Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information for

1,4-Additions of tricyclic 1,4-diphosphinines – a novel system to study σ-bond activation and π–π dispersion interactions

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1. General Considerations

The lithiation/phosphanylation reactions were executed carefully under an argon atmosphere, using standard Schlenk-line techniques and dry solvents. Tetrahydrofuran, diethyl ether, pentane and toluene were dried over sodium wire/benzophenone, dichloro-methane over calcium hydride and further purified by subsequent distillation. All NMR spectra were recorded on a Bruker AX-300 spectrometer (300.1 MHz for ^{1}H, 75.5 MHz for ^{13}C, 121.5 MHz for ^{31}P). The ^{1}H and ^{13}C spectra were referenced to the residual proton resonances and the ^{13}C signals of the deuterated solvents and ^{31}P signals to 85% H_3PO_4 as the external standard, respectively. Elemental analyses were carried out on a Elementar Vario Micro elemental analyzer. Melting points were determined in one side melted off capillaries using Büchi Type apparatus. Mass spectrometric data were collected on a Kratos MS 50 spectrometer using EI, 70 eV. The X-ray diffraction analyses were performed on a Bruker D8-Venture or a Bruker X8-KappaApex TT type diffractometer at 123(2) or 100(2) K, respectively. The structures were solved by direct methods refined by the full matrix least-squares technique in anisotropic approximation for non-hydrogen atoms using the SHELXS97 and SHELXL9725 program packages. Hydrogen atoms were located from Fourier synthesis and refined isotopically. The crystallographic data for the structures reported in this paper have been deposited in the Cambridge Crystallographic Data Centre having the corresponding numbers: 1589254 (**2a**), 1589255 (**2b**), 1589256 (**3a**) and 1589257 (**3b**).

2. Common protocol for 2a,b

A solution of **1** (0.48 g, 1 mmol) in toluene (20 ml) was heated with 0.12 ml of dimethyl acetylene dicarboxylate (for **2a**; heated for 1 h at 50 °C) or *N*-phenylmaleimide (0.17 g for **2b**; heated at 110 °C for 3h) in a Schlenk tube. The color of the reaction mixture turned dark reddish brown for **2a** and light red-orange for **2b**. Afterwards the solvent was removed under reduced pressure (8× 10^{-3} mbar) and the residue was washed with *n*-pentane (3×5 ml). Finally it was dried under vacuum (8× 10^{-3} mbar) to get **2a,b** in pure form.

2.1 Compound 2a

Analytical data

2a: Yield: 0.59 g (0.95 mmol, 95.0 %) , brick red powder. m.p. decom. at 180°C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.99 (t, 12H, $^{3}J_{H,H}$ = 7.3 Hz, $NCH_2CH_2CH_2\underline{Me}$), 1.39 (tq, 8H, $^{3}J_{H,H}$ = 7.3 Hz = 14.9 Hz, $^{3}J_{H,H}$ = 7.49 Hz, $NCH_2CH_2\underline{CH_2}Me$), 1.69-1.86 (m, 8H, $NCH_2\underline{CH_2}CH_2Me$), 3.87 (s, 6H, $-CO_2\underline{Me}$), 4.27 (t, 8H, $^{3}J_{H,H}$ = 7.4 Hz $N\underline{CH_2}CH_2CH_2Me$). ^{13}C NMR (75.0 MHz, $CDCl_3$): δ = 13.8 (s, $NCH_2CH_2CH_2\underline{Me}$), 20.1 (s, $NCH_2CH_2\underline{CH_2}Me$), 31.6 (s, $NCH_2\underline{CH_2}CH_2Me$), 47.8 (dd, $^{3}J_{P,C}$ = 4.6 Hz, $N\underline{CH_2}CH_2CH_2Me$), 53.4 (s, $-CO_2\underline{Me}$), 128.6 (d, $^{1}J_{P,C}$ = 61.2 Hz, P-$\underline{C}O_2Me$), 142.5 (t, $J_{P,C}$ = 4.1 Hz, *P-C* of the middle ring), 160.5 (dd, $^{2}J_{P,C}$ = 14.1 Hz, $^{2}J_{P,C}$ = 11.9 Hz, $-\underline{C}O_2Me$) 164.3 (s, *C=S*), 166.1 (dd, $^{2}J_{P,C}$ = 16.8 Hz, $-\underline{C}O_2Me$). ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = -87.3 (s). IR [cm^{-1}]: ṽ = 2957 (w), 2933 (w), 2873 (w), 1721 (s), 1435 (m), 1404 (s), 1245 (s), 1217 (s). MS (EI, 70 eV): m/z (%) = 624.1 (10) $[M]^{\cdot+}$, 482.2 (100) $[M\text{-}C_6H_6O_4]^{\cdot+}$HRMS: theor./exp. for $[C_{28}H_{42}N_4O_4P_2S_2]$: 624.2123/624.2123. EA [%]: theor./exp. C 53.83/53.55 , H 6.78/6.73, N 8.97/8.82, S 10.26/9.84.

Figure 1. ^{1}H NMR spectrum of 2a in $CDCl_3$ (300.1 MHz, 25 °C)

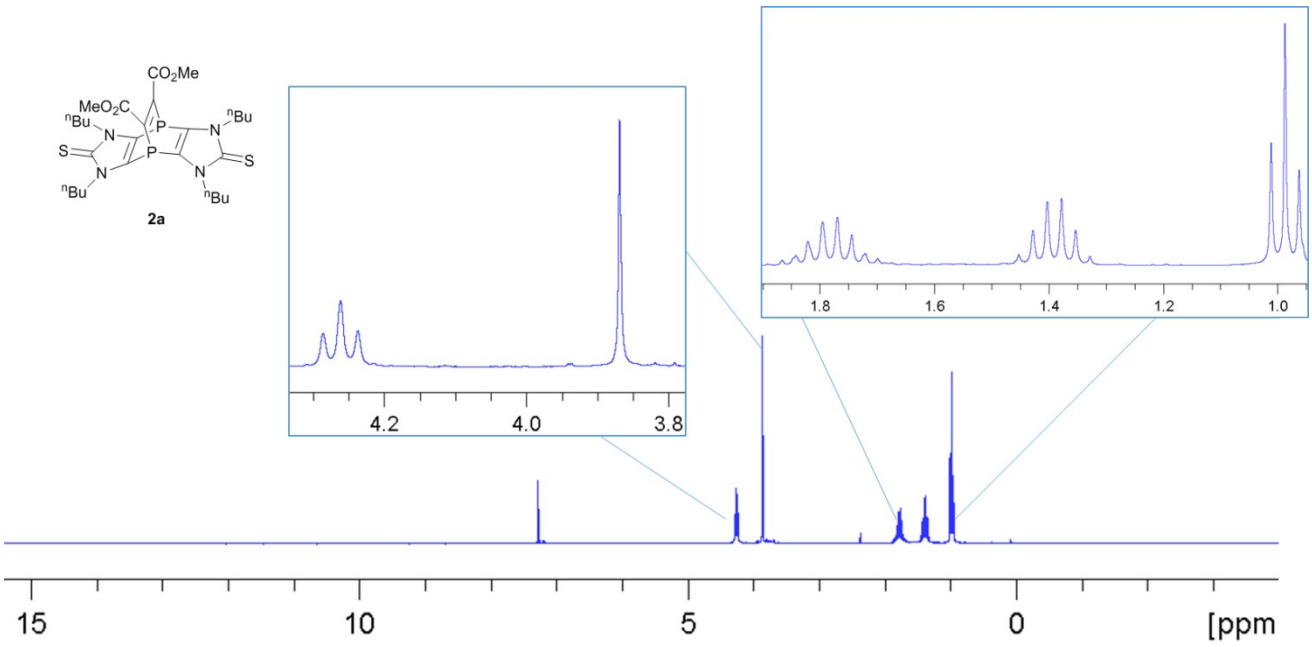


Figure 2. ^{13}C {^{1}H} NMR spectrum of 2a in $CDCl_3$ (75.5 MHz, 25 °C)

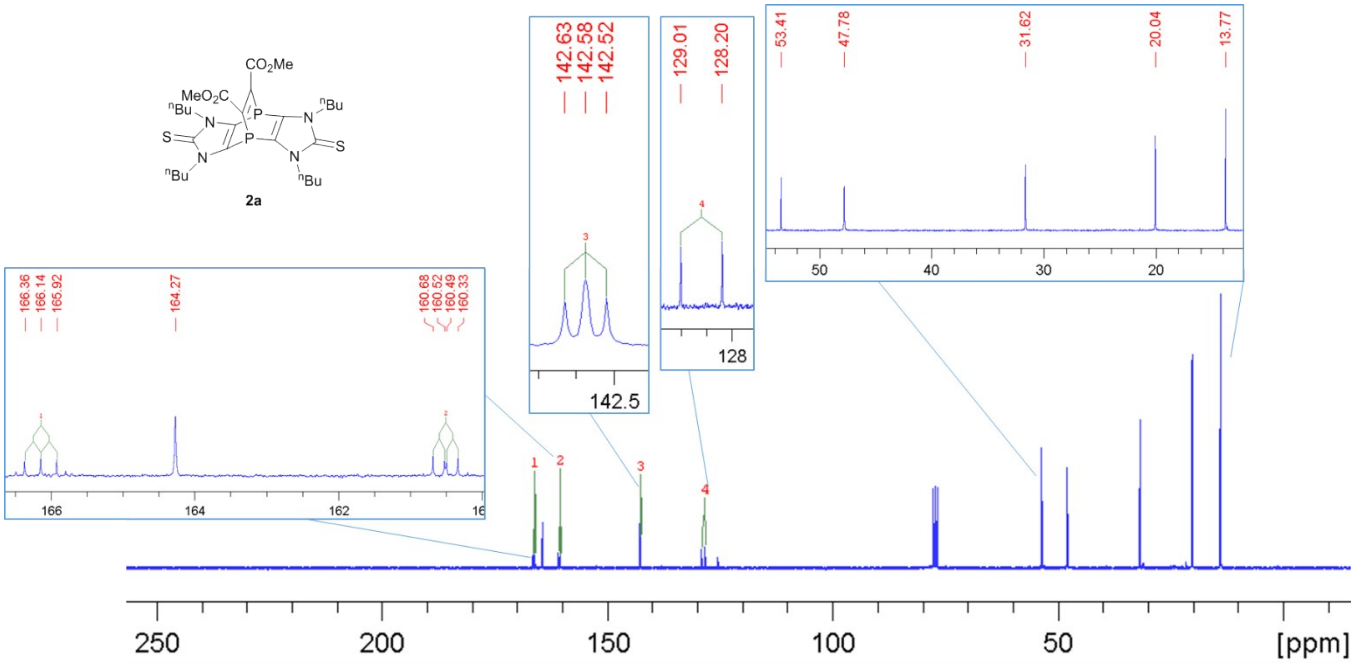
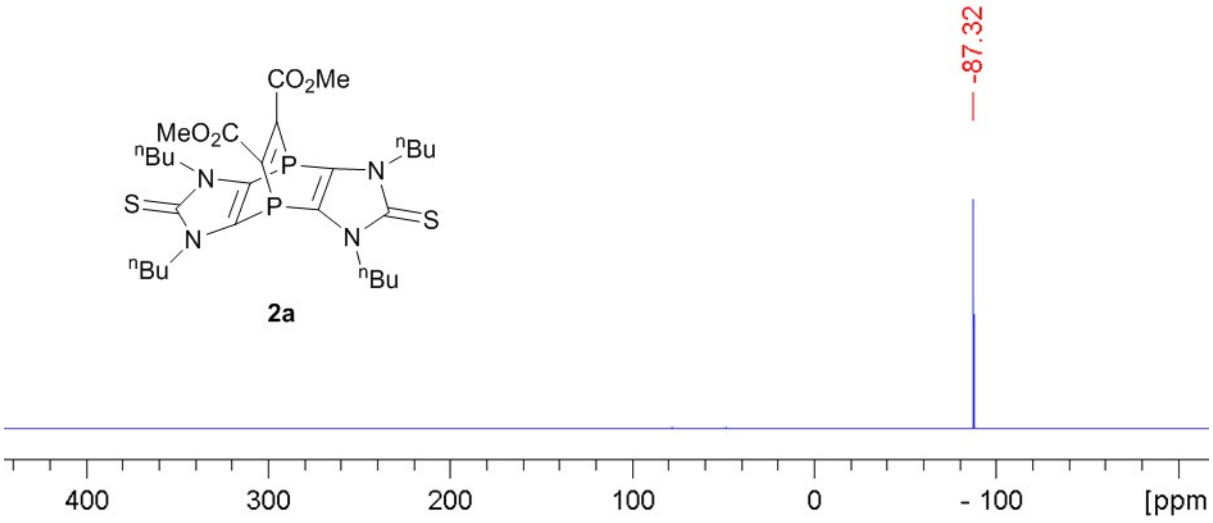


Figure 3. ^{31}P NMR spectrum of 2a in $CDCl_3$ (121.5 MHz, 25 °C)



2.2 Compound 2b

Analytical data

2b: Yield: 0.59 g (0.91 mmol, 91.0 %), orange powder. m.p. decomp. at 160°C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 0.89 (t, 6H, $^{3}J_{H,H}$ = 7.3 Hz, $NCH_2CH_2CH_2\underline{Me}$), 1.01 (t, 6H, $^{3}J_{H,H}$ = 7.3 Hz, $NCH_2CH_2CH_2\underline{Me}$), 1.29-1.49 (m, 8H, $NCH_2CH_2\underline{CH_2}Me$), 1.63-1.84 (m, 8H, $NCH_2\underline{CH_2}CH_2Me$), 3.72 (t, 2H, $^{3}J_{P,H}$ = 4.9 Hz, P-$\underline{CH}$), 4.09-4.39 (m, 8H, $N\underline{CH_2}CH_2CH_2Me$), 6.75-7.45 (m, 5H, *Ph ring protons*). ^{13}C{1H} NMR (75.0 MHz, $CDCl_3$): δ = 13.5 & 13.8 (s, $NCH_2CH_2CH_2\underline{Me}$), 19.9 & 20.1 (s, $NCH_2CH_2\underline{CH_2}Me$), 31.5 & 31.7 (s, $NCH_2\underline{CH_2}CH_2Me$), 44.5 (dd, $^{3}J_{P,C}$ = 8.4 Hz, P-$\underline{CH}$), 47.3 (t, $^{3}J_{P,C}$ = 1.9 Hz, $N\underline{CH_2}CH_2CH_2Me$), 47.5 (t, $^{3}J_{P,C}$ = 2.1 Hz, $N\underline{CH_2}CH_2CH_2Me$), 126.3 (s, *Ph ring C*), 129.5 (s, *Ph ring C*), 129.6 (s, *Ph ring C*), 130.5 (s, *Ph ring C*), 133.0 (dd, $J_{P,C}$ = 6.4 Hz, *P-C* of the middle ring), 134.5 (dd, $J_{P,C}$ = 3.5 Hz, *P-C* of the middle ring), 167.4 (s, -*C*(O)-), 172.4 (t, $^{3}J_{P,C}$ = 3.3 Hz, *C=S*). ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = -86.3 (t, $^{2}J_{P,H}$ = 4.9 Hz). IR [cm^{-1}]: ṽ = 2956 (w), 2930 (w), 2870 (w), 1768 (w), 1704 (s), 1404 (s), 1373 (s), 1217 (w), 1162 (s). Pos-ESI-MS: for $C_{32}H_{43}N_5O_2P_2S_2H$ theor./exp. 656.2417/656.2406. EA [%]:theor./exp. C 58.61/58.02 , H 6.61/6.76, N 10.68/10.12, S 9.78/9.10.

