C	0.0000010	3.6554420	2.3748660
C	0.0000010	4.2134340	1.0999500
C	0.0000000	3.3915320	-0.0284520
C	-0.0000010	2.0091850	0.1212620
C	-4.9664370	-0.3561500	-0.3527210
C	-5.1434090	1.0040440	-0.6482740
C	-6.3988730	1.5058890	-0.9536700
C	-7.4763330	0.6298080	-0.9744610
C	-7.3387830	-0.7233450	-0.6975980

C	-6.0784740	-1.2096840	-0.3831080
N	-8.8087040	1.1536280	-1.3057440
O	-9.7345710	0.3638480	-1.3230880
N	8.8087070	1.1536300	-1.3057320
O	9.7345700	0.3638460	-1.3230970
O	-0.0000010	-0.7002640	3.1315260
O	-8.9006300	2.3441820	-1.5420400
O	8.9006280	2.3441780	-1.5420620
H	0.0000000	1.8095790	3.5138310
H	0.0000010	4.2973420	3.2500840
H	0.0000010	5.2926470	0.9805450
H	-0.0000000	3.8299960	-1.0216890
H	-0.0000010	1.3645200	-0.7556230
H	-1.1528820	-4.3593730	0.2639040
H	-2.6627000	0.8809890	0.8312660
H	-4.2839580	1.6664040	-0.6576300
H	-6.5558710	2.5521120	-1.1858070
H	-8.2100920	-1.3660630	-0.7217590
H	-5.9592300	-2.2610960	-0.1381830
H	1.1528810	-4.3593720	0.2639030
H	2.6626990	0.8809890	0.8312670
H	4.2839580	1.6664040	-0.6576280
H	6.5558720	2.5521130	-1.1858010
H	8.2100940	-1.3660620	-0.7217490
H	5.9592290	-2.2610960	-0.1381800

5 ax- $\perp$ (ground state, M06-2X/6-31G*)

-2290.818211270			
S	3.2093930	-0.8697680	1.7688560
C	1.5862590	-0.3199600	1.4635270
C	1.4331050	-0.0194860	0.1230510
C	2.6065410	-0.2707200	-0.6424790
C	3.6588420	-0.7376270	0.1005700
C	5.0044930	-1.1073990	-0.3594010
C	5.7751670	-2.0463550	0.3367960
C	7.0416260	-2.3974980	-0.1150090
C	7.5559580	-1.8225600	-1.2740900
C	6.7965360	-0.8876330	-1.9742320
C	5.5343350	-0.5266940	-1.5189380
C	0.6734770	-0.2930000	2.5859790
C	-0.6795100	-0.3015770	2.5816620
C	-1.5842470	-0.3428660	1.4534780
S	-3.2008160	-0.9195320	1.7461170
C	-3.6435730	-0.7785290	0.0773590
C	-2.5889660	-0.3079800	-0.6599690

C	-1.4225450	-0.0487390	0.1125260
P	0.0012760	0.6828720	-0.7124890
C	-0.0178180	2.4592890	-0.3358200
C	-0.0033350	2.9569560	0.9704400
C	-0.0222730	4.3302860	1.1861280
C	-0.0554950	5.2069170	0.1017020
C	-0.0696060	4.7120110	-1.1990480
C	-0.0507310	3.3368290	-1.4205160
C	-4.9838320	-1.1522070	-0.3939420
C	-5.1577270	-1.6046150	-1.7083030
C	-6.4202620	-1.9519430	-2.1725310
C	-7.5266550	-1.8657910	-1.3301940
C	-7.3619130	-1.4251340	-0.0195930
C	-6.1015510	-1.0671830	0.4447470
O	0.0079800	0.4397540	-2.1875350
H	1.1478270	-0.3307770	3.5641700
H	2.6333920	-0.1331620	-1.7180880
H	5.3700120	-2.5207890	1.2267910
H	7.6236420	-3.1300510	0.4355230
H	8.5432660	-2.1003740	-1.6292800
H	7.1928090	-0.4296020	-2.8751820
H	4.9587510	0.2235790	-2.0526300
H	-1.1595650	-0.3437470	3.5568160
H	-2.6283050	-0.1208590	-1.7276000
H	-4.2931060	-1.7020550	-2.3580920
H	-6.5384320	-2.3033650	-3.1928200
H	-8.5113060	-2.1438760	-1.6925080
H	-8.2188610	-1.3525740	0.6429240
H	-5.9845030	-0.6993770	1.4609260
H	0.0228830	2.2753580	1.8171570
H	-0.0106090	4.7193200	2.1996190
H	-0.0701300	6.2789380	0.2743990
H	-0.0952280	5.3957480	-2.0419190
H	-0.0605800	2.9245940	-2.4255430

5 ax-|| (ground state, M06-2X/6-31G*)

-2290.817728430			
P	0.0042590	0.6669440	-0.9970230
C	1.4291600	0.1034420	-0.0560420
C	1.5840850	0.2628630	1.3063630
C	0.6745090	0.7638900	2.3160900
C	-0.6789770	0.7443820	2.3121210
C	-1.5695760	0.2162820	1.2994150
C	-1.4004990	0.0478900	-0.0605500
C	-0.0381410	2.4662210	-0.7352270

C	1.1506830	3.1948810	-0.6467900
C	1.1122040	4.5794840	-0.5130590
C	-0.1129930	5.2402810	-0.4665960
C	-1.3010690	4.5182710	-0.5550790
C	-1.2646400	3.1339780	-0.6884790
C	2.5648270	-0.4709960	-0.6896410
C	3.5950750	-0.7346110	0.1757830
S	3.1659790	-0.2689810	1.7927680
C	-2.5241470	-0.5431900	-0.6999240
C	-3.5584440	-0.8117400	0.1591600
S	-3.1419850	-0.3485820	1.7795350
C	4.9070900	-1.3241070	-0.1244090
C	5.6307230	-2.0195310	0.8518690
C	6.8666030	-2.5800420	0.5519190
C	7.3966840	-2.4624340	-0.7302530
C	6.6836850	-1.7733450	-1.7090330
C	5.4527870	-1.2029640	-1.4092500
C	-4.8651980	-1.4068470	-0.1512760
C	-4.9895750	-2.2974730	-1.2251940
C	-6.2232950	-2.8541630	-1.5391900
C	-7.3491230	-2.5414120	-0.7799810
C	-7.2331300	-1.6635270	0.2945640
C	-6.0023590	-1.0975090	0.6050750
O	0.0162760	0.2163610	-2.4216350
H	1.1460440	1.1415630	3.2205670
H	2.5861870	-0.6884030	-1.7520970
H	5.2115860	-2.1405920	1.8473520
H	7.4119520	-3.1182360	1.3209120
H	8.3602750	-2.9035600	-0.9650530
H	7.0928860	-1.6698010	-2.7092070
H	4.9144790	-0.6441840	-2.1689160
H	-1.1662390	1.1101410	3.2131340
H	-2.5591120	-0.7151810	-1.7704060
H	-4.1083840	-2.5659860	-1.8001470
H	-6.3033660	-3.5443080	-2.3733270
H	-8.3109760	-2.9817190	-1.0233810
H	-8.1056360	-1.4105000	0.8888170
H	-5.9239730	-0.3932600	1.4293520
H	-2.1919180	2.5689780	-0.7492320
H	-2.2558650	5.0334370	-0.5155100
H	-0.1423090	6.3203280	-0.3580700
H	2.0379430	5.1420580	-0.4417280
H	2.1067550	2.6773570	-0.6758060

5 eq (ground state, M06-2X/6-31G*)

-2290.817354490

O	-0.0056080	0.1170600	2.9074060
C	0.0028640	1.8779340	0.7912750
C	0.0140560	2.1806400	-0.5748140
H	0.0270350	1.3777170	-1.3094450
C	0.0108070	3.5076900	-0.9897790
H	0.0215130	3.7449240	-2.0491690
C	-0.0047080	4.5327670	-0.0429960
H	-0.0072820	5.5684190	-0.3696660
C	-0.0164170	4.2328840	1.3161040
H	-0.0291220	5.0330350	2.0498010
C	-0.0123810	2.9037900	1.7360140
H	-0.0215210	2.6419650	2.7906260
C	0.6641960	-3.0712740	0.6999760
H	1.1369790	-4.0430460	0.8212950
C	1.5744820	-1.9710850	0.4820860
C	1.4205650	-0.6037670	0.6269720
C	2.5973260	0.1200880	0.2729130
H	2.6588220	1.2026860	0.3030200
C	3.6365480	-0.6750530	-0.1296910
C	4.9792400	-0.2577370	-0.5569940
C	5.7292470	-1.0229580	-1.4580170
H	5.3112880	-1.9416040	-1.8614240
C	6.9930160	-0.6046480	-1.8591430
H	7.5609630	-1.2084700	-2.5600980
C	7.5243760	0.5868680	-1.3725390
H	8.5097570	0.9140810	-1.6887570
C	6.7862180	1.3538920	-0.4738080
H	7.1971220	2.2785970	-0.0806700
C	5.5273740	0.9331880	-0.0631640
H	4.9697900	1.5167780	0.6632130
C	-0.6888530	-3.0661500	0.7000640
H	-1.1692130	-4.0339840	0.8225530
C	-1.5897960	-1.9593390	0.4782350
C	-1.4222300	-0.5928840	0.6152790
C	-2.5910890	0.1412090	0.2568170
H	-2.6623610	1.2205880	0.3386410
C	-3.6367000	-0.6455560	-0.1454240
C	-4.9720180	-0.2171140	-0.5827090
C	-5.1365470	1.0323800	-1.1947600
H	-4.2667970	1.6581790	-1.3723580
C	-6.3956930	1.4596740	-1.5977560
H	-6.5073740	2.4304080	-2.0708760
C	-7.5078960	0.6423170	-1.4098090
H	-8.4898650	0.9752580	-1.7306290
C	-7.3524440	-0.6055500	-0.8113750