Figure 4. ^{1}H NMR spectrum of 2b in $CDCl_3$ (300.1 MHz, 25 °C)

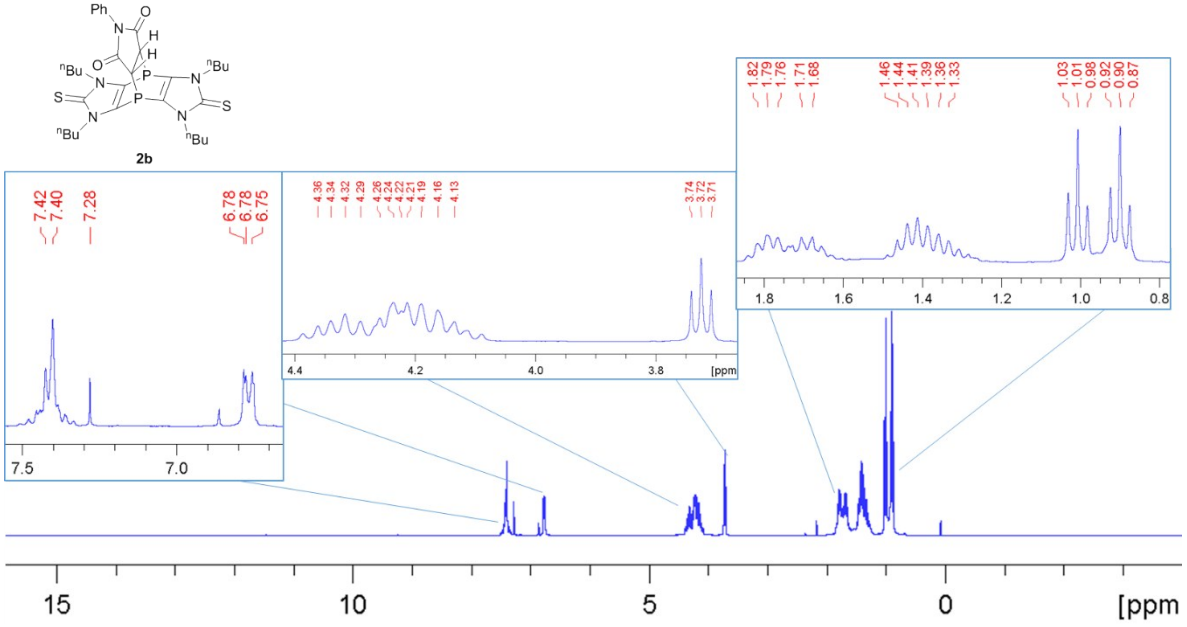


Figure 5. ^{13}C {^{1}H} NMR spectrum of 2b in $CDCl_3$ (75.5 MHz, 25 °C)

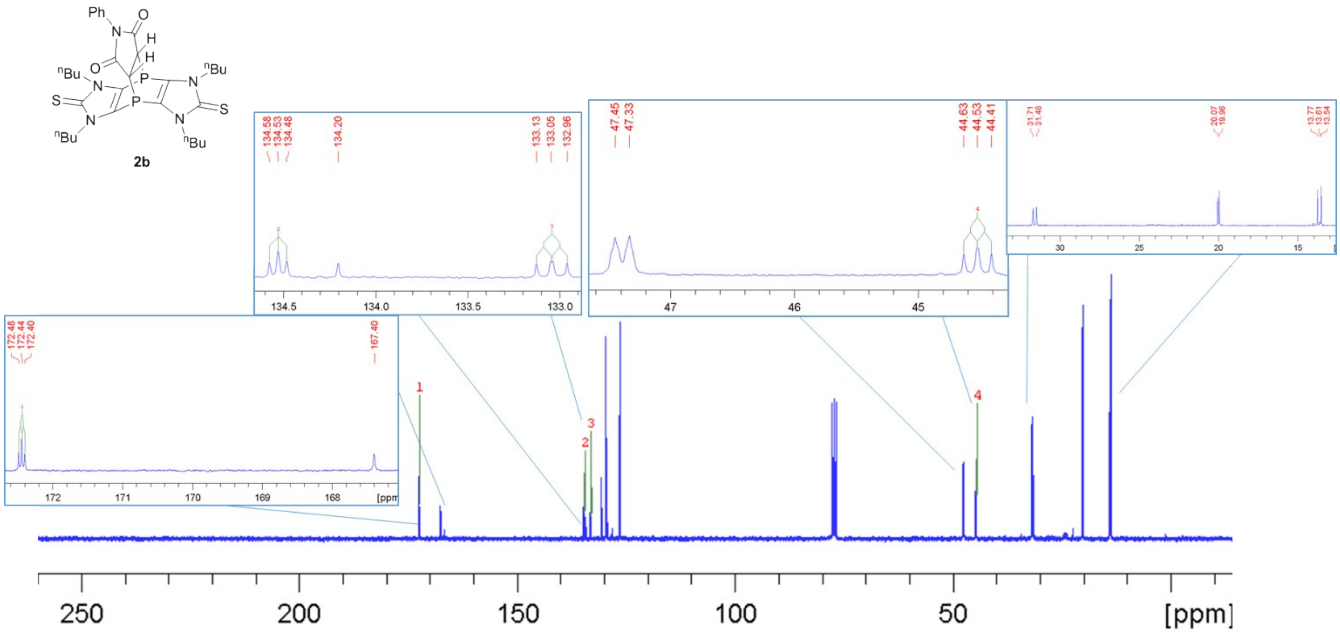
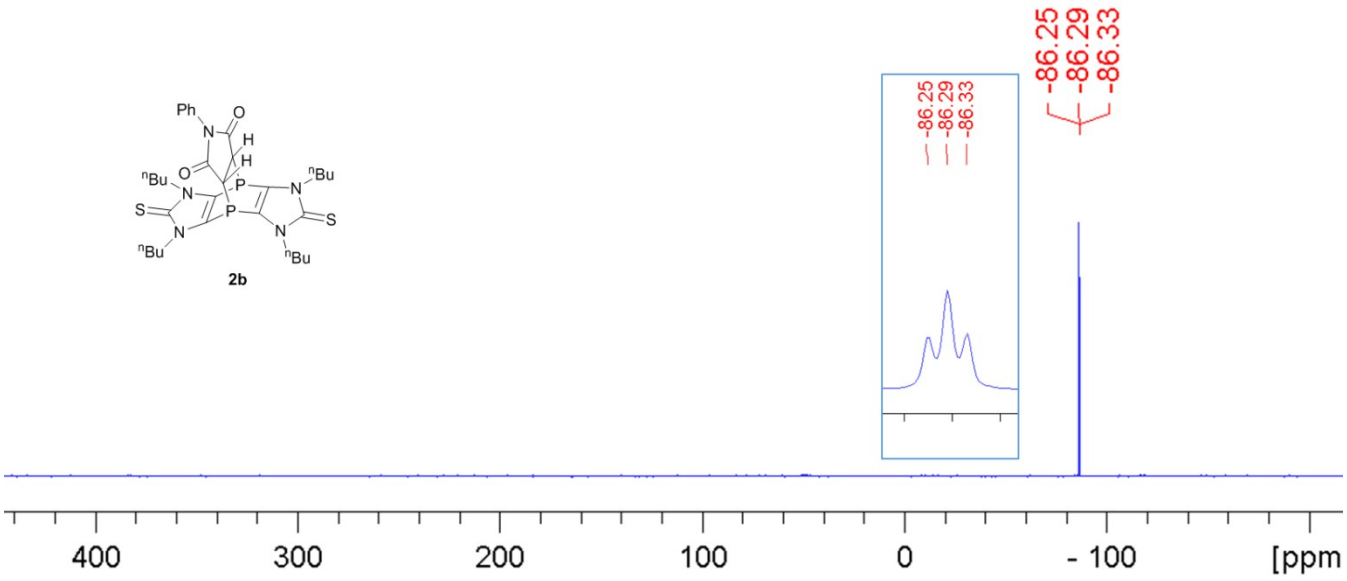


Figure 6. ^{31}P NMR spectrum of 2b in $CDCl_3$ (121.5 MHz, 25 °C)



3. Synthetic protocol for Compounds 3a,b

A solution of 1 (0.48 g, 1 mmol) in toluene (20 ml) was heated with 0.22 g of diphenyl disulfide (for 3a; heated for 2 days) or 0.31 g of diphenyl diselenide (for 3b; heated for 6h) or 0.41 g of diphenyl ditelluride at 110°C in a Schlenk tube. The color of the reaction mixture turned yellow in cases of Ph_2S_2 and Ph_2Se_2 from dark blood red during the course of the reaction. After the complete consumption of the starting materials the solvent was removed under reduced pressure (8× 10^{-3} mbar) and Afterwards the solvent was removed under reduced pressure (8× 10^{-3} mbar) and the residue was washed with *n*-pentane (3×5 ml). Finally it was dried under vacuum (8× 10^{-3} mbar) to get 3a,b in pure form as yellow powders. But in case of Ph_2Te_2 no reaction could be observed even after heating at 110°C for a week.

3.1 Compound 3a

Analytical data

Yield: 0.55 g (0.78 mmol, 78.0 %), yellow powder. M.p. decom. 195°C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.06 (t, 12H, $^3J_{H,H}$ = 7.3 Hz, $NCH_2CH_2CH_2\underline{Me}$), 1.42-1.54 (m, 8H, $NCH_2CH_2\underline{CH_2}Me$), 1.58-1.73 (m, 4H, $NCH_2\underline{CH_2}CH_2Me$), 1.82-1.97 (m, 4H, $NCH_2\underline{CH_2}CH_2Me$), 3.98-4.08 (m, 4H, $N\underline{CH_2}CH_2CH_2Me$), 4.47-4.57 (m, 4H, $N\underline{CH_2}CH_2CH_2Me$), 6.33 (d, 4H, $^3J_{H,H}$ = 7.9 Hz, *o-protons of Ph ring*), 7.07 (t, 4H, $^3J_{H,H}$ = 7.5 Hz, *m-protons of Ph ring*), 7.29 (t, 2H, $^3J_{H,H}$ = 7.5 Hz, *p-protons of Ph ring*). ^{13}C{1H} NMR (75.0 MHz, $CDCl_3$): δ 13.8 (s, $NCH_2CH_2CH_2\underline{Me}$), 20.1 (s, $NCH_2CH_2\underline{CH_2}Me$), 31.1 (s, $NCH_2\underline{CH_2}CH_2Me$), 46.9 (t, $^3J_{P,C}$ = 3.4 Hz, $N\underline{CH_2}CH_2CH_2Me$), 125.4 (dd, , $^3J_{P,C}$ = 7.4 Hz, $^3J_{P,C}$ = 6.5 Hz, *ipso-C of Ph ring*), 126.3 (t, $J_{P,C}$ = 4.1 Hz, *P-C* of the middle ring), 128.9 (s, *Ph ring C*) 129.2 (s, *p-C of Ph ring*), 134.9 (s, *Ph ring C*), 167.5 (t, $^3J_{P,C}$ = 1.6 Hz *C=S*). ^{31}P NMR (121.5 MHz, $CDCl_3$, 25 °C): δ = -34.2 (s). IR [cm^{-1}]: ν̃ = 2958 (w), 2931 (w), 2871 (w), 1436 (s), 1398 (s), 1286 (s), 1216 (s), 1159 (s), 861 (s), 745 (s). Pos-ESI-MS: for $C_{34}H_{46}N_4P_2S_4H$ theor./exp. 701.2165/701.2153. EA [%]: theor./exp. C 58.26/58.01, H 6.61/6.66, N 7.99/7.83, S 18.29/17.43.

Figure 10. ^{1}H NMR spectrum of 3a in THF-d_8 (300.1 MHz, 25 °C)

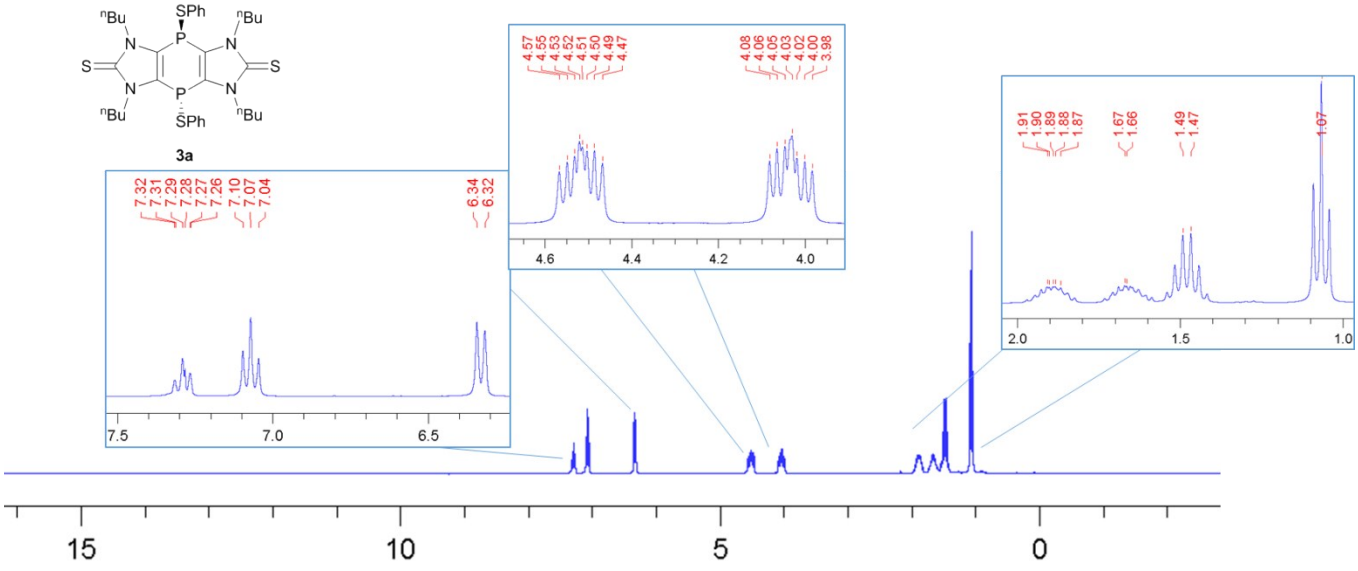


Figure 11. ^{13}C {^{1}H} NMR spectrum of 3a in THF-d_8 (75.5 MHz, 25 °C)

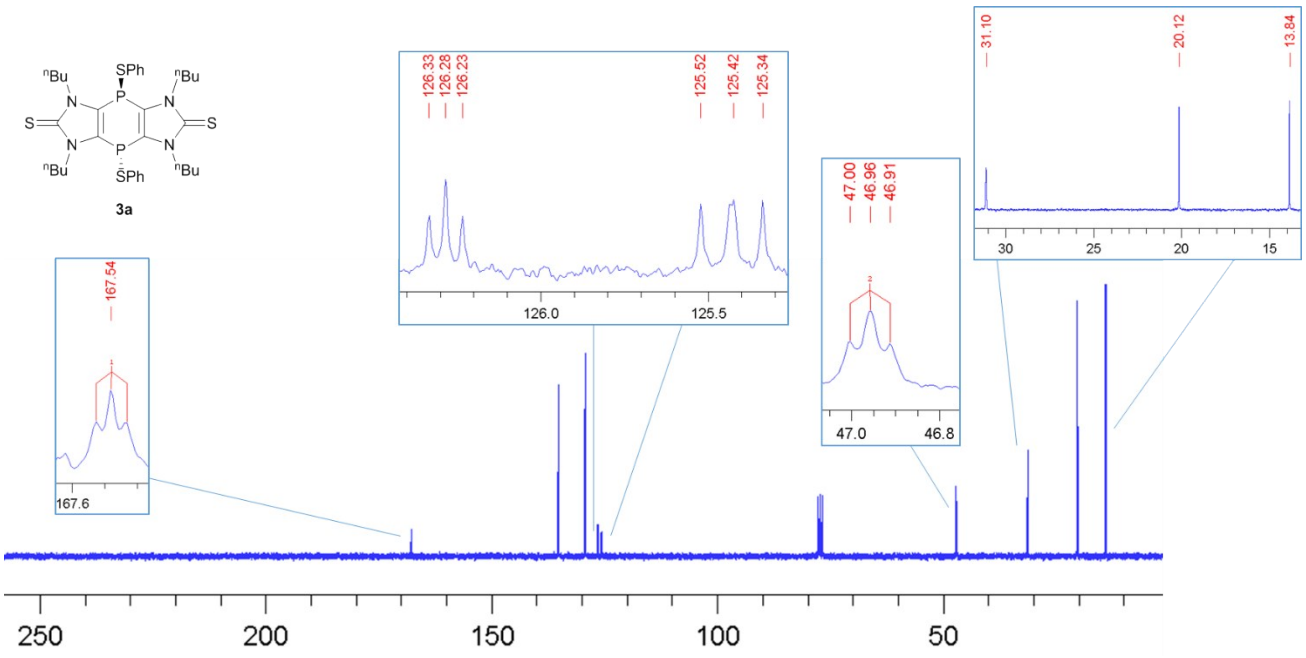
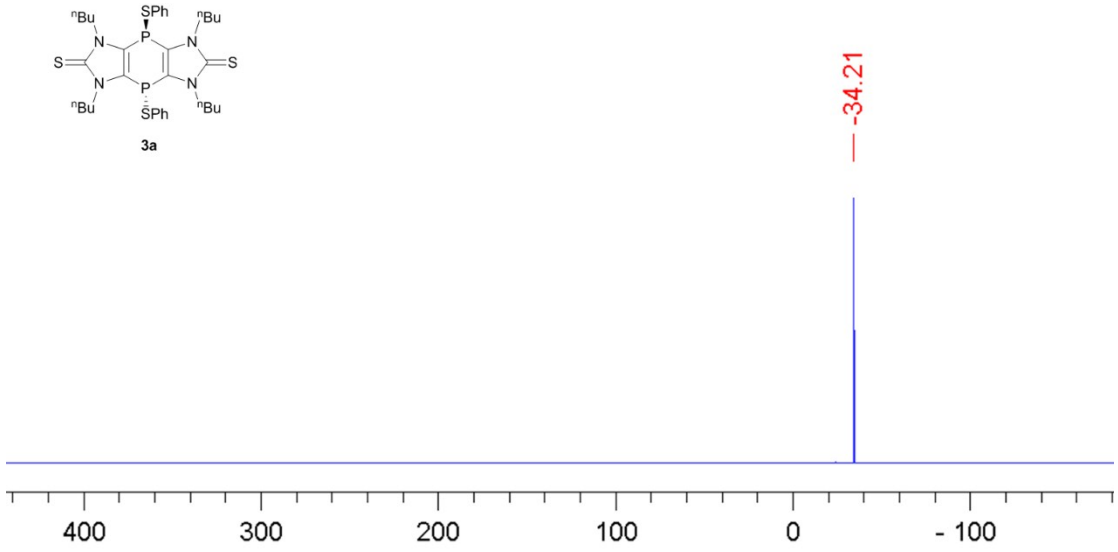


Figure 12. ^{31}P NMR spectrum of 3a in THF-d_8 (116.6 MHz, 25 °C)



3.2 Compound 3b

Analytical data for 3b

Yield: 0.59 g (0.75 mmol, 75.0 %), yellow solid, m.p.: 188 °C , ^{1}H NMR (300.1 MHz, C_6D_6, 25 °C): δ = 0.91 (t, 12H, $^{3}J_{H,H}$ = 7.2 Hz, $NCH_2CH_2CH_2\underline{\textit{Me}}$), 1.25-1.35 (m, 8H, $NCH_2CH_2\underline{\textit{CH}_2}Me$), 1.67-1.78 (m, 4H, $NCH_2\underline{\textit{CH}_2}CH_2Me$), 1.92-2.03(m, 4H, $NCH_2\underline{\textit{CH}_2}CH_2Me$), 4.01-4.08 (m, 4H, $N\underline{\textit{CH}_2}CH_2CH_2Me$), 4.60-4.68 (m, 4H, $N\underline{\textit{CH}_2}CH_2CH_2Me$), 6.42 (d, 4H, $^{3}J_{H,H}$ = 7.6 Hz, *o-protons of Ph ring*), 6.77 (t, 4H, $^{3}J_{H,H}$ = 6.8 Hz, *m-protons of Ph ring*), 6.91 (tt, 2H, $^{3}J_{H,H}$ = 7.5 Hz, $^{3}J_{H,H}$ = 1.2 Hz *p-protons of Ph ring*). $^{13}C\{^{1}H\}$ NMR (75.5 MHz, C_6D_6, 25 °C): δ = 13.6 (s, $NCH_2CH_2CH_2\underline{\textit{Me}}$), 20.1 (s, $NCH_2CH_2\underline{\textit{CH}_2}Me$), 30.9 (s, $NCH_2\underline{\textit{CH}_2}CH_2Me$), 46.7 (t, $^{3}J_{P,C}$ = 3.8 Hz, $N\underline{\textit{CH}_2}CH_2CH_2Me$), 124.1 (t, $J_{P,C}$ = 4.1 Hz, *P-C* of the middle ring), 124.6 (dd, , $^{3}J_{P,C}$ = 9.5 Hz, $^{3}J_{P,C}$ = 7.9 Hz, *ipso-C of Ph ring*), 128.7 (s, *Ph ring C*) 129.0 (s, *p-C of Ph ring*), 136.3 (s, *Ph ring C*), 168.9 (br, *C=S*). ^{31}P NMR (121.5 MHz, C_6D_6, 25 °C): δ = -44.6 (s). IR [cm^{-1}]: $\tilde{\nu}$ = 2957 (w), 2930 (w), 2871 (w), 1436 (s), 1396 (s), 1285 (s), 1216 (s), 1157 (s), 861 (s), 739 (s). Pos-ESI-MS: for $C_{34}H_{46}N_4P_2Se_2S_2H$ theor./exp. 797.1052/797.1047. EA [%]: theor./exp. C 51.38/50.71, H 5.83/5.83, N 7.05/6.92, S 8.07/8.12.

Figure 13. ^{1}H NMR spectrum of 3b in $CDCl_3$ (300.1 MHz, 25 °C)

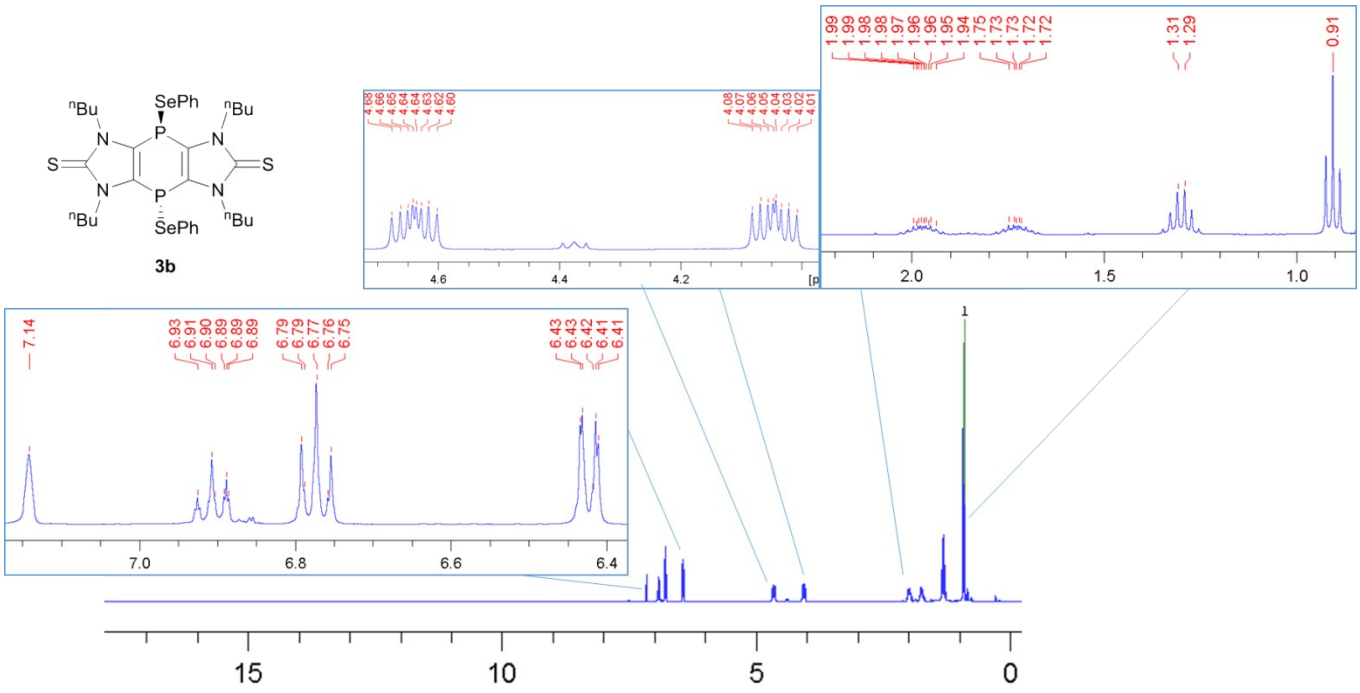


Figure 14. $^{13}C\ \{^{1}H\}$ NMR spectrum of 3b in $CDCl_3$ (75.5 MHz, 25 °C)

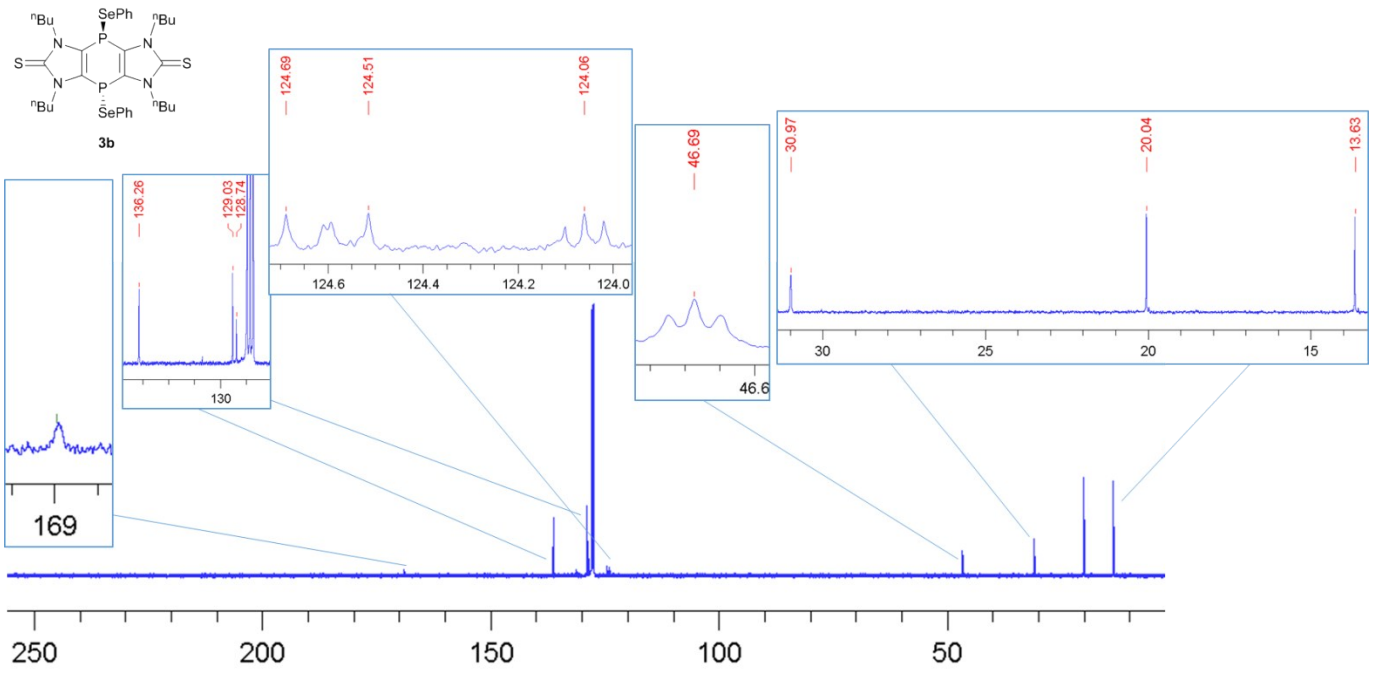
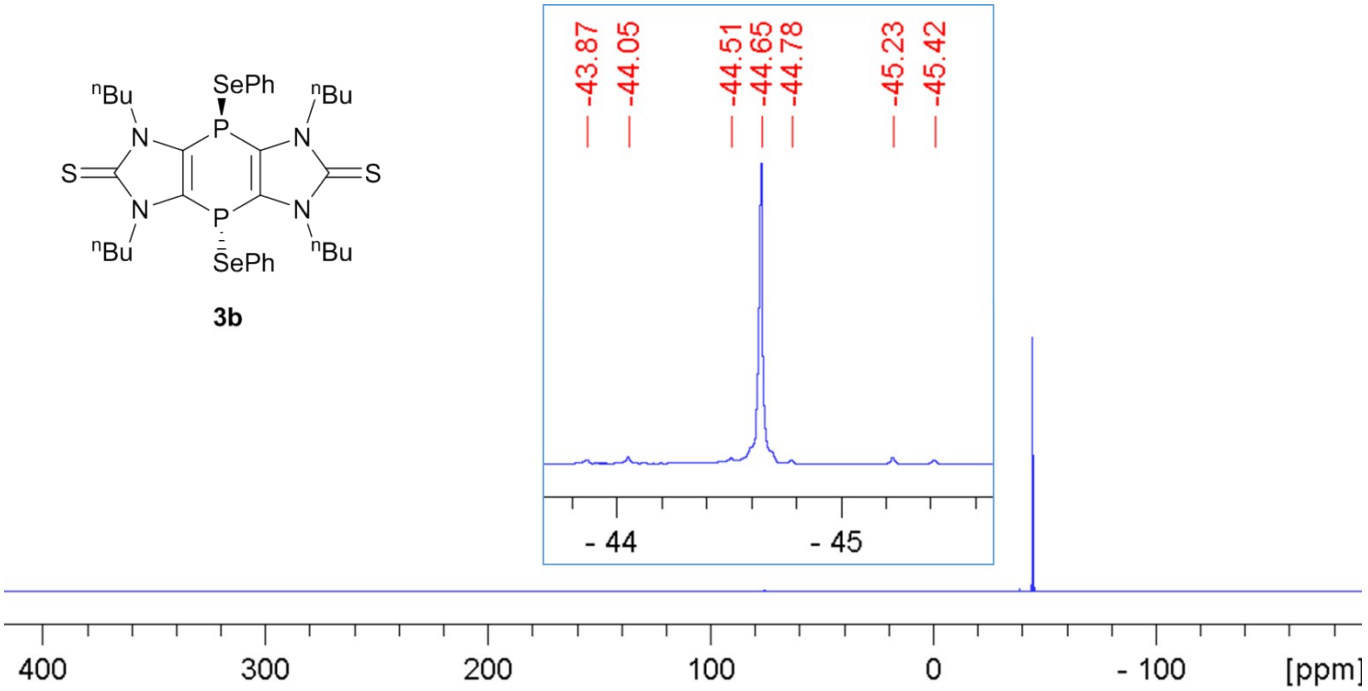
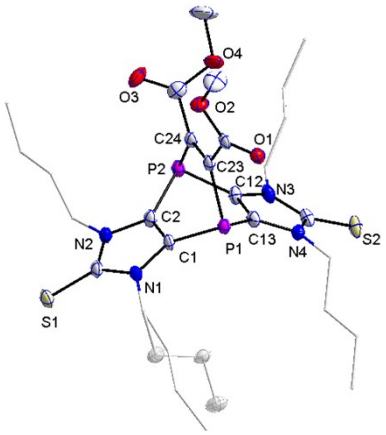


Figure 15. ^{31}P NMR spectrum of 3b in $CDCl_3$ (121.5 MHz, 25 °C)



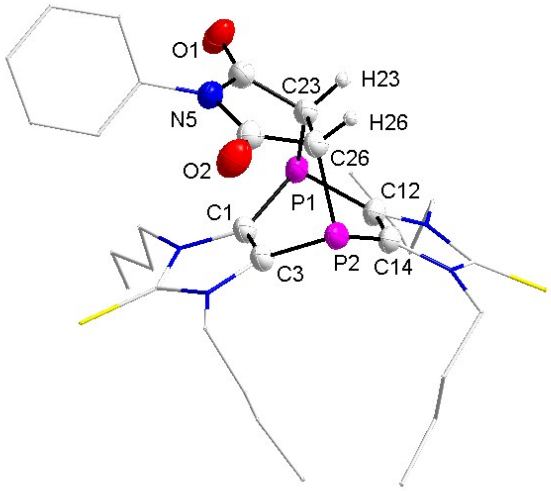
X-ray data of the compounds

Compound 2a



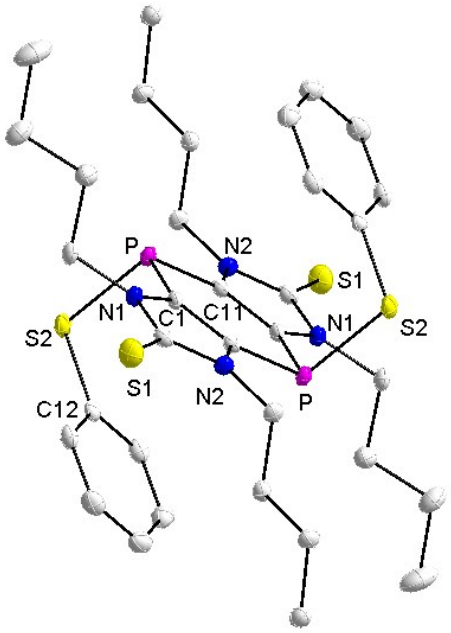
$C_{63}H_{92}N_8O_8P_4S_4$, $2(C_{28}H_{42}N_4O_4P_2S_2)$, C_7H_8, M = 1341.56, crystal size 0.36 × 0.06 × 0.02 mm^3, triclinic, space group P-1, Z = 2, a = 14.6456(8) Å, b = 15.5637(9) Å, c = 17.4714(10) Å, α = 67.920(3)°, β = 78.389(3)°, γ = 73.028(3)°. V = 3510.8(4)$Å^3$, d_c = 1.269 $g.cm^{-3}$, μ = 0.283 mm^{-1}, T = 100 K, $2\theta_{max}$ = 51.998°, independent reflections 23083, R_1[for I>=2σ (I)] = 0.0970, wR_2 (for all data) = 0.2482, goodness of fit 1.067, ΔF(max/min) = 1.30/-0.86 e $Å^{-3}$.