H	-8.2139810	-1.2477770	-0.6569190
C	-6.0953910	-1.0313270	-0.3976480
H	-5.9850620	-1.9954880	0.0919240
P	-0.0011600	0.1712640	1.4152430
S	3.1817710	-2.3467380	-0.0685170
S	-3.1947290	-2.3209470	-0.0884100

6 ax- $\perp$ (ground state, M06-2X/6-31G*)

-3325.302305940

C	11.2184800	-0.8294920	-0.8244960
C	10.0700310	-0.4906690	-0.1017630
C	10.0513840	0.6942080	0.6414880
C	11.1617610	1.5308560	0.6470670
C	12.3080900	1.1902390	-0.0675540
C	12.3307220	0.0040930	-0.7974380
N	8.9402060	-1.3483210	-0.1169950
C	9.1364920	-2.7487610	-0.0069880
C	8.4055310	-3.6357590	-0.8042120
C	8.6059000	-5.0064670	-0.6856830
C	9.5476790	-5.5096830	0.2090380
C	10.2837890	-4.6255890	0.9940450
C	10.0768750	-3.2544950	0.8969280
C	7.6434530	-0.8146740	-0.2484300
C	6.5487620	-1.4288040	0.3773070
C	5.2723970	-0.9097290	0.2341090
C	5.0410970	0.2544940	-0.5109790
C	6.1407600	0.8680550	-1.1234060
C	7.4177750	0.3411710	-1.0077230
C	3.6858000	0.7991720	-0.6320140
S	3.2288690	1.8019340	-1.9712920
C	1.5968320	1.9841940	-1.3904400
C	1.4385730	1.2920240	-0.2042970
C	2.6201040	0.6179940	0.2115360
P	0.0054320	1.2382950	0.8843950
C	-1.4254670	1.2975550	-0.2071730
C	-1.5807970	1.9946390	-1.3910130
S	-3.2149170	1.8252950	-1.9705410
C	-3.6760570	0.8222980	-0.6337780
C	-2.6109100	0.6297000	0.2077380
C	-0.6662050	2.7634400	-2.2045350
C	0.6874320	2.7583840	-2.2046440
C	-5.0360820	0.2920940	-0.5066260
C	-5.2655840	-0.9025730	0.1895550
C	-6.5454110	-1.4115360	0.3362570
C	-7.6476530	-0.7367510	-0.2075880

C	-7.4253560	0.4539360	-0.9111740
C	-6.1401700	0.9528550	-1.0587980
N	-8.9510710	-1.2478220	-0.0466110
C	-9.9132270	-1.0917600	-1.0760280
C	-11.2310420	-0.7427430	-0.7625830
C	-12.1747520	-0.6036050	-1.7739810
C	-11.8170410	-0.7911200	-3.1068740
C	-10.5028550	-1.1310460	-3.4194840
C	-9.5561940	-1.2908930	-2.4138780
O	0.0020680	0.0479100	1.7890290
C	0.0066970	2.7870140	1.8320310
C	0.0127990	4.0432810	1.2193210
C	0.0127530	5.1927190	2.0015610
C	0.0066250	5.0899940	3.3925510
C	0.0006870	3.8393480	4.0031360
C	0.0007220	2.6846980	3.2236450
C	-9.3208360	-1.8878440	1.1638240
C	-10.1275160	-3.0306410	1.1378580
C	-10.4986800	-3.6489490	2.3262460
C	-10.0596870	-3.1512420	3.5509630
C	-9.2510170	-2.0173860	3.5762340
C	-8.8900750	-1.3806550	2.3944380
H	0.0176640	4.1240730	0.1347020
H	0.0176640	6.1700290	1.5285910
H	0.0065720	5.9899260	4.0003130
H	-0.0039870	3.7618150	5.0860410
H	-0.0037760	1.6964270	3.6748550
H	-1.1393830	3.3918070	-2.9557600
H	-2.6569970	0.0507760	1.1236960
H	-4.4232260	-1.4561840	0.5940110
H	-6.7018540	-2.3457290	0.8660200
H	-8.2695850	0.9914810	-1.3308240
H	-5.9969350	1.8949350	-1.5821160
H	-10.4609310	-3.4237440	0.1822970
H	-11.1251700	-4.5350910	2.2921180
H	-10.3448270	-3.6420340	4.4758050
H	-8.9064210	-1.6145230	4.5238020
H	-8.2705710	-0.4893560	2.4146120
H	-11.5058190	-0.5857330	0.2759720
H	-13.1945570	-0.3339290	-1.5165020
H	-12.5552220	-0.6740820	-3.8935390
H	-10.2120100	-1.2883770	-4.4537430
H	-8.5346360	-1.5685460	-2.6555610
H	1.1651200	3.3828160	-2.9563180
H	2.6601190	0.0394460	1.1279370
H	4.4377670	-1.4189620	0.7064200