Compound 2b



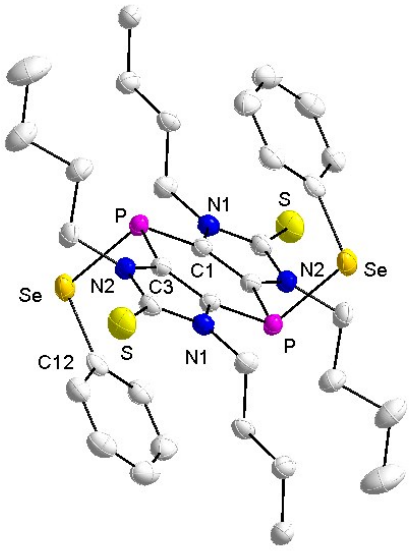
$C_{129}H_{174}Cl_2N_{20}O_8P_8S_8$, $4(C_{32}H_{43}N_5O_2P_2S_2)$,$CH_2Cl_2$, M = 2708.01, crystal size 0.18×0.12×0.07mm^3, monoclinic, space group C2/c, Z = 2, a = 27.7111(12) Å, b = 14.5378(7) Å, c = 21.9682(16) Å, α = 90°, β = 126.3663(11)°, γ = 90°. V = 7126.5(7) $Å^3$, d_c = 1.262 $g.cm^{-3}$, μ = 0.313 mm^{-1}, T = 100 K, $2\theta_{max}$ = 56 °, independent reflections 8586, R_{int} = 0.0533, R_1[for I>=2σ (I)] = 0.0729, wR_2 (for all data) = 0.2277, goodness of fit 1.062, ΔF(max/min) = 1.26/-0.51 e $Å^{-3}$.

Compound 3a



$C_{34}H_{46}N_4P_2S_4$, *M* = 700.93, crystal size 0.18 × 0.14 × 0.05 mm^3, monoclinic, space group $P2_1/c$, *Z* = 4, a = 18.465(3) Å, b = 13.1095(18) Å, c = 15.633(2) Å, α = 90°, β = 103.230(5)°, γ = 90°. V = 3683.8(9) Å^3, d_c = 1.264 g.cm^{-3}, μ = 0.374 mm^{-1}, *T* = 100.01 K, $2\theta_{max}$ = 56°, independent reflections 8895, R_{int} = 0.0776, R_1[for I>=2σ (I)] = 0.0466, wR_2 (for all data) = 0.0975, goodness of fit 1.078, ΔF(max/min) = 0.54/-0.40 e Å^{-3}.

Compound 3b



$C_{34}H_{46}N_4P_2S_2Se_2$, *M* = 794.73, crystal size 0.24 × 0.12 × 0.08 mm^3, monoclinic, space group $P2_1/c$, *Z* = 4, a = 18.5972(7) Å, b = 13.2665(5) Å, c = 15.6185(6) Å, α = 90 °, β = 103.2796(13) °, γ = 90 °. V = 3750.4(2) Å^3, d_c = 1.408 g.cm^{-3}, μ = 2.197 mm^{-1}, *T* = 100 K, $2\theta_{max}$ = 55.998°, independent reflections 9047, R_{int} = 0.0775, R_1[for I>=2σ (I)] = 0.0353, wR_2 (for all data) = 0.0754, goodness of fit 1.007, ΔF(max/min) = 0.39/-0.40e Å^{-3}.

4. Computation details

All calculations were carried out with the Gaussian 09 program package.[1] For H, C, N, O, P, S, Se atoms the 6-311+G** basis set were used (as it was implemented in G09), while for Te the def-2-TZVP basis set[2] was used. Full geometry optimization calculations were performed, followed by calculation of the harmonic vibrational at the optimized structures to establish the nature of the stationary points obtained, as characterized by none or a single negative eigenvalue of the Hessian for minima and transition structures, respectively. The Gibbs free energies were calculated based on the harmonic vibrational frequencies (atmospheric pressure, 298.15 ˇK). **1** and their derivatives were calculated with methyl substituents at the nitrogen atoms (instead of the *n*-buthyl) to reduce the computational time and they were labeled by the special character ‘. For the visualization of the molecular structures and the molecular orbitals the MOLDEN program was used.[3]

Table 1. Reaction energies and Gibbs free energies of the [4π+2π]-cyclo-addition reactions and the related reaction barriers in kcal.mol^{-1} unit at M06-2X/6-311+G level of theory**

	$\Delta E^{\#}$	$\Delta G^{\#}$	ΔE	ΔG
C_2H_2	16,3	24,6	-18,6	-2,5
C_2Ph_2	18,8	35,9	-13,9	5,4
DMAD	8,5	25,3	-24,6	-4,9
maleimide	0,3	18,2	-21,6	-2,3

Figure 16. Gibbs free energy profile of the possible formation of 3a' and 3b' compounds via 3cis intermediate at M06-2X/6-311+G level of theory and in kcal.mol^{-1} unit**

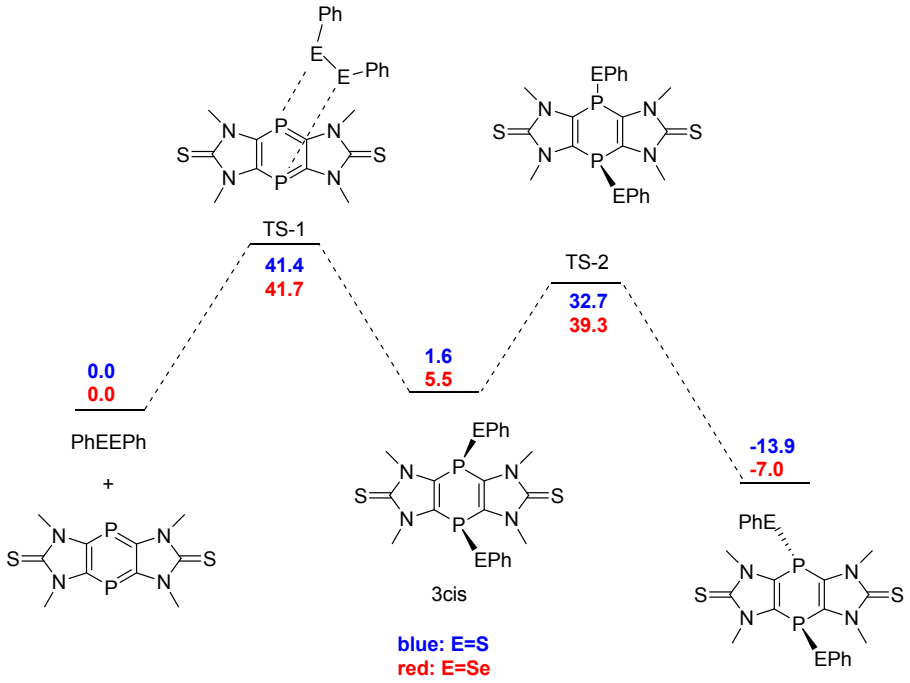


Figure 17. Gibbs free energy profile of the possible formation of 3a' and 3b' compounds via 3ipso intermediate at M06-2X/6-311+G level of theory and in kcal.mol^{-1} unit**

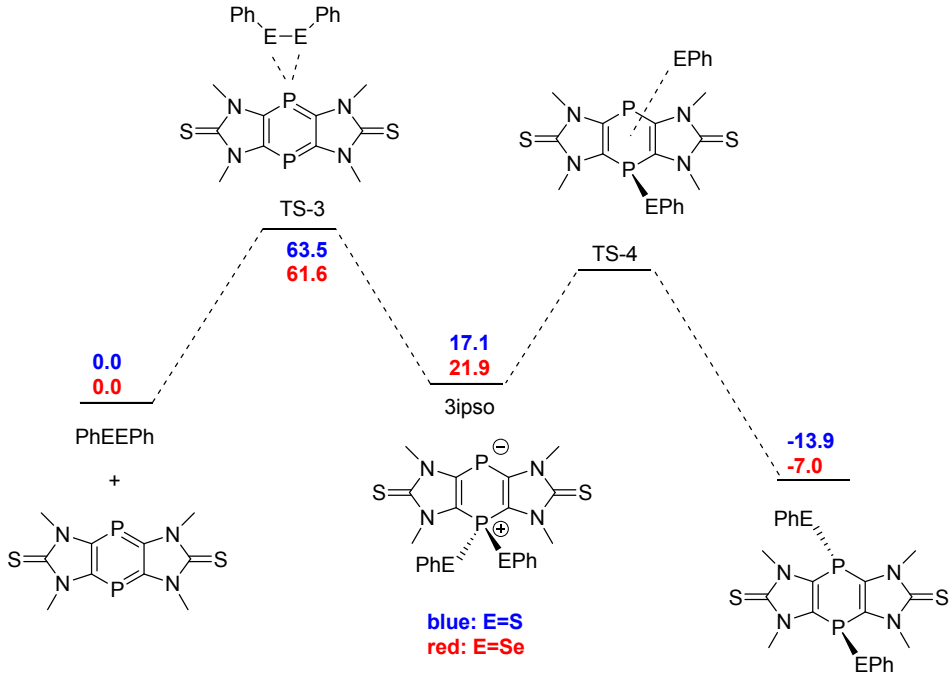


Figure 18. The in/in, in/out and out/out rotamers of 3a'

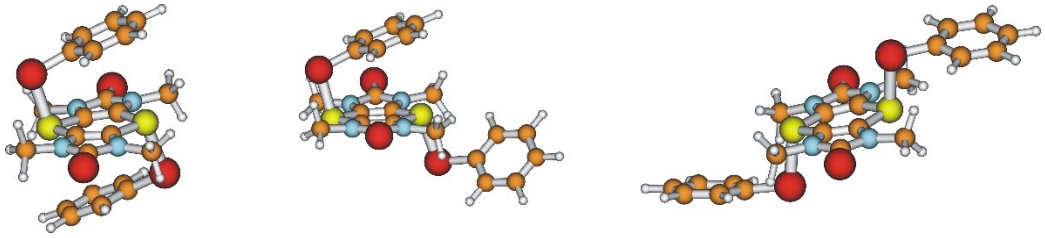


Table 2. Relative stability of the different rotamers in case of 3a' and 3b' at M06-2X-6-311+G level of theory and in kcal/mol unit**

	In/in	In/out	Out/Out
E=S	0.0	7.6	13.5
E=Se	0.0	5.9	13.8

Table 3. NICS(0) and NICS(1) values of the rotamers of 3a'

	In/in		In/out		Out/Out	
	NICS(0)	NICS(1)	NICS(0)	NICS(1)	NICS(0)	NICS(1)
Ph(1)	8.5	10.5; 11.3	8.5	10.9; 11.2	7.8	9.8; 10.5
Middle ring of the tricycle	6.1	7.6; 7.6	3.2	6.2; 2.1	0.6	1.0; 1.0
Ph(2)	8.5	10.5; 11.3	7.7	9.8; 10.2	7.8	9.8; 10.5

Table 4. NICS(0) and NICS(1) values of the rotamers of 4a'

	In/in		In/out		Out/Out	
	NICS(0)	NICS(1)	NICS(0)	NICS(1)	NICS(0)	NICS(1)
Ph(1)	8.4	10.5; 11.4	8.4	11.8 ; 10.6	7.2	9.7; 9.7
Middle ring of the tricycle	5.2	6.8; 6.8	3.8	6.3; 2.9	1.1	1.8; 1.8
Ph(2)	8.4	10.5; 11.4	7.1	9.9; 9.5	7.2	9.6; 9.7

XYZ geometries and total energies of the investigated systems

C_2H_2

G(M06-2X/6-311+G**)= -3345.507291

E(M06-2X/6-311+G**)= -77.316277

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.064284
H	-0.002339	0.000000	3.325454
C	-0.002240	0.000000	2.261196

C_2Ph_2

G(M06-2X/6-311+G**)= -539.204993

E(M06-2X/6-311+G**)= -539.359455

C	0.019076	0.017367	0.119593
C	0.005502	0.025204	1.330407
C	0.035329	0.007992	-1.303597
C	-0.010744	0.034592	2.753597
C	-1.005109	0.608492	-2.036679
C	-0.985067	0.596941	-3.426670
C	0.067697	-0.010646	-4.111243
C	1.104299	-0.608934	-3.394555
C	1.092291	-0.602025	-2.004449
H	-1.822210	1.080089	-1.504154
H	-1.793639	1.063627	-3.977995
H	0.080206	-0.017840	-5.195144
H	1.925280	-1.082768	-3.920876

H	1.896834	-1.066390	-1.447042
C	1.029524	-0.566204	3.486679
C	1.009500	-0.554622	4.876670
C	-0.043068	0.053304	5.561243
C	-1.079502	0.651884	4.844555
C	-1.067514	0.644939	3.454449
H	1.846489	-1.038036	2.954154
H	1.817947	-1.021524	5.427995
H	-0.055552	0.060540	6.645144
H	-1.900344	1.125958	5.370876
H	-1.871937	1.109512	2.897042

DMAD

G(M06-2X/6-311+G**)= -532.944216

E(M06-2X/6-311+G**)= -533.022403

C	0.000218	-0.000458	-0.000245
O	-0.000464	-0.000751	1.432818
C	1.205557	0.000000	1.995780
O	2.246524	-0.001169	1.403357
C	1.104879	0.002463	3.449617
C	1.082664	0.000502	4.648997
C	1.045999	0.070903	6.104142
O	0.965308	1.097099	6.716529
O	1.113537	-1.144007	6.643470
C	1.085740	-1.173214	8.075935
H	-1.046290	-0.000928	-0.290339
H	0.506851	0.889318	-0.373982
H	0.508066	-0.889229	-0.374645
H	1.146896	-2.223453	8.345358
H	1.933521	-0.618707	8.478216
H	0.158994	-0.731198	8.441621

Maleimide

G(M06-2X/6-311+G**)= -590.290056

E(M06-2X/6-311+G**)= -590.404109

C	-0.003681	0.035398	0.003987
C	-0.000300	0.000301	1.395937
C	1.198807	-0.035095	2.102801
C	2.400572	-0.042982	1.405835
C	2.408624	-0.000295	0.015756
C	1.205351	0.042688	-0.680300
N	-1.235812	0.000591	2.103805
C	-1.525201	-0.799657	3.220042
C	-2.931473	-0.460413	3.624453
C	-3.404533	0.463580	2.798392
C	-2.344850	0.801158	1.788763
O	-0.790065	-1.591348	3.737583
O	-2.419079	1.593079	0.892994
H	-4.369443	0.948197	2.780925

H	-3.404262	-0.944049	4.466343
H	1.187544	-0.067003	3.184099
H	3.333430	-0.076205	1.955576
H	3.348409	-0.000527	-0.522689
H	1.202871	0.075679	-1.763098
H	-0.942198	0.067535	-0.533137

Ts(C_2H_2)

G(M06-2X/6-311+G**)= -2163.401963

E(M06-2X/6-311+G**)= -2163.597380

C	-0.113405	0.294311	0.124436
S	0.014130	1.008700	3.207690
C	3.051270	0.276893	3.892152
C	1.217838	0.424943	2.214281
N	1.115976	0.131484	0.879109
N	2.511368	0.120582	2.554257
C	3.206269	-0.354750	1.453574
C	2.321157	-0.348526	0.389861
C	7.396743	-2.361212	0.266972
N	6.207235	-2.123987	-0.529624
C	6.070770	-2.522798	-1.835001
S	7.178253	-3.343634	-2.771143
H	4.566114	-3.359651	-3.850238
C	4.263159	-2.364669	-3.527330
C	5.059969	-1.480734	-0.093468
P	2.728445	-0.484446	-1.318787
N	4.815993	-2.116056	-2.208226
C	4.176163	-1.475450	-1.158219
P	4.959559	-0.504358	1.369377
C	4.978364	1.547033	-0.101353
C	4.189810	1.552631	-1.050590
H	4.640080	-1.633190	-4.244618
H	3.177528	-2.300646	-3.467051
H	-0.062468	-0.334826	-0.763224
H	-0.950415	-0.005688	0.753273
H	-0.249200	1.337779	-0.166048
H	2.233446	0.175347	4.603104
H	3.798957	-0.497710	4.062032
H	3.506835	1.262206	4.011974
H	7.896610	-3.245414	-0.124019
H	8.078452	-1.510171	0.205954
H	7.099921	-2.521465	1.303433
H	5.746178	2.000985	0.488508
H	3.754352	2.016462	-1.910201