H	6.7065400	-2.3251780	0.9683090
H	8.2524410	0.8286840	-1.5005630
H	5.9981790	1.7787880	-1.6998180
H	7.6814780	-3.2423990	-1.5112420
H	8.0292990	-5.6833290	-1.3088220
H	9.7060730	-6.5798950	0.2934930
H	11.0169430	-5.0047050	1.6994750
H	10.6426330	-2.5648100	1.5158250
H	9.1623740	0.9518480	1.2091920
H	11.1341950	2.4479590	1.2275980
H	13.1757760	1.8417120	-0.0547460
H	13.2157900	-0.2709840	-1.3629750
H	11.2297620	-1.7488220	-1.4018960

6 ax-|| (ground state, M06-2X/6-31G*)

-3325.301767600

P	0.0298750	2.0660770	1.0290520
O	0.0212480	1.2398200	2.2742020
S	-3.1339590	1.9258280	-1.9080480
C	0.0748900	3.8674440	1.2753550
C	1.3027160	4.5204510	1.4101950
H	2.2286420	3.9591470	1.3082610
C	1.3422900	5.8873300	1.6659840
H	2.2984540	6.3912280	1.7679610
C	0.1556940	6.6070400	1.7869870
H	0.1868230	7.6746260	1.9830460
C	-1.0708590	5.9603990	1.6543150
H	-1.9956230	6.5217400	1.7457450
C	-1.1124810	4.5930840	1.3987950
H	-2.0695710	4.0889410	1.2873090
C	-1.3950670	1.7808580	-0.0290030
C	-1.5546850	2.3180160	-1.2909750
C	-0.6485370	3.0842190	-2.1200870
H	-1.1227750	3.7009560	-2.8802300
C	-2.5282180	1.0531300	0.4242100
H	-2.5675740	0.5947170	1.4065140
C	-3.5625530	1.0386590	-0.4769100
C	-4.8666080	0.3836560	-0.3448670
C	-5.0139530	-0.7231630	0.5021680
H	-4.1472940	-1.1122060	1.0284490
C	-6.2358840	-1.3591130	0.6475020
H	-6.3235070	-2.2244080	1.2965810
C	-7.3625570	-0.9046900	-0.0526080
C	-7.2232240	0.2011580	-0.9018950
H	-8.0887970	0.5700330	-1.4426410

C	-5.9950270	0.8280390	-1.0448450
H	-5.9207530	1.6991820	-1.6911280
N	-8.6072210	-1.5485070	0.0905050
C	-8.9841660	-2.1121020	1.3364200
C	-9.6190440	-3.3574840	1.3807230
H	-9.8117740	-3.8880240	0.4533210
C	-9.9999100	-3.9026060	2.6013680
H	-10.4930360	-4.8698210	2.6217830
C	-9.7393250	-3.2263300	3.7908030
H	-10.0321650	-3.6583990	4.7422100
C	-9.1002580	-1.9894850	3.7470250
H	-8.8964850	-1.4484250	4.6660530
C	-8.7325170	-1.4272890	2.5299850
H	-8.2460230	-0.4571770	2.4938110
C	-9.4903910	-1.6511400	-1.0145300
C	-10.8630300	-1.4476920	-0.8388150
H	-11.2406760	-1.2018380	0.1490090
C	-11.7291830	-1.5643610	-1.9198750
H	-12.7925710	-1.4049570	-1.7688640
C	-11.2408320	-1.8658080	-3.1889660
H	-11.9195420	-1.9484050	-4.0316120
C	-9.8729270	-2.0609350	-3.3652360
H	-9.4791980	-2.3043240	-4.3474890
C	-9.0009860	-1.9651020	-2.2867860
H	-7.9363560	-2.1308590	-2.4212500
S	3.1592300	1.8374510	-1.9377430
C	1.4286250	1.7249270	-0.0483620
C	1.5953800	2.2673750	-1.3072760
C	0.7057510	3.0635570	-2.1260090
H	1.1919550	3.6661120	-2.8898960
C	2.5435700	0.9602680	0.3906090
H	2.5786290	0.4919280	1.3685910
C	3.5715130	0.9273260	-0.5165600
C	4.8611290	0.2394540	-0.3977640
C	4.9653970	-0.9301680	0.3667660
H	4.0800110	-1.3328370	0.8497300
C	6.1774180	-1.5868320	0.5099700
H	6.2402930	-2.4875460	1.1122650
C	7.3263490	-1.1052850	-0.1314610
C	7.2268840	0.0553730	-0.9089040
H	8.1101580	0.4371730	-1.4109200
C	6.0151600	0.7187950	-1.0293230
H	5.9669640	1.6287830	-1.6219880
N	8.5592630	-1.7787840	0.0001680
C	8.5969810	-3.1956290	0.0171400
C	7.7652630	-3.9348500	-0.8312340

H	7.0938230	-3.4122090	-1.5056880
C	7.7996980	-5.3241670	-0.8053990
H	7.1473000	-5.8851320	-1.4677780
C	8.6731910	-5.9950200	0.0468540
H	8.7023860	-7.0796450	0.0592820
C	9.5093280	-5.2589430	0.8832640
H	10.1915550	-5.7684820	1.5571130
C	9.4689410	-3.8693870	0.8788300
H	10.1118470	-3.2947100	1.5385160
C	9.7649520	-1.0391400	0.0906580
C	9.8203610	0.1254070	0.8644990
H	8.9327780	0.4509600	1.3984620
C	11.0011160	0.8543440	0.9453690
H	11.0282070	1.7563400	1.5491760
C	12.1448170	0.4256430	0.2758890
H	13.0671220	0.9930040	0.3465550
C	12.0927530	-0.7397260	-0.4850750
H	12.9752830	-1.0823250	-1.0169610
C	10.9114330	-1.4656360	-0.5879220
H	10.8684790	-2.3674740	-1.1907380

6 eq (ground state, M06-2X/6-31G*)

-3325.301270750			
C	-11.2332590	-0.1168530	-0.6089760
C	-10.0040840	0.0291080	0.0418650
C	-9.8570850	-0.4515520	1.3471910
C	-10.9219110	-1.0801870	1.9827440
C	-12.1482560	-1.2195420	1.3373500
C	-12.2980610	-0.7296210	0.0419750
N	-8.9203510	0.6671870	-0.6158830
C	-9.1566710	1.8577270	-1.3476210
C	-8.5094580	2.0831190	-2.5675770
C	-8.7504890	3.2533160	-3.2784720
C	-9.6491030	4.2028880	-2.7974000
C	-10.2997440	3.9741800	-1.5873240
C	-10.0514830	2.8163110	-0.8598270
C	-7.6153800	0.1512460	-0.4839930
C	-6.5065240	1.0045660	-0.4017140
C	-5.2290970	0.4851280	-0.2587170
C	-5.0132330	-0.8959390	-0.1672370
C	-6.1256310	-1.7420670	-0.2554770
C	-7.4036580	-1.2325900	-0.4222710
C	-3.6605150	-1.4232110	0.0372850
S	-3.1997340	-2.9926680	-0.5384800
C	-1.5861250	-2.8419620	0.0989140

C	-1.4291370	-1.6184240	0.7260530
C	-2.6116060	-0.8227990	0.6817130
P	-0.0115190	-1.1758440	1.7445170
C	1.4202520	-1.6245140	0.7483760
C	1.5844140	-2.8494590	0.1256500
S	3.2081610	-3.0055390	-0.4847880
C	3.6625480	-1.4361540	0.0947200
C	2.6048520	-0.8318760	0.7213120
C	0.6754890	-3.9474080	-0.0987180
C	-0.6781490	-3.9438790	-0.1105640
C	5.0160980	-0.9062220	-0.0916920
C	5.2225850	0.4762660	-0.1922660
C	6.4962460	1.0020010	-0.3322780
C	7.6152870	0.1576600	-0.3694180
C	7.4155330	-1.2262280	-0.2842730
C	6.1357860	-1.7444270	-0.1527200
N	8.9115340	0.6991910	-0.4821290
C	9.9259340	-0.0068340	-1.1766650
C	11.2168450	-0.0947200	-0.6454860
C	12.2094360	-0.7812270	-1.3357390
C	11.9274800	-1.4021910	-2.5499260
C	10.6398230	-1.3207330	-3.0754030
C	9.6454470	-0.6203490	-2.4023510
C	-0.0074060	0.6418190	1.7407600
O	-0.0230640	-1.7359000	3.1289720
C	9.2374190	1.9020960	0.1958110
C	10.0545220	2.8565780	-0.4186360
C	10.3825220	4.0290230	0.2529770
C	9.8895790	4.2739430	1.5325380
C	9.0712950	3.3257640	2.1416410
C	8.7534670	2.1418260	1.4859960
H	1.1508840	-4.8933500	-0.3473580
H	2.6802740	0.1393200	1.1988040
H	4.3666590	1.1449000	-0.1893570
H	6.6371360	2.0746970	-0.4187990
H	8.2724020	-1.8916120	-0.3036650
H	6.0080180	-2.8194870	-0.0539450
H	10.4295610	2.6691740	-1.4202900
H	11.0183900	4.7615750	-0.2349830
H	10.1413200	5.1937900	2.0501860
H	8.6862060	3.4990480	3.1419550
H	8.1266630	1.3963050	1.9656650
H	11.4324570	0.3792680	0.3071450
H	13.2071330	-0.8423780	-0.9116270
H	12.7034200	-1.9432990	-3.0815110
H	10.4081700	-1.7943500	-4.0246270