Ts(C_2Ph_2)

G(M06-2X/6-311+G**)= -2625.283250

E(M06-2X/6-311+G**)= -2625.6366206

C	0.224718	-2.529422	2.582487

C	-0.687171	-1.596192	2.077812
C	-2.045729	-1.723446	2.383005
C	-2.481726	-2.765626	3.192828
C	-1.571601	-3.686025	3.703574
C	-0.218373	-3.561094	3.398158
C	-0.248616	-0.500855	1.231052
C	0.002093	0.717519	1.141819
C	0.186036	1.978945	1.837809
C	-0.909329	2.810656	2.088580
C	-0.727889	4.020253	2.748222
C	0.542312	4.413516	3.159316
C	1.634171	3.586582	2.909766
C	1.462693	2.377402	2.248116
P	-0.091752	-1.825805	-0.874178
C	1.424020	-1.019097	-1.277912
C	1.616589	0.347537	-1.371975
N	2.982261	0.566720	-1.327343
C	3.658217	-0.623809	-1.226884
N	2.686336	-1.588460	-1.183567
P	0.406617	1.611365	-1.152419
C	-1.007865	0.710848	-1.693730
C	-1.205679	-0.652116	-1.573867
N	-2.563012	-0.874986	-1.727395
C	-3.228629	0.308141	-1.932804
N	-2.255252	1.274789	-1.915318
C	-3.206615	-2.172685	-1.628848
S	-4.866709	0.521902	-2.162516
C	-2.512035	2.693801	-2.081824
C	3.611369	1.872296	-1.405822
S	5.306204	-0.876603	-1.192178
C	2.998952	-3.005190	-1.113521
H	-4.144751	-2.128117	-2.177899
H	-3.407913	-2.423820	-0.583916
H	-2.544509	-2.923391	-2.060807
H	2.080901	-3.571938	-1.258327
H	3.722470	-3.250092	-1.891151
H	3.439803	-3.245191	-0.144971
H	4.687080	1.718482	-1.460451
H	3.258941	2.393165	-2.297750
H	3.366871	2.464419	-0.520700
H	-3.453948	2.808047	-2.614679
H	-2.585369	3.186710	-1.109545
H	-1.696384	3.136186	-2.653906
H	-1.897892	2.501187	1.766773
H	-1.583425	4.656356	2.941858
H	0.683174	5.356828	3.672859
H	2.625357	3.882720	3.234017
H	2.309926	1.728716	2.053973
H	-2.749217	-0.999620	1.986120

H	-3.535533	-2.855620	3.428247
H	-1.914219	-4.497039	4.334599
H	0.495682	-4.272931	3.795682
H	1.276244	-2.431312	2.337282

Ts(DMAD)

G(M06-2X/6-311+G**)= -2619.039318

E(M06-2X/6-311+G**)= -2619.315978

C	0.024729	0.037649	0.013373
C	0.010706	0.015802	1.398331
N	1.326987	0.023272	1.813865
C	2.175879	0.063478	0.733667
N	1.353811	0.074362	-0.366761
P	-1.347091	-0.376282	2.450005
C	-2.666735	0.059994	1.369295
N	-3.993435	0.131680	1.751520
C	-4.817268	0.141025	0.651547
N	-3.970095	0.074875	-0.428986
C	-2.653703	0.030281	-0.014898
C	-4.470334	0.149451	3.122348
P	-1.302462	-0.396393	-1.060789
C	-4.405865	-0.021313	-1.811206
S	-6.478537	0.233236	0.637861
C	1.754855	-0.098394	3.196914
S	3.839066	0.109977	0.738952
C	1.846864	0.078804	-1.732159
C	-1.307883	-2.620544	1.331989
C	-1.323408	-2.630168	0.093312
C	-1.391934	-3.368753	-1.168609
O	-2.414879	-3.686279	-1.710308
C	-1.174242	-3.330862	2.605099
O	-0.125244	-3.528242	3.155684
O	-2.365174	-3.691981	3.085442
C	-2.329185	-4.364377	4.350388
O	-0.169425	-3.607493	-1.650491
C	-0.137344	-4.303399	-2.902309
H	-5.456202	0.258481	-1.849752
H	-4.284568	-1.046264	-2.169632
H	-3.812299	0.658571	-2.423795
H	1.093579	0.532470	-2.375575
H	2.768100	0.657738	-1.762716
H	2.054647	-0.940886	-2.063268
H	2.829764	0.064874	3.226351
H	1.245133	0.652562	3.802430
H	1.522194	-1.099567	3.567552
H	-5.457883	0.606304	3.129658
H	-4.540424	-0.868251	3.513273
H	-3.779129	0.733220	3.730578
H	0.915316	-4.408191	-3.149452

H	-0.608691	-5.280829	-2.801541
H	-0.661794	-3.727247	-3.665191
H	-3.365632	-4.579348	4.594383
H	-1.751986	-5.285240	4.271041
H	-1.877304	-3.719251	5.104408

TS(Melimid)

G(M06-2X/6-311+G**)= -2676.396430

E(M06-2X/6-311+G**)= -2676.7107141

C	-3.755012	0.136150	-1.019041
C	-3.117285	-1.094936	-0.910511
C	-3.855766	-2.259587	-0.703254
C	-5.237103	-2.178701	-0.589582
C	-5.882233	-0.950057	-0.692499
C	-5.138139	0.202521	-0.909981
N	-1.695871	-1.174918	-1.023662
C	-0.924118	-0.466881	-1.959271
C	0.504255	-0.858173	-1.719832
C	0.524686	-1.784028	-0.686917
C	-0.887656	-2.020087	-0.249499
O	-1.350961	0.305143	-2.775751
O	-1.278324	-2.768330	0.607798
P	1.238884	1.455375	-1.092829
C	0.084584	1.374348	0.239274
C	0.053616	0.453159	1.272410
N	-1.174075	0.591564	1.894417
C	-1.897510	1.609853	1.320119
N	-1.123918	2.045866	0.266599
P	1.179500	-0.875792	1.558138
C	2.601092	-0.174932	0.777325
C	2.622484	0.732277	-0.268247
N	3.914176	0.735889	-0.769034
C	4.706073	-0.139286	-0.068303
N	3.882346	-0.693300	0.878857
C	4.397584	1.548489	-1.871552
C	4.356235	-1.653467	1.861590
S	6.321382	-0.461368	-0.299865
C	-1.625672	-0.218937	3.015205
S	-3.364552	2.220026	1.817245
C	-1.486917	3.114452	-0.650415
H	4.514315	-2.627211	1.395279
H	3.615864	-1.736512	2.655592
H	5.305372	-1.302358	2.265032
H	-2.587376	0.172983	3.338197
H	-1.734493	-1.257509	2.696496
H	-0.901915	-0.149614	3.829442
H	-1.510097	2.729201	-1.672661
H	-2.472005	3.475606	-0.361607
H	-0.759996	3.925689	-0.576698

H	3.827006	2.476288	-1.901897
H	5.452264	1.758829	-1.703064
H	4.289463	1.017146	-2.819479
H	-3.351697	-3.212284	-0.619098
H	-5.809166	-3.082929	-0.420564
H	-6.960081	-0.892561	-0.600450
H	-5.627262	1.166266	-0.978859
H	-3.180099	1.035536	-1.186959
H	1.205062	-0.822290	-2.541414
H	1.256285	-2.569838	-0.563733

Cycloadditon product with C_2H_2

G(M06-2X/6-311+G**)= -2163,653148

E(M06-2X/6-311+G**)= -2163.653148

N	0.002801	0.001335	0.013278
C	-0.000502	0.006211	1.395859
C	1.291749	0.006264	1.804655
N	2.084212	0.001336	0.671719
C	1.293792	0.007076	-0.448683
P	-1.401169	-0.084706	2.576111
C	-0.669232	-1.510427	3.559251
C	0.594672	-1.510381	3.959078
P	1.758781	-0.084590	3.575744
C	0.568351	1.211655	4.091255
N	0.724332	2.267448	4.970195
C	-0.464336	2.936777	5.108625
N	-1.357086	2.267353	4.311777
C	-0.723900	1.211610	3.682456
C	1.937630	2.685825	5.648262
C	-2.739650	2.685618	4.168682
S	-0.760091	4.291115	6.043384
C	3.533879	0.025793	0.602641
S	1.798036	0.028303	-2.042660
C	-1.143387	0.025789	-0.876982
H	-2.776528	3.694155	3.754858
H	-3.218344	2.697894	5.148120
H	-3.247162	1.986328	3.506519
H	-1.120742	0.935230	-1.478781
H	-1.099900	-0.832156	-1.548277
H	-2.050488	-0.007595	-0.276077
H	3.884391	-0.832143	0.028459
H	3.861463	0.935242	0.097322
H	3.930345	-0.007603	1.615920
H	2.205680	3.694399	5.330954
H	1.765960	2.698058	6.724821
H	2.733703	1.986627	5.398416
H	1.014290	-2.335056	4.526569
H	-1.338833	-2.335141	3.782174

Cycloadditon product with C_2Ph_2

G(M06-2X/6-311+G**)= -2625.331758

E(M06-2X/6-311+G**)= -2625.6887423

C	2.451759	-0.889804	2.558174
C	2.290476	0.029772	1.518106
C	3.281735	0.992396	1.304595
C	4.414856	1.022663	2.107726
C	4.577157	0.089483	3.127594
C	3.593309	-0.868801	3.349999
C	1.072981	-0.011154	0.669550
C	1.073033	-0.000742	-0.669192
C	2.290080	-0.050025	-1.517930
C	2.457270	0.869425	-2.557161
C	3.598296	0.841544	-3.349382
C	4.575720	-0.123581	-3.128282
C	4.407495	-1.056696	-2.109265
C	3.274868	-1.019608	-1.305650
P	-0.554370	-0.040504	1.647925
C	-1.317053	1.334834	0.712921
C	-1.324235	1.362508	-0.641884
N	-1.866808	2.574416	-1.027971
C	-2.212697	3.303109	0.080677
N	-1.856677	2.528823	1.154659
P	-0.553900	0.043156	-1.647622
C	-1.329319	-1.325021	-0.712678
C	-1.336877	-1.352643	0.642164
N	-1.891003	-2.559354	1.028142
C	-2.243641	-3.284697	-0.080593
N	-1.880250	-2.513788	-1.154518
C	-2.133879	-3.030737	2.379198
C	-2.102373	-2.932722	-2.526435
S	-2.973009	-4.789119	-0.114825
C	-2.104721	3.048145	-2.379084
S	-2.927709	4.814428	0.114584
C	-2.074813	2.949911	2.526545
H	-3.142504	3.086224	2.703386
H	-1.573078	3.902705	2.696313
H	-1.674375	2.186759	3.191485
H	-3.205254	-3.164744	2.534518
H	-1.643397	-3.994009	2.521678
H	-1.740054	-2.295235	3.078878
H	-1.609245	-3.889975	-2.696375
H	-3.171282	-3.059434	-2.703080
H	-1.695242	-2.173107	-3.191363
H	-3.174680	3.192584	-2.534706
H	-1.604817	4.006577	-2.521397
H	-1.717856	2.308852	-3.078655
H	1.693726	1.619942	-2.737758
H	3.721636	1.569869	-4.142004

H	5.461631	-0.152109	-3.751352
H	5.160899	-1.816769	-1.939548
H	3.146310	-1.742141	-0.507814
H	3.157742	1.715060	0.506163
H	5.173241	1.777536	1.937015
H	5.463447	0.112729	3.750352
H	3.712045	-1.597119	4.143334
H	1.683224	-1.634942	2.739787

Cycloadditon product with DMAD

G(M06-2X/6-311+G**)= -2619.087438

E(M06-2X/6-311+G**)= -2619.368830

N	0.109501	0.054894	-0.037550
C	0.098150	0.040630	1.343691
C	1.386739	0.114492	1.758877
N	2.184841	0.170150	0.632975
C	1.401748	0.142626	-0.492493
P	-1.306600	-0.183511	2.497991
C	-0.478683	-1.612142	3.428038
C	-1.256515	-2.868332	3.667575
O	-0.789742	-3.885177	4.105941
P	1.851031	0.012615	3.523406
C	0.783349	-1.522813	3.841332
C	1.537914	-2.643528	4.495203
O	2.353873	-3.293362	3.905000
C	3.633529	0.252056	0.575039
S	1.910172	0.209168	-2.081270
C	-1.030781	0.007860	-0.935031
C	0.561050	1.173764	4.094609
N	0.623607	2.165761	5.055244
C	-0.619061	2.716719	5.235303
N	-1.449282	2.035764	4.380491
C	-0.726363	1.092139	3.676863
C	1.793467	2.626793	5.781210
C	-2.865895	2.333858	4.268191
S	-1.033297	3.962301	6.266983
O	1.254343	-2.744074	5.788465
C	1.866240	-3.855510	6.455505
O	-2.541484	-2.726789	3.329765
C	-3.357725	-3.886563	3.526247
H	-2.996244	3.377952	3.982179
H	-3.348657	2.177155	5.233279
H	-3.300283	1.677000	3.516647
H	-1.020970	0.887084	-1.579864
H	-0.965933	-0.881724	-1.562317
H	-1.940875	-0.016078	-0.338224
H	4.023874	-0.607978	0.030528
H	3.926620	1.160326	0.047619
H	4.021328	0.259882	1.592106

H	1.952473	3.686897	5.581263
H	1.632044	2.496919	6.851752
H	2.655174	2.046403	5.455972
H	-4.349839	-3.608346	3.182397
H	-2.964727	-4.722021	2.947005
H	-3.374340	-4.157692	4.581860
H	1.559480	-3.778338	7.494523
H	1.504587	-4.783336	6.011515
H	2.950802	-3.802245	6.363734

Cycloadditon product with Melaimid

G(M06-2X/6-311+G**)= -2676.429095

E(M06-2X/6-311+G**)= -2676.7456706

C	4.111448	-2.443869	-0.322312
C	3.330979	-1.310700	-0.515681
C	3.895755	-0.042189	-0.554037
C	5.269015	0.093105	-0.395124
C	6.062809	-1.032627	-0.201975
C	5.483955	-2.297823	-0.164743
N	1.911398	-1.445316	-0.639142
C	1.121440	-2.049533	0.339510
C	-0.336996	-1.816057	-0.016935
C	-0.311787	-1.159504	-1.398609
C	1.164359	-0.900733	-1.681260
P	-1.036606	-0.796775	1.449848
C	-0.120868	0.710104	0.970100
C	-0.194930	1.269550	-0.270477
N	0.831984	2.189478	-0.368439
C	1.543493	2.225452	0.803827
N	0.955255	1.292387	1.617502
P	-1.161114	0.539918	-1.639808
C	-2.636116	0.150199	-0.653315
N	-3.971060	0.250850	-1.003068
C	-4.758702	-0.202485	0.023863
N	-3.887744	-0.591563	1.009592
C	-2.585155	-0.372502	0.599961
C	-4.528274	0.776696	-2.237009
C	-4.340661	-1.118855	2.285109
S	-6.425932	-0.264607	0.068554
C	1.450374	0.997862	2.952800
S	2.852895	3.200439	1.158488
C	1.164685	3.015632	-1.517743
O	1.535465	-2.600896	1.321093
O	1.612575	-0.293648	-2.614778
H	-5.169024	1.629860	-2.012074
H	-5.132604	0.008748	-2.720581
H	-3.709340	1.079517	-2.887041
H	1.188650	4.062413	-1.214556
H	2.147306	2.735303	-1.900187