H	8.6450610	-0.5440260	-2.8176980
H	-1.1539120	-4.8873630	-0.3676870
H	-2.6914730	0.1479460	1.1594660
H	-4.3809240	1.1622650	-0.2173180
H	-6.6543130	2.0784020	-0.4543480
H	-8.2530610	-1.9046870	-0.4887300
H	-5.9904180	-2.8179600	-0.1798500
H	-7.8205520	1.3365580	-2.9510810
H	-8.2426130	3.4147770	-4.2245210
H	-9.8417610	5.1104610	-3.3601460
H	-10.9988730	4.7075270	-1.1970540
H	-10.5503350	2.6423360	0.0884820
H	-8.9043190	-0.3310900	1.8537510
H	-10.7935350	-1.4513620	2.9949620
H	-12.9790410	-1.7049200	1.8390260
H	-13.2476860	-0.8359650	-0.4736300
H	-11.3447870	0.2573100	-1.6221170
C	-0.0120470	1.2882460	2.9762590
C	-0.0087970	2.6813150	3.0295270
C	-0.0010360	3.4223090	1.8513930
C	0.0035880	2.7769770	0.6140620
C	0.0004740	1.3877090	0.5571560
H	-0.0181870	0.6852640	3.8801680
H	-0.0126080	3.1869490	3.9902620
H	0.0013570	4.5074400	1.8938280
H	0.0094960	3.3583290	-0.3028450
H	0.0041030	0.8788110	-0.4048540

8 ax- $\perp$ (ground state, M06-2X/6-31G*)

-3012.487459070

C	-2.9142580	-2.3420600	-1.9972890
C	-3.7130740	-1.3862080	-1.2612780
C	-1.5739820	-2.5280800	-1.9649840
C	-0.5731900	-1.8346160	-1.1853470
C	-0.6455020	-1.0568570	-0.0445530
P	-2.0683610	-0.7440390	1.0127930
C	-3.4701230	-0.6503630	-0.1162740
S	1.0728900	-1.9038670	-1.7524630
C	1.6415760	-0.8563190	-0.4942380
C	0.6056690	-0.4972570	0.3310290
S	-5.2776400	-0.9841680	-1.9107360
C	-5.5858700	0.1781850	-0.6626070
C	-4.5295710	0.2399370	0.2080840
C	-6.8304950	0.9521340	-0.6158570
H	-4.4937680	0.8802860	1.0827950

H	0.7034580	0.1782840	1.1737780
O	-1.9226620	0.4861030	1.8495790
C	-2.3070500	-2.2232210	2.0360920
C	-2.3388340	-2.0463920	3.4201800
C	-2.5198670	-3.1472760	4.2542380
C	-2.6692520	-4.4181240	3.7062290
C	-2.6378090	-4.5950370	2.3230580
C	-2.4561260	-3.5001370	1.4864400
H	-2.2198270	-1.0449020	3.8236880
H	-2.5443540	-3.0121620	5.3311210
H	-2.8105900	-5.2755760	4.3574920
H	-2.7541100	-5.5874350	1.8986700
H	-2.4296030	-3.6402310	0.4085620
H	-1.1809630	-3.2638330	-2.6631560
H	-3.4646560	-2.9464830	-2.7143530
C	-8.0093640	0.4784980	-1.2095030
C	-9.1824700	1.2162960	-1.1483330
C	-9.1664430	2.4323470	-0.4793380
C	-8.0180990	2.9348750	0.1192750
C	-6.8503900	2.1925020	0.0403030
H	-8.0136900	-0.4866120	-1.7078820
H	-10.1031440	0.8638610	-1.5970270
N	-10.4061600	3.2161430	-0.4043260
H	-8.0518160	3.8937210	0.6218160
H	-5.9364310	2.5844340	0.4740040
O	-10.3682140	4.2714090	0.2015210
O	-11.3938410	2.7608300	-0.9517780
C	3.0475850	-0.4548440	-0.4020460
C	3.8999710	-0.4788810	-1.5129230
C	5.2182150	-0.0602830	-1.4186830
C	5.7333110	0.3938890	-0.1971810
C	4.8905840	0.4035760	0.9241160
C	3.5740880	-0.0113210	0.8192410
H	3.5178260	-0.7959630	-2.4800140
H	5.8547340	-0.0669130	-2.2974220
N	7.0648490	0.8388570	-0.0911700
H	5.2814550	0.7350630	1.8806580
H	2.9487470	-0.0178620	1.7067930
C	7.3789400	1.9308580	0.7598220
C	8.0904900	0.2397000	-0.8647280
C	8.1240820	-1.1474860	-1.0450270
C	9.1310700	-1.7271820	-1.8082030
C	10.1265530	-0.9404760	-2.3827760
C	10.0994470	0.4390010	-2.1932540
C	9.0859390	1.0305260	-1.4479650
H	7.3572190	-1.7626790	-0.5840620