H	0.412900	2.854352	-2.287855
H	2.475287	0.631147	2.884299
H	1.441638	1.907839	3.553179
H	0.811551	0.238443	3.399988
H	-4.966037	-0.378017	2.784182
H	-4.936072	-2.016604	2.116732
H	-3.469346	-1.351469	2.894786
H	3.644245	-3.419598	-0.278780
H	6.100475	-3.174374	-0.007633
H	7.133148	-0.924114	-0.073917
H	5.707846	1.083083	-0.409584
H	3.269989	0.830071	-0.696142
H	-0.875994	-2.763685	0.002192
H	-0.712325	-1.818219	-2.171624

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G(M06-2X/6-311+G**)= -3345.507291

E(M06-2X/6-311+G**)= -2086.307153

C	-0.006619	-0.033098	0.010543
C	-0.007378	-0.037494	1.417912
N	1.321641	-0.098231	1.804817
C	2.156959	-0.130475	0.715113
N	1.322932	-0.089339	-0.375274
P	-1.323281	0.019501	2.561684
C	-2.638147	0.078111	1.416796
C	-2.637392	0.082603	0.009437
N	-3.966428	0.143236	-0.377465
C	-4.801739	0.175355	0.712259
N	-3.967705	0.134161	1.802633
P	-1.321484	0.025456	-1.134344
C	-4.408728	0.151570	3.183601
S	-6.462691	0.248226	0.711639
C	-4.406159	0.164800	-1.758803
C	1.761376	-0.119161	3.186150
S	3.817888	-0.203570	0.715790
C	1.763997	-0.106310	-1.756233
H	1.312654	-0.970719	3.702110
H	2.844831	-0.211020	3.190320
H	1.465116	0.806225	3.685092
H	2.851339	-0.109243	-1.759456
H	1.388684	-1.002155	-2.255885
H	1.391620	0.781320	-2.272143
H	-4.038590	-0.737143	3.699258
H	-5.496063	0.157036	3.186795
H	-4.031306	1.046377	3.683509
H	-4.106492	-0.758731	-2.259101
H	-3.960741	1.018849	-2.273507
H	-5.489939	0.252671	-1.762794

PhSSPh

G(M06-2X/6-311+G**)= -1259.437823

E(M06-2X/6-311+G**)= -1259.582652

S	-0.357761	-0.687690	-0.010907
S	-0.416676	-0.653675	2.040907
C	1.302867	-0.166075	-0.431884
C	-0.795259	1.045279	2.461884
C	1.685517	-0.388052	-1.755794
C	2.937483	0.025906	-2.191807
C	3.816690	0.649860	-1.311840
C	3.432316	0.858517	0.007333
C	2.177009	0.456118	0.453497
H	1.007462	-0.885751	-2.440739
H	3.228381	-0.149708	-3.220683
H	4.794644	0.967674	-1.651830
H	4.109911	1.341672	0.701370
H	1.887736	0.620575	1.484261
C	-1.178821	1.265674	3.785794
C	-1.446306	2.556888	4.221807
C	-1.345550	3.630281	3.341840
C	-0.972660	3.401732	2.022667
C	-0.693495	2.113404	1.576503
H	-1.270814	0.429612	4.470739
H	-1.743841	2.721006	5.250683
H	-1.559291	4.636120	3.681830
H	-0.893033	4.230123	1.328630
H	-0.406434	1.945115	0.545739

Ts_1 E=S

G(M06-2X/6-311+G**)= -3345.507291

E(M06-2X/6-311+G**)= -3345.8483611

N	-3.153845	-1.322185	-0.863215
C	-1.767360	-1.336718	-0.932212
C	-1.332806	-2.250179	0.032455
N	-2.475357	-2.744275	0.639488
C	-3.607845	-2.191763	0.095943
P	-0.868238	-0.244270	-1.966027
C	0.735466	-0.855153	-1.611809
C	1.181527	-1.753326	-0.635779
N	2.562998	-1.772435	-0.729516
C	3.005999	-0.927038	-1.714206
N	1.871350	-0.380355	-2.254428
P	0.285409	-2.568851	0.635958
C	1.852344	0.606195	-3.318445
S	4.589484	-0.613735	-2.146023
C	3.431720	-2.475432	0.196700
C	-2.464026	-3.701685	1.727834
S	-5.193285	-2.519209	0.499681
C	-3.998075	-0.479478	-1.684434

S	0.001982	0.031033	1.696776
C	1.726401	0.347728	1.974879
C	2.305818	0.031009	3.210361
C	3.675799	0.195187	3.394430
C	4.466752	0.699339	2.364447
C	3.889625	1.025862	1.138810
C	2.526908	0.841968	0.940630
S	-0.825229	1.676923	0.113338
C	-1.281253	3.399108	0.192983
C	-2.621266	3.766572	0.367229
C	-2.982957	5.108643	0.345350
C	-2.010392	6.087561	0.153186
C	-0.678322	5.729542	-0.040651
C	-0.313089	4.388526	-0.029225
H	2.870835	0.730333	-3.678339
H	1.476649	1.559146	-2.931910
H	1.204962	0.263782	-4.127488
H	-5.032320	-0.695590	-1.428114
H	-3.774480	0.573001	-1.484102
H	-3.822898	-0.695260	-2.740504
H	-2.033026	-3.244857	2.622877
H	-3.492953	-3.995855	1.926425
H	-1.873149	-4.572435	1.443177
H	4.430433	-2.501944	-0.233086
H	3.455734	-1.948925	1.154441
H	3.054419	-3.488425	0.339856
H	1.681252	-0.336138	4.014903
H	4.122458	-0.056096	4.348911
H	5.530621	0.837323	2.515094
H	4.500634	1.397186	0.325331
H	2.070271	1.092050	-0.011200
H	0.718092	4.093161	-0.174465
H	0.073300	6.493787	-0.196631
H	-2.293898	7.135176	0.152835
H	-4.019623	5.392054	0.487016
H	-3.364514	2.994964	0.531028

Ts_3 E=S

G(M06-2X/6-311+G**)= -3345.472092

E(M06-2X/6-311+G**)= -3345.815599

C	-4.594581	-3.199708	-0.497397
C	-3.995648	-1.928156	-0.621189
C	-4.836288	-0.797494	-0.721040
C	-6.214614	-0.934948	-0.692604
C	-6.788034	-2.200329	-0.566271
C	-5.973881	-3.330268	-0.473409
S	-2.272590	-1.736192	-0.633091
S	-0.472610	-0.838941	1.532464
C	-1.279410	0.707476	1.738983

C	-2.678527	0.758725	1.788741
C	-3.320194	1.970929	1.989703
C	-2.574805	3.142580	2.125467
C	-1.183013	3.096049	2.088458
C	-0.532956	1.882092	1.902917
P	0.555958	-0.594370	-0.722504
C	2.148578	-1.223819	-0.340356
C	3.364281	-0.568406	-0.152332
N	4.295342	-1.562072	0.104733
C	3.709511	-2.805173	0.107114
N	2.383213	-2.573605	-0.163576
P	3.754875	1.141240	-0.126324
C	2.162555	1.758516	-0.539910
N	1.912701	3.116390	-0.663977
C	0.594763	3.351242	-0.969254
N	0.015466	2.114008	-1.052934
C	0.940128	1.119054	-0.782368
C	2.921206	4.146480	-0.510975
C	-1.402928	1.943255	-1.330546
S	-0.168369	4.816089	-1.178828
C	1.358071	-3.599749	-0.253621
S	4.445042	-4.274023	0.371882
C	5.701438	-1.310229	0.355184
H	-1.629122	2.370002	-2.308659
H	3.365056	4.086641	0.485428
H	-1.649113	0.881820	-1.311497
H	-1.981068	2.471321	-0.569363
H	0.848116	-3.523389	-1.215232
H	1.847948	-4.567570	-0.162412
H	0.629496	-3.478119	0.551485
H	6.198933	-2.271617	0.460202
H	6.130044	-0.755861	-0.482686
H	5.818928	-0.731198	1.274011
H	2.435612	5.110713	-0.644488
H	3.702545	4.015987	-1.263711
H	0.551145	1.833580	1.872602
H	-0.606620	4.008439	2.181481
H	-3.077618	4.093017	2.253336
H	-4.402964	2.006638	2.026746
H	-3.245321	-0.155845	1.657629
H	-3.954103	-4.069919	-0.425310
H	-6.421066	-4.312412	-0.379761
H	-7.865998	-2.306794	-0.544581
H	-6.847932	-0.058660	-0.770849
H	-4.380050	0.181327	-0.824684

3cis E=S

G(M06-2X/6-311+G**)= -3345.570737

E(M06-2X/6-311+G**)= -3345.921440

C	-0.953850	1.199265	-1.075084
C	-1.506827	-0.048313	-1.133703
N	-2.874906	0.125365	-1.293267
C	-3.191223	1.456930	-1.288998
N	-1.990929	2.109203	-1.180446
P	-0.776941	-1.691353	-0.894969
C	0.954019	-1.188070	-1.064698
C	1.509576	0.056876	-1.136608
N	2.877684	-0.122092	-1.301497
C	3.191324	-1.451020	-1.289730
N	1.991029	-2.100648	-1.167943
P	0.779731	1.705100	-0.920818
S	0.763357	1.891254	1.269413
C	2.495366	1.589114	1.585744
C	2.930364	0.274079	1.762315
C	4.271137	0.018112	2.022970
C	5.175035	1.073535	2.126024
C	4.738181	2.384305	1.961818
C	3.399969	2.646240	1.688708
C	3.897717	0.905940	-1.443679
S	4.710466	-2.140152	-1.386156
C	1.897921	-3.550457	-1.110592
C	-3.892321	-0.902605	-1.435686
S	-4.710373	2.140757	-1.385317
C	-1.900573	3.559052	-1.137213
S	-0.747654	-1.826265	1.295214
C	-2.492872	-1.584753	1.600965
C	-2.969922	-0.285590	1.780957
C	-4.323893	-0.071782	2.028410
C	-5.193665	-1.156148	2.117498
C	-4.712123	-2.453706	1.947243
C	-3.363370	-2.670811	1.684701
H	4.523261	0.928530	-0.550174
H	3.414950	1.870023	-1.585597
H	4.517651	0.664227	-2.306389
H	-0.851564	3.849153	-1.213941
H	-2.470365	3.978410	-1.965823
H	-2.321275	3.928746	-0.201075
H	-4.523609	-0.927418	-0.545140
H	-4.511789	-0.663810	-2.301456
H	-3.406984	-1.866816	-1.576925
H	2.461560	-3.978255	-1.940347
H	2.324515	-3.914264	-0.175933
H	0.849082	-3.840622	-1.178863
H	2.210759	-0.535963	1.685515
H	4.613136	-1.004316	2.128635
H	6.218606	0.871982	2.327963
H	5.440993	3.205848	2.045996
H	3.047461	3.665043	1.556579

H	-2.276605	0.548175	1.712622
H	-4.697385	0.937443	2.139968
H	-6.245147	-0.988870	2.311520
H	-5.391322	-3.296315	2.014903
H	-2.976690	-3.676404	1.552045

TS_2 E=S

G(M06-2X/6-311+G**)= -3345.521050

E(M06-2X/6-311+G**)= -3345.8639389

N	-2.202915	-1.024032	1.397507
C	-1.305003	-0.134229	0.803447
C	-0.308371	-0.909446	0.273036
N	-0.604813	-2.227578	0.531715
C	-1.806605	-2.312089	1.208759
P	-1.639631	1.629529	0.585590
C	0.078452	2.167754	0.391185
C	1.154615	1.478037	-0.102703
N	2.250249	2.312022	-0.078193
C	1.883257	3.547347	0.412282
N	0.558372	3.440389	0.707866
P	1.086039	-0.223880	-0.551041
S	2.357576	-1.193584	-1.769805
C	3.699374	-1.852217	-0.741816
C	4.706968	-2.501907	-1.450678
C	5.782049	-3.050854	-0.761401
C	5.851022	-2.951624	0.624513
C	4.838926	-2.300749	1.321285
C	3.757220	-1.748790	0.641305
C	3.596251	1.960347	-0.494970
S	2.849168	4.896430	0.615120
C	-0.204754	4.550605	1.251326
C	0.213520	-3.369630	0.161397
S	-2.590731	-3.718668	1.670826
C	-3.436028	-0.632078	2.058662
S	-2.199796	1.652946	-1.548760
C	-3.633534	0.603166	-1.341886
C	-4.884996	1.152959	-1.060637
C	-5.976238	0.316554	-0.846790
C	-5.819704	-1.065882	-0.898402
C	-4.572634	-1.615989	-1.182333
C	-3.483414	-0.783304	-1.415303
H	4.261397	2.746191	-0.142444
H	3.654557	1.892140	-1.582537
H	3.877412	1.003935	-0.049309
H	1.257876	-3.157317	0.398127
H	-0.135291	-4.224046	0.737613
H	0.114221	-3.583369	-0.904269
H	-3.876628	-1.529528	2.487149
H	-3.213848	0.089964	2.845235

H	-4.127103	-0.191975	1.336105
H	-1.231161	4.225757	1.410744
H	0.240470	4.870980	2.193491
H	-0.177434	5.386914	0.552155
H	4.654182	-2.577586	-2.531762
H	6.567201	-3.555838	-1.311279
H	6.690124	-3.380042	1.158500
H	4.885772	-2.219444	2.400690
H	2.968559	-1.237759	1.185299
H	-2.506539	-1.201141	-1.635464
H	-4.440058	-2.691216	-1.204654
H	-6.667146	-1.715233	-0.713921
H	-6.947442	0.746565	-0.631757
H	-4.993206	2.229839	-1.007984

3a'

G(M06-2X/6-311+G**)=-3345,596157

E(M06-2X/6-311+G**)= -3345.940991

C	-0.705686	3.095166	-0.046556
C	-1.531983	2.440952	0.868074
C	-2.847478	2.124220	0.520801
C	-3.322191	2.427825	-0.749161
C	-2.490053	3.058926	-1.671245
C	-1.189138	3.403187	-1.314912
S	-0.887373	1.905800	2.440929
P	0.024717	-0.008024	1.883004
C	1.253527	0.501177	0.664706
N	2.523950	0.895514	1.059511
C	3.306831	1.153000	-0.031430
N	2.480406	0.974635	-1.110487
C	1.225192	0.557926	-0.699309
C	2.989376	0.941224	2.434815
S	4.928399	1.560736	-0.076172
C	2.940030	1.124062	-2.481375
P	-0.024755	0.008509	-1.882876
S	0.887217	-1.905401	-2.441120
C	1.531743	-2.440769	-0.868315
C	0.705306	-3.094821	0.046295
C	1.188694	-3.402964	1.314641
C	2.489676	-3.058975	1.670987
C	3.321959	-2.428045	0.748909
C	2.847323	-2.124341	-0.521056
C	-1.225109	-0.557666	0.699453
N	-2.480216	-0.974643	1.110703
C	-3.306612	-1.153299	0.031662
N	-2.523742	-0.895892	-1.059294
C	-1.253407	-0.501190	-0.664566
C	-2.939481	-1.123970	2.481725
C	-2.989259	-0.941828	-2.434568

S	-4.928149	-1.561237	0.076173
H	3.573130	2.008162	-2.538822
H	2.075782	1.233475	-3.135434
H	3.521191	0.250787	-2.785030
H	-2.341363	-1.594587	-3.022030
H	-4.002963	-1.336703	-2.424285
H	-2.986757	0.064946	-2.858141
H	-3.575421	-2.006051	2.538469
H	-2.075146	-1.237032	3.135086
H	-3.517471	-0.249093	2.786872
H	4.004688	1.331946	2.424201
H	2.344153	1.597327	3.021526
H	2.982602	-0.065042	2.859522
H	-0.310703	-3.347961	-0.234756
H	0.544371	-3.906269	2.026169
H	2.858091	-3.293214	2.663030
H	4.338725	-2.160837	1.014588
H	3.490975	-1.624816	-1.236430
H	-3.491051	1.624590	1.236171
H	-4.338907	2.160416	-1.014837
H	-2.858513	3.293044	-2.663298
H	-0.544938	3.906628	-2.026453
H	0.310252	3.348558	0.234517

3a'

G(B3LYP/6-311+G**)= -3346.205744

E(B3LYP/6-311+G**)= -3346.536604

N	-2.694659	0.116686	1.086913
C	-1.362818	0.075228	0.681571
C	-1.362825	-0.075256	-0.681178
N	-2.694667	-0.117085	-1.086465
C	-3.535220	-0.000388	0.000251
P	0.000159	0.229874	1.864141
C	1.363161	0.075539	0.681562
N	2.694992	0.117116	1.086926
C	3.535575	0.000029	0.000283
N	2.695056	-0.116649	-1.086449
C	1.363198	-0.074986	-0.681191
C	3.162084	0.248563	2.461942
S	5.213551	-0.000288	0.000208
C	3.162449	-0.249379	-2.461228
P	0.000195	-0.229149	-1.863804
S	0.000472	-2.401743	-2.309366
C	0.000115	-3.224423	-0.716463
C	-1.211066	-3.572942	-0.107385
C	-1.207446	-4.262526	1.103242
C	-0.000460	-4.607417	1.710325
C	1.206813	-4.261479	1.104414
C	1.211005	-3.571914	-0.106225