H	9.1440870	-2.8048060	-1.9406060
H	10.9157890	-1.3982710	-2.9702030
H	10.8660930	1.0656350	-2.6388930
H	9.0586530	2.1068240	-1.3092600
C	8.5283840	1.8960490	1.5555500
C	8.8375520	2.9724900	2.3794770
C	8.0005550	4.0846510	2.4349030
C	6.8525960	4.1160710	1.6467560
C	6.5453600	3.0530570	0.8052800
H	9.1729290	1.0229890	1.5197180
H	9.7331790	2.9345640	2.9920370
H	8.2417550	4.9196790	3.0845360
H	6.1963790	4.9805580	1.6736700
H	5.6578030	3.0819170	0.1806030

8 ax-|| (ground state, M06-2X/6-31G*)

-3012.486866220

P	-2.1104340	-1.1403400	1.1794260
C	-0.6639850	-1.2181970	0.1155880
C	-0.6018590	-1.9018570	-1.0828160
C	-1.6259130	-2.5833010	-1.8460140
C	-2.9590710	-2.3471280	-1.8714480
C	-3.7054120	-1.3404410	-1.1449530
C	-3.4435230	-0.7033030	0.0520840
C	-2.4569640	-2.8650750	1.6371680
C	-1.4264740	-3.8014940	1.7465840
C	-3.7681680	-3.2370700	1.9481550
C	-4.0456830	-4.5339540	2.3657010
C	-3.0145180	-5.4653390	2.4718880
C	-1.7067280	-5.0995220	2.1637930
C	-4.4177080	0.2719380	0.3955290
C	-5.4339250	0.3691410	-0.5200180
S	-5.1854590	-0.7398490	-1.8319630
C	0.5746510	-0.6424340	0.5034100
C	1.5950980	-0.8976280	-0.3789060
S	1.0230500	-1.8647370	-1.7028720
O	-1.9705370	-0.1802050	2.3153990
C	2.9908870	-0.4582020	-0.2987270
C	3.8162750	-0.4016830	-1.4288630
C	5.1246260	0.0490670	-1.3445190
C	5.6572980	0.4562810	-0.1144730
C	4.8423890	0.3862740	1.0250410
C	3.5357240	-0.0609910	0.9304370
C	-6.6041270	1.2518080	-0.4760830
C	-7.7957220	0.9120780	-1.1330670

C	-8.9001540	1.7491670	-1.0824840
C	-8.8032340	2.9305880	-0.3599920
C	-7.6407410	3.3009770	0.3041020
C	-6.5414370	2.4592410	0.2367160
N	-9.9698100	3.8207540	-0.2974710
O	-10.9777800	3.4682010	-0.8825450
N	6.9782140	0.9344690	-0.0168280
C	8.0005860	0.4036470	-0.8425600
C	8.0675310	-0.9719250	-1.0900030
C	9.0691540	-1.4861970	-1.9050800
C	10.0272320	-0.6452950	-2.4665350
C	9.9676640	0.7222290	-2.2100930
C	8.9586220	1.2491340	-1.4120500
O	-9.8555940	4.8547550	0.3347410
C	7.2778010	2.0001200	0.8720640
C	8.4470200	1.9724460	1.6385720
C	8.7384070	3.0231930	2.5014100
C	7.8650110	4.1013530	2.6243010
C	6.6979830	4.1255780	1.8644750
C	6.4075970	3.0891330	0.9849420
H	-4.3653500	0.8406860	1.3180760
H	0.6766020	-0.0480130	1.4047660
H	-0.4062560	-3.5173540	1.5007800
H	-0.9047450	-5.8265110	2.2461820
H	-3.2317640	-6.4794190	2.7936370
H	-5.0653180	-4.8195440	2.6047920
H	-4.5729570	-2.5110060	1.8571110
H	-1.2617880	-3.3385750	-2.5389880
H	-3.5387830	-2.9367300	-2.5776090
H	-7.8649000	-0.0271240	-1.6742280
H	-9.8287640	1.5005560	-1.5813760
H	-7.6100350	4.2369970	0.8482780
H	-5.6157000	2.7464690	0.7244650
H	3.4205120	-0.6804820	-2.4023200
H	5.7394150	0.1020840	-2.2370990
H	5.2472310	0.6819230	1.9875660
H	2.9336690	-0.1268470	1.8316530
H	7.3303690	-1.6304140	-0.6406650
H	9.1074900	-2.5555120	-2.0896320
H	10.8116300	-1.0515210	-3.0967380
H	10.7046270	1.3910980	-2.6441840
H	8.9058830	2.3165750	-1.2215610
H	9.1208910	1.1257190	1.5493220
H	9.6491380	2.9907450	3.0916050
H	8.0921170	4.9152700	3.3050830
H	6.0122650	4.9635340	1.9444000