C	-3.161877	-0.248724	-2.461421
S	-5.213204	-0.000764	0.000248
C	-3.161762	0.247756	2.461962
S	-0.000194	2.402650	2.308974
C	-0.000441	3.224901	0.715858
C	-1.211589	3.572592	0.106240
C	-1.207893	4.261878	-1.104558
C	-0.000868	4.607314	-1.711252
C	1.206368	4.262215	-1.104788
C	1.210490	3.572932	0.106012
H	4.234353	-0.060227	-2.459663
H	2.656439	0.480609	-3.095492
H	2.968816	-1.255573	-2.837721
H	-2.963007	-1.252923	-2.840455
H	-4.234753	-0.065171	-2.458853
H	-2.660157	0.485593	-3.094137
H	-4.234968	0.066143	2.459056
H	-2.661520	-0.488134	3.094038
H	-2.961061	1.251214	2.841972
H	4.235380	0.067483	2.459007
H	2.960884	1.251961	2.841842
H	2.662256	-0.487516	3.094128
H	-2.148030	-3.315295	-0.585806
H	-2.148821	-4.535213	1.566703
H	-0.000683	-5.149432	2.649181
H	2.147977	-4.533370	1.568771
H	2.148207	-3.313541	-0.583786
H	-2.148587	3.314572	0.584394
H	-2.149245	4.533923	-1.568443
H	-0.001030	5.149099	-2.650241
H	2.147554	4.534519	-1.568859
H	2.147653	3.315173	0.583982

E(ωB97X-D/6-311+G**)= -3346.086629
G (ωB97X-D/6-311+G**)= -3345.739681

C	0.594663	-3.200825	0.069086
C	-0.395197	-2.858502	-0.850957
C	-1.740958	-3.020847	-0.521820
C	-2.095940	-3.500777	0.731363
C	-1.109434	-3.823302	1.657409
C	0.232739	-3.680511	1.323031
S	0.034550	-2.125869	-2.418544
P	0.248091	-0.027139	-1.869918
C	1.601008	-0.084424	-0.677503
N	2.925360	-0.145339	-1.085187
C	3.761289	-0.155019	-0.000633
N	2.930999	-0.106414	1.086658
C	1.604345	-0.060982	0.684635
C	3.381271	-0.243511	-2.458950

S	5.432541	-0.209517	0.002472
C	3.406586	-0.040425	2.455794
P	0.255167	0.015109	1.879812
S	0.260909	2.126976	2.416512
C	-0.063039	2.893311	0.840057
C	-1.379200	3.184486	0.481226
C	-1.656339	3.702915	-0.776196
C	-0.622462	3.934396	-1.677439
C	0.691415	3.659543	-1.314538
C	0.975615	3.140470	-0.056363
C	-1.093480	0.106478	-0.672413
N	-2.416906	0.176795	-1.073088
C	-3.249390	0.114512	0.009831
N	-2.418633	0.016981	1.091674
C	-1.095052	0.000222	0.685428
C	-2.883342	0.274459	-2.442451
C	-2.874789	-0.087901	2.464340
S	-4.923579	0.143294	0.001650
H	4.391472	-0.503372	2.492802
H	2.716207	-0.581231	3.104496
H	3.484498	0.997602	2.786330
H	-2.624817	0.819133	3.019459
H	-3.955973	-0.214898	2.440294
H	-2.408849	-0.953832	2.938390
H	-3.865595	0.744036	-2.430858
H	-2.184704	0.884262	-3.016446
H	-2.963973	-0.716501	-2.895467
H	4.448750	-0.029181	-2.469024
H	3.209693	-1.249725	-2.847461
H	2.849861	0.483489	-3.075369
H	-2.183663	2.984417	1.179553
H	-2.682916	3.916869	-1.050986
H	-0.838968	4.336455	-2.660724
H	1.499477	3.846692	-2.012618
H	1.997852	2.918625	0.227545
H	-2.507429	-2.748083	-1.237902
H	-3.144536	-3.612440	0.982651
H	-1.385836	-4.194667	2.637893
H	1.002794	-3.941044	2.040192
H	1.639462	-3.081073	-0.192624

3a' in/out

G(M06-2X/6-311+G**)= -3345.583246

E(M06-2X/6-311+G**)= -3345.9307058

C	-3.372843	-2.734459	0.476913
C	-3.390163	-1.939302	-0.669537
C	-4.603336	-1.475396	-1.176584
C	-5.794076	-1.806756	-0.537972

C	-5.777184	-2.584361	0.614810
C	-4.564695	-3.044599	1.121125
S	-1.890349	-1.517938	-1.550919
P	-0.745152	-0.693321	0.091771
C	-0.779131	1.078830	-0.264373
N	-1.864245	1.860416	0.097781
C	-1.612051	3.181892	-0.161560
N	-0.350051	3.206060	-0.690568
C	0.175124	1.921675	-0.758268
C	-3.149783	1.385092	0.583934
S	-2.627346	4.479924	0.111701
C	0.334847	4.438967	-1.041664
P	1.846430	1.612815	-1.366590
S	3.047594	2.189085	0.370755
C	2.412319	1.061289	1.594105
C	3.065297	-0.153228	1.812673
C	2.520350	-1.085158	2.688509
C	1.330919	-0.801451	3.355396
C	0.694668	0.421286	3.159095
C	1.231397	1.355955	2.278607
C	0.914502	-1.005287	-0.546110
N	1.517079	-2.242642	-0.381962
C	2.820565	-2.197952	-0.795861
N	2.996362	-0.928887	-1.277503
C	1.841416	-0.178437	-1.112682
C	0.888768	-3.401454	0.227715
C	4.268373	-0.462572	-1.804314
S	3.981626	-3.398610	-0.704883
H	-0.402594	5.137973	-1.432668
H	1.088189	4.226413	-1.799575
H	0.809289	4.873180	-0.159641
H	4.963542	-0.253170	-0.988759
H	4.687480	-1.243805	-2.436438
H	4.100492	0.442960	-2.385740
H	1.603194	-4.220983	0.184382
H	0.641748	-3.181388	1.269529
H	-0.013912	-3.664012	-0.326930
H	-3.523856	2.097422	1.317537
H	-3.863030	1.314185	-0.239520
H	-3.024188	0.402942	1.041602
H	3.985512	-0.377609	1.284516
H	3.024866	-2.033231	2.837535
H	0.905026	-1.528463	4.037353
H	-0.224495	0.648539	3.686588
H	0.737287	2.307385	2.113213
H	-4.608801	-0.852623	-2.063749
H	-6.734103	-1.445082	-0.937625
H	-6.704226	-2.833227	1.116654
H	-4.546501	-3.657347	2.014713

H	-2.430192	-3.103907	0.864883

3a' out/out

G(M06-2X/6-311+G**)= -3345.573774

E(M06-2X/6-311+G**)= -3345.917459

C	0.656178	-1.044885	0.187095
C	-0.656271	-1.044891	-0.187039
N	-1.044122	-2.371309	-0.302059
C	-2.381951	-2.861142	-0.590963
P	1.791968	0.306660	0.577675
S	3.015607	0.392106	-1.206412
C	4.549975	-0.234974	-0.532992
C	5.146938	-1.333197	-1.150433
C	6.354301	-1.828212	-0.667179
C	6.958476	-1.242044	0.439677
C	6.360638	-0.146078	1.055095
C	5.165072	0.365581	0.565232
C	0.000008	-3.203485	-0.000086
N	1.044093	-2.371279	0.302010
C	2.382021	-2.860981	0.590644
S	0.000061	-4.873651	-0.000230
P	-1.792113	0.306631	-0.577507
S	-3.015621	0.392259	1.206630
C	-4.549959	-0.234948	0.533249
C	-5.146724	-1.333360	1.150537
C	-6.354028	-1.828483	0.667239
C	-6.958324	-1.242230	-0.439505
C	-6.360674	-0.146078	-1.054775
C	-5.165175	0.365686	-0.564868
C	0.655204	1.660381	0.191369
N	1.040297	2.987897	0.312091
C	-0.000042	3.822784	-0.000106
N	-1.040381	2.987880	-0.312220
C	-0.655279	1.660361	-0.191445
C	2.366037	3.460363	0.672170
C	-2.366105	3.460300	-0.672410
S	-0.000025	5.493654	-0.000193
H	-2.295720	-3.751399	-1.211988
H	-2.945881	-2.089693	-1.116507
H	-2.896605	-3.120989	0.335963
H	-3.014933	3.484862	0.205086
H	-2.261551	4.464482	-1.078589
H	-2.785872	2.795040	-1.428123
H	2.261480	4.464521	1.078404
H	2.785913	2.795079	1.427799
H	3.014773	3.485002	-0.205390
H	2.295964	-3.751706	1.211019
H	2.896812	-3.120018	-0.336432
H	2.945729	-2.089769	1.116779

H	-4.662231	-1.797862	2.001590
H	-6.815122	-2.680749	1.151886
H	-7.893224	-1.635316	-0.820317
H	-6.830818	0.320050	-1.912412
H	-4.708332	1.228656	-1.034719
H	4.662569	-1.797622	-2.001598
H	6.815537	-2.680330	-1.151951
H	7.893422	-1.635050	0.820457
H	6.830685	0.319998	1.912812
H	4.708110	1.228419	1.035210

3a' out/out

G(B3LYP/6-311+G**)= -3346.196090

E(B3LYP/6-311+G**)= -3346.529726

C	-0.646547	1.632400	-0.229795
C	0.646502	1.632419	0.229808
N	1.025623	2.965215	0.375928
C	-0.000055	3.805205	0.000008
N	-1.025702	2.965184	-0.375931
P	1.770341	0.267557	0.641680
S	3.064970	0.375442	-1.144704
C	4.641926	-0.207928	-0.506211
C	5.260397	-1.276851	-1.163398
C	6.519497	-1.713248	-0.754641
C	7.159180	-1.102013	0.321826
C	6.539625	-0.041182	0.981946
C	5.291403	0.414584	0.564930
C	2.323020	3.446165	0.830083
S	-0.000074	5.480753	-0.000008
C	-2.323102	3.446098	-0.830113
P	-1.770346	0.267503	-0.641664
S	-3.064973	0.375350	1.144726
C	-4.641930	-0.208008	0.506222
C	-5.260476	-1.276847	1.163474
C	-6.519580	-1.713221	0.754705
C	-7.159191	-1.102047	-0.321839
C	-6.539562	-0.041299	-0.982023
C	-5.291336	0.414445	-0.564996
C	0.645449	-1.096486	0.233302
C	-0.645409	-1.096505	-0.233295
N	-1.024061	-2.428494	-0.380605
C	0.000061	-3.266129	-0.000015
N	1.024147	-2.428462	0.380603
C	-2.318632	-2.925326	-0.827609
S	0.000089	-4.940598	-0.000016
C	2.318730	-2.925255	0.827617
H	-2.155491	-3.792805	-1.466065
H	-2.831253	-2.142654	-1.385659
H	-2.930537	-3.228037	0.024203

H	-3.046511	3.438651	-0.012105
H	-2.190710	4.467150	-1.183808
H	-2.678918	2.813231	-1.644405
H	2.190606	4.467215	1.183777
H	2.678866	2.813311	1.644372
H	3.046416	3.438735	0.012063
H	2.155613	-3.792729	1.466087
H	2.930642	-3.227963	-0.024191
H	2.831331	-2.142561	1.385655
H	-4.756147	-1.760803	1.991476
H	-6.993874	-2.538276	1.274002
H	-8.134853	-1.447471	-0.643445
H	-7.033730	0.443222	-1.816632
H	-4.827432	1.252961	-1.069148
H	4.756011	-1.760857	-1.991335
H	6.993732	-2.538369	-1.273886
H	8.134838	-1.447455	0.643424
H	7.033847	0.443386	1.816495
H	4.827558	1.253163	1.069031

3a' out/out

G(ωB97X-D/6-311+G**)= -3345.716938

E(ωB97X-D/6-311+G**)= -3346.061949

C	-0.648694	1.666533	-0.208464
C	0.648873	1.666387	0.207750
N	1.031991	2.992965	0.339438
C	0.000313	3.826223	-0.000303
N	-1.031537	2.993202	-0.340064
P	1.780882	0.309022	0.586851
S	2.996821	0.396928	-1.196605
C	4.538660	-0.235167	-0.542603
C	5.090204	-1.374961	-1.123724
C	6.300801	-1.874394	-0.657352
C	6.954831	-1.249286	0.397238
C	6.403371	-0.111477	0.976495
C	5.204110	0.403353	0.502543
C	2.345048	3.464182	0.734930
S	0.000433	5.496990	-0.000210
C	-2.344557	3.464734	-0.735314
P	-1.781197	0.309464	-0.587176
S	-2.996382	0.397813	1.196825
C	-4.538391	-0.234589	0.543484
C	-5.089279	-1.374818	1.124371
C	-6.299873	-1.874506	0.658268
C	-6.954553	-1.249211	-0.395812
C	-6.403768	-0.110945	-0.974813
C	-5.204506	0.404127	-0.501121
C	0.647857	-1.047912	0.209813
C	-0.648337	-1.047754	-0.210677

N	-1.032989	-2.373574	-0.339932
C	-0.000554	-3.203613	-0.000222
N	1.032075	-2.373799	0.339518
C	-2.344003	-2.869162	-0.715460
S	-0.000778	-4.873475	-0.000328
C	2.343350	-2.869561	0.713886
H	-2.222386	-3.684752	-1.427995
H	-2.921050	-2.063728	-1.170235
H	-2.872926	-3.244560	0.162288
H	-3.017316	3.497200	0.124366
H	-2.231098	4.467388	-1.144674
H	-2.749688	2.797338	-1.497923
H	2.231801	4.467121	1.143652
H	2.749613	2.797091	1.498111
H	3.018173	3.495885	-0.124488
H	2.222079	-3.686609	1.424787
H	2.872347	-3.242984	-0.164672
H	2.920130	-2.064805	1.170220
H	-4.567366	-1.869391	1.935611
H	-6.724887	-2.760912	1.115058
H	-7.892753	-1.646692	-0.765326
H	-6.913420	0.384618	-1.793235
H	-4.785854	1.300674	-0.943165
H	4.568810	-1.869400	-1.935379
H	6.726309	-2.760464	-1.114333
H	7.893040	-1.646552	0.766964
H	6.912505	0.383935	1.795331
H	4.784962	1.299555	0.944812

PhSeSePh

G(M06-2X/6-311+G**)= -5266.192308

E(M06-2X/6-311+G**)= -5266.3310827

C	-0.004742	-0.079123	0.138387
C	-0.196555	-0.002062	1.517822
C	0.872035	-0.207694	2.388836
C	2.136220	-0.487851	1.876616
C	2.329479	-0.566298	0.502402
C	1.258665	-0.362997	-0.365647
Se	-1.940029	0.350154	2.251172
Se	-2.754064	-1.859602	2.172388
C	-1.503424	-2.628523	3.415862
C	-0.358993	-3.252319	2.921916
C	0.569419	-3.793159	3.807675
C	0.356901	-3.706669	5.178557
C	-0.786744	-3.079976	5.669293
C	-1.719386	-2.541601	4.791136
H	0.708066	-0.165993	3.459614
H	2.965228	-0.651349	2.555083

H	3.313325	-0.785670	0.104736
H	1.408768	-0.422529	-1.437228
H	-0.843657	0.074796	-0.529819
H	-2.608475	-2.047857	5.164913
H	-0.953927	-3.013377	6.737926
H	1.080582	-4.126642	5.867124
H	1.460593	-4.274400	3.422298
H	-0.190443	-3.296349	1.851943