H	5.5047830	3.1131640	0.3823300
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8 eq (ground state, M06-2X/6-31G*)

-3012.486427160

C	6.5780370	2.6848430	-1.0438020
C	7.3797510	1.7023610	-0.4526970
C	8.5647160	2.0788550	0.1880800
C	8.9395310	3.4168570	0.2309690
C	8.1351010	4.3964890	-0.3456060
C	6.9520390	4.0220900	-0.9785070
N	7.0006230	0.3372620	-0.5084460
C	7.9977350	-0.6534190	-0.7056360
C	8.0072210	-1.8143400	0.0742850
C	8.9880790	-2.7794670	-0.1248670
C	9.9790330	-2.5924100	-1.0858030
C	9.9754510	-1.4308690	-1.8548860
C	8.9877270	-0.4688000	-1.6759530
C	5.6618090	-0.0433340	-0.2982260
C	5.1250590	-1.1537490	-0.9636230
C	3.8118840	-1.5376960	-0.7445100
C	2.9837820	-0.8304100	0.1363010
C	3.5272120	0.2798750	0.7965680
C	4.8402480	0.6686800	0.5875700
C	1.5938500	-1.2301230	0.3748930
S	1.0647650	-2.8569510	0.0940670
C	-0.5666940	-2.4980390	0.5815090
C	-0.6728080	-1.1736590	0.9692730
C	0.5568100	-0.4645740	0.8424240
C	-1.5348200	-3.5660900	0.5130890
C	-2.8829360	-3.4922730	0.4223610
C	-3.7202670	-2.3174630	0.3648740
C	-3.5062590	-1.0106600	0.7678080
C	-4.6171070	-0.1643230	0.4859060
C	-5.6647550	-0.8086320	-0.1167690
S	-5.2965980	-2.4857480	-0.3526460
P	-2.1178010	-0.4812000	1.7890380
O	-2.2449050	-0.8089430	3.2398910
C	-6.9523790	-0.2377680	-0.5248890
C	-8.1014450	-1.0355090	-0.6262880
C	-9.3182390	-0.4861990	-1.0018150
C	-9.3767160	0.8745610	-1.2690250
C	-8.2605890	1.6967050	-1.1804050
C	-7.0489070	1.1319640	-0.8147700
N	-10.6623090	1.4657170	-1.6626850
O	-11.6240120	0.7229320	-1.7355030

C	-2.0042010	1.3078560	1.4966330
O	-10.6845550	2.6614740	-1.8909580
H	-4.6472850	0.8828690	0.7680140
H	0.6591300	0.5885680	1.0804970
H	-1.1109880	-4.5667770	0.4674160
H	-3.4071930	-4.4387690	0.3162420
H	-8.0468960	-2.0936560	-0.3877750
H	-10.2165950	-1.0863250	-1.0792540
H	-8.3537370	2.7514840	-1.4082280
H	-6.1600120	1.7527440	-0.7722910
H	3.4155100	-2.3893530	-1.2918650
H	5.7455730	-1.7098490	-1.6588230
H	5.2469900	1.5196370	1.1243620
H	2.9231900	0.8251580	1.5157020
H	7.2430520	-1.9521480	0.8331550
H	8.9844780	-3.6763930	0.4868600
H	10.7472620	-3.3444150	-1.2331420
H	10.7394880	-1.2757710	-2.6104650
H	8.9768630	0.4330520	-2.2804850
H	9.1859460	1.3164150	0.6477040
H	9.8617620	3.6945280	0.7322950
H	8.4274340	5.4406750	-0.3037950
H	6.3191170	4.7742430	-1.4397380
H	5.6638450	2.3916080	-1.5509830
C	-2.0629230	2.1413670	2.6135440
C	-1.9845440	3.5235200	2.4514990
C	-1.8481760	4.0674940	1.1776550
C	-1.7896550	3.2349290	0.0589500
C	-1.8677180	1.8556050	0.2162860
H	-2.1691820	1.6900650	3.5962620
H	-2.0285240	4.1738420	3.3195320
H	-1.7859360	5.1443230	1.0520090
H	-1.6806680	3.6631240	-0.9326770
H	-1.8203100	1.2022690	-0.6527650