Ts_1 E=Se

G(M06-2X/6-311+G**)= -7352.261287

E(M06-2X/6-311+G**)= -7352.601457

C	3.307295	3.366006	-0.398728
C	1.943953	3.239808	-0.111812
C	1.184515	4.382168	0.162083
C	1.785238	5.634912	0.157754
C	3.143873	5.754056	-0.124303
C	3.903895	4.620796	-0.403377
Se	1.110855	1.495348	-0.105020
Se	-0.128548	-0.275517	-1.759270
C	-1.911986	0.402622	-1.950078
C	-2.623546	0.137897	-3.122253
C	-3.954406	0.531446	-3.225615
C	-4.567958	1.204027	-2.173047
C	-3.850927	1.487851	-1.012533
C	-2.525486	1.085724	-0.897755
P	0.812783	-0.370416	2.026621
C	-0.898123	-0.711206	1.743914
C	-1.523925	-1.569729	0.848441
N	-2.884257	-1.347511	0.972483
C	-3.139625	-0.380874	1.911225
N	-1.907265	-0.006395	2.381926
P	-0.820984	-2.601580	-0.405715
C	0.846549	-2.578699	0.184847
C	1.465163	-1.697969	1.061103
N	2.825988	-1.941827	0.970484
C	3.087235	-2.941970	0.069202
N	1.854573	-3.318880	-0.406533
C	3.836694	-1.212548	1.713637
S	4.571911	-3.574434	-0.349447
C	1.637103	-4.334315	-1.420336
C	-3.895401	-1.951066	0.122059
S	-4.627922	0.218258	2.375161
C	-1.677824	1.022311	3.379586
H	-1.106547	1.843019	2.937774
H	-1.125335	0.603714	4.222780
H	-2.647803	1.383697	3.713288
H	4.810272	-1.576385	1.393048
H	3.748070	-0.145204	1.497215

H	3.710334	-1.384514	2.784399
H	1.286834	-3.871023	-2.346035
H	2.586349	-4.834628	-1.598274
H	0.894593	-5.050409	-1.064274
H	-4.867279	-1.767834	0.574653
H	-3.862221	-1.496065	-0.872939
H	-3.709484	-3.023472	0.048661
H	-2.135847	-0.376145	-3.941835
H	-4.507849	0.316453	-4.132151
H	-5.604103	1.509988	-2.255129
H	-4.327840	1.997475	-0.184151
H	-1.960808	1.303487	0.003013
H	0.126206	4.280564	0.374103
H	1.195841	6.518522	0.372769
H	3.610607	6.732053	-0.129642
H	4.960012	4.716644	-0.626226
H	3.889632	2.479378	-0.622782

TS_3 E=Se

G(M06-2X/6-311+G**)= -7352.229460

E(M06-2X/6-311+G**)= -7352.5669929

C	-5.178332	0.153478	-0.917410
C	-4.396194	-0.995953	-0.719373
C	-5.013838	-2.255748	-0.766880
C	-6.375723	-2.360552	-1.011091
C	-7.141046	-1.213050	-1.209684
C	-6.539799	0.043124	-1.162313
Se	-2.537245	-0.842957	-0.380319
P	0.462630	-0.488754	-0.526275
Se	-0.429238	-0.361580	1.858232
C	-0.592147	1.537902	1.938006
C	-1.861034	2.114719	2.032952
C	-1.979834	3.494164	2.144783
C	-0.841009	4.297784	2.138563
C	0.422878	3.721921	2.041126
C	0.552370	2.340668	1.950088
C	1.373162	0.979498	-0.826914
C	2.764011	1.155648	-0.853438
N	2.970972	2.501721	-1.105919
C	1.778302	3.167703	-1.250290
N	0.808695	2.217004	-1.092719
P	4.102037	0.039946	-0.635679
C	3.157699	-1.421218	-0.402208
C	1.779874	-1.626889	-0.310314
N	1.589637	-2.963578	-0.013438
C	2.793751	-3.614157	0.087306
N	3.742480	-2.655488	-0.169738
C	4.279003	3.116643	-1.224070
S	1.533240	4.788401	-1.542989

C	-0.606748	2.539138	-1.198612
C	0.310576	-3.609066	0.238747
S	3.032440	-5.219354	0.450317
C	5.173518	-2.889442	-0.166806
H	-0.818580	2.890211	-2.209453
H	4.838950	2.977610	-0.296871
H	-1.199325	1.652697	-0.977162
H	-0.844052	3.333591	-0.490215
H	-0.477847	-3.070942	-0.288910
H	0.368583	-4.634746	-0.120819
H	0.096144	-3.620980	1.309768
H	5.335704	-3.957498	-0.040413
H	5.600702	-2.554897	-1.114064
H	5.640803	-2.344843	0.656819
H	4.130556	4.177527	-1.413028
H	4.828504	2.662864	-2.051651
H	1.533235	1.882845	1.874511
H	1.306270	4.348917	2.020696
H	-0.937846	5.375224	2.199386
H	-2.962398	3.944330	2.222483
H	-2.739392	1.480477	2.000342
H	-4.414003	-3.144500	-0.611314
H	-6.843511	-3.337318	-1.048462
H	-8.204182	-1.297684	-1.401398
H	-7.134175	0.935796	-1.317988
H	-4.703729	1.127454	-0.879580

3cis E=Se

G(M06-2X/6-311+G**)= -7352.319009

E(M06-2X/6-311+G**)= -7352.66156

N	-2.880974	0.130551	-1.465653
C	-1.511968	-0.052681	-1.316479
C	-0.949672	1.192395	-1.264970
N	-1.985422	2.108330	-1.360494
C	-3.188121	1.460769	-1.460993
P	-0.783469	-1.700845	-1.139080
C	0.949275	-1.188837	-1.267346
C	1.511553	0.056261	-1.317550
N	2.880595	-0.126937	-1.466660
C	3.187702	-1.457135	-1.463657
N	1.984857	-2.104744	-1.364563
P	0.783167	1.704064	-1.135855
Se	0.781912	1.970708	1.197008
C	2.622326	1.489207	1.500172
C	2.963809	0.138689	1.588285
C	4.288054	-0.225445	1.806378
C	5.263123	0.756776	1.965489
C	4.916387	2.102713	1.896072
C	3.596379	2.474700	1.655688

C	3.907277	0.896086	-1.585381
S	4.705659	-2.150967	-1.550297
C	1.883734	-3.554154	-1.322031
C	-1.885530	3.557805	-1.317064
S	-4.705797	2.155157	-1.547294
C	-3.907503	-0.892397	-1.586364
Se	-0.781461	-1.973971	1.193041
C	-2.621773	-1.493100	1.497927
C	-3.595633	-2.479013	1.651945
C	-4.915605	-2.107644	1.893518
C	-5.262519	-0.761884	1.965408
C	-4.287621	0.220738	1.807781
C	-2.963379	-0.142815	1.588721
H	4.542913	0.884136	-0.699000
H	3.431430	1.869148	-1.693229
H	4.518181	0.678307	-2.461458
H	-0.839976	3.845918	-1.419784
H	-2.472242	3.978134	-2.133236
H	-2.285267	3.930276	-0.372500
H	-4.542124	-0.883602	-0.699223
H	-4.519550	-0.671666	-2.460900
H	-3.431521	-1.864953	-1.698080
H	2.484713	-3.974178	-2.127787
H	2.266569	-3.927009	-0.370584
H	0.840082	-3.841912	-1.443600
H	2.192163	-0.615375	1.472080
H	4.559094	-1.274054	1.836307
H	6.293892	0.470589	2.136848
H	5.674209	2.867024	2.022597
H	3.320249	3.520078	1.589641
H	-2.191860	0.611563	1.473819
H	-4.558760	1.269258	1.839793
H	-6.293274	-0.476152	2.137606
H	-5.673269	-2.872286	2.018984
H	-3.319391	-3.524214	1.583821

TS_2 Se

G(M06-2X/6-311+G**)= -7352.265090

E(M06-2X/6-311+G**)= -7352.6056444

C	-5.086279	0.531890	-0.902566
C	-3.771245	0.157845	-1.180027
C	-3.418925	-1.192694	-1.206232
C	-4.374132	-2.166067	-0.931198
C	-5.686908	-1.792880	-0.655470
C	-6.043128	-0.447199	-0.648810
Se	-2.412687	1.493018	-1.474019
P	-1.789725	1.507506	0.796022
C	-0.116638	2.177518	0.600569

C	1.008893	1.574460	0.104420
N	2.040561	2.487197	0.148322
C	1.581219	3.684805	0.652539
N	0.265135	3.477188	0.936931
P	1.062761	-0.121240	-0.384388
Se	2.481294	-1.036844	-1.708668
C	3.948817	-1.596116	-0.545242
C	5.030906	-2.183820	-1.195021
C	6.119906	-2.621144	-0.448442
C	6.127224	-2.470420	0.934560
C	5.040531	-1.881120	1.571458
C	3.944935	-1.441106	0.833770
C	3.412567	2.246123	-0.262021
S	2.445426	5.097048	0.882182
C	-0.577867	4.517244	1.501119
C	-1.316053	-0.225130	0.999217
C	-0.257592	-0.916122	0.472535
N	-0.437125	-2.252046	0.751376
C	-1.622475	-2.431329	1.437569
N	-2.127302	-1.180072	1.614984
C	-3.400129	-0.896999	2.257049
S	-2.281358	-3.892106	1.926528
C	0.474354	-3.326452	0.396470
H	4.014036	3.069390	0.118466
H	3.486835	2.211520	-1.350143
H	3.759271	1.301293	0.160739
H	1.498627	-3.017319	0.612459
H	0.208647	-4.193618	0.997502
H	0.381715	-3.574974	-0.662270
H	-3.681504	-1.775722	2.833112
H	-3.286797	-0.035099	2.914369
H	-4.165340	-0.693448	1.503579
H	-0.166805	4.840750	2.457834
H	-0.599997	5.373045	0.825855
H	-1.581374	4.118830	1.638437
H	5.031159	-2.302972	-2.273787
H	6.962951	-3.079363	-0.951649
H	6.977348	-2.809642	1.513507
H	5.040309	-1.759953	2.648163
H	3.098615	-0.978121	1.332603
H	-2.393636	-1.474275	-1.423419
H	-4.086910	-3.210865	-0.915462
H	-6.430059	-2.551904	-0.442062
H	-7.065183	-0.156144	-0.436053
H	-5.351958	1.582023	-0.883087

3ipso E=Se

G(M06-2X/6-311+G**)= -7352.292741

E(M06-2X/6-311+G**)= -7352.6348747

C	1.399517	0.205327	2.551140
C	0.484185	-0.784781	2.194701
C	0.883751	-2.117634	2.088824
C	2.213171	-2.456320	2.315474
C	3.133876	-1.467563	2.654036
C	2.726468	-0.142914	2.780807
Se	-1.298648	-0.298014	1.655979
P	-0.355387	0.228558	-0.452523
C	0.622936	1.657294	-0.474990
C	2.012251	1.709565	-0.629794
N	2.344560	3.045916	-0.481308
C	1.242836	3.821830	-0.208150
N	0.188168	2.959110	-0.185390
P	3.257580	0.485731	-0.885544
C	2.150666	-0.889128	-0.950403
C	0.758870	-1.007968	-0.934213
N	0.459127	-2.376480	-0.983622
C	1.608240	-3.106150	-1.032231
N	2.627179	-2.185973	-1.033137
C	-0.868742	-2.955219	-1.069818
S	1.753788	-4.772885	-1.058751
C	4.038791	-2.517078	-1.023777
C	3.700843	3.548516	-0.585812
S	1.204432	5.472847	0.041784
C	-1.178786	3.374556	0.068483
Se	-2.153391	0.436198	-1.847579
C	-3.585369	-0.032328	-0.649763
C	-4.138161	0.935933	0.187720
C	-5.153440	0.581445	1.069369
C	-5.625198	-0.726909	1.099839
C	-5.095564	-1.682157	0.236893
C	-4.074690	-1.338253	-0.640794
H	-1.137532	4.337626	0.574088
H	4.321478	3.100920	0.193809
H	-1.733591	3.477198	-0.866467
H	-1.661528	2.640437	0.715330
H	-1.309206	-2.742436	-2.046730
H	-0.762059	-4.030978	-0.941672
H	-1.503378	-2.551101	-0.278636
H	4.129214	-3.598908	-1.084695
H	4.532468	-2.048779	-1.877551
H	4.489486	-2.149570	-0.098226
H	3.666620	4.628309	-0.462667
H	4.111016	3.292466	-1.564749
H	0.170130	-2.882467	1.802926
H	2.525296	-3.488856	2.204802
H	4.172187	-1.729807	2.821799
H	3.444653	0.625473	3.040770

H	1.080047	1.238904	2.622584
H	-3.660567	-2.076112	-1.316674
H	-5.474090	-2.697014	0.249051
H	-6.414929	-1.000592	1.789092
H	-5.575718	1.328810	1.730127
H	-3.777047	1.956094	0.149512

3b'

G(M06-2X/6-311+G**)= -7352.338864

E(M06-2X/6-311+G**)= -7352.683752

C	-3.213049	-1.574645	0.794247
C	-1.981850	-2.230688	0.753018
C	-1.182233	-2.299818	1.893930
C	-1.610467	-1.689002	3.069886
C	-2.825537	-1.010865	3.105181
C	-3.630101	-0.959423	1.969097
Se	-1.341474	-2.922256	-0.919863
P	-0.116737	-1.041921	-1.567011
C	1.133678	-0.949342	-0.269422
N	2.314686	-1.671141	-0.373708
C	3.148517	-1.379369	0.668763
N	2.439752	-0.513764	1.459451
C	1.210145	-0.225720	0.887928
C	2.659942	-2.543796	-1.481999
S	4.713619	-1.910815	0.930892
C	2.988071	0.059954	2.676949
P	0.116805	1.042128	1.567107
Se	1.341493	2.922308	0.919610
C	1.981861	2.230578	-0.753200
C	1.182257	2.299703	-1.894133
C	1.610523	1.688947	-3.070102
C	2.825632	1.010871	-3.105394
C	3.630161	0.959409	-1.969290
C	3.213065	1.574554	-0.794417
C	-1.210165	0.225758	-0.887723
C	-1.133702	0.949393	0.269613
N	-2.314718	1.671161	0.373906
C	-3.148566	1.379337	-0.668536
N	-2.439767	0.513787	-1.459257
C	-2.988029	-0.059938	-2.676773
S	-4.713749	1.910623	-0.930551
C	-2.660042	2.543786	1.482192
H	3.510254	-0.724134	3.223296
H	2.173130	0.462375	3.277374
H	3.694941	0.857277	2.437873
H	-1.895822	3.314662	1.595802
H	-3.618819	3.003631	1.251508
H	-2.740640	1.958676	2.401226

H	-3.510629	0.724039	-3.222876
H	-2.173007	-0.461886	-3.277410
H	-3.694523	-0.857611	-2.437754
H	3.619125	-3.003002	-1.251731
H	1.896137	-3.315172	-1.595054
H	2.739661	-1.958808	-2.401183
H	0.231057	2.817862	-1.855823
H	0.988755	1.736974	-3.956748
H	3.149925	0.530693	-4.021565
H	4.577350	0.431597	-1.985212
H	3.835638	1.525010	0.091956
H	-3.835673	-1.525153	-0.092092
H	-4.577259	-0.431556	1.984970
H	-3.149751	-0.530619	4.021346
H	-0.988702	-1.737032	3.956534
H	-0.231055	-2.818013	1.855620

3b' in/out

G(M06-2X/6-311+G**)= -7352.329418

E(M06-2X/6-311+G**)= -7352.671357

N	0.979579	-2.507090	-0.300034
C	0.625008	-1.176961	-0.467597
C	1.672206	-0.557566	-1.090020
N	2.645703	-1.525805	-1.289137
C	2.242113	-2.729262	-0.777315
P	-0.927272	-0.538024	0.202282
C	-0.625205	1.199961	-0.190139
N	-1.529185	2.187365	0.171408
C	-1.043145	3.425987	-0.151954
N	0.179924	3.191421	-0.720113
C	0.452754	1.829972	-0.745797
C	-2.861793	1.989930	0.718833
S	-1.789381	4.899983	0.093817
C	1.067076	4.255650	-1.157952
P	1.998724	1.190064	-1.423648
Se	3.464130	1.616666	0.343234
C	2.611600	0.477704	1.632435
C	3.058034	-0.835815	1.785231
C	2.371904	-1.706155	2.625073
C	1.249574	-1.262471	3.320128
C	0.821070	0.055364	3.186932
C	1.497820	0.930382	2.341399
C	3.956023	-1.329636	-1.886952
S	3.139413	-4.139975	-0.718819
C	0.161355	-3.515747	0.349940
Se	-2.350958	-1.189906	-1.493625
C	-3.932648	-1.259255	-0.391619
C	-5.037298	-0.488530	-0.750250

C	-6.188865	-0.525809	0.030845
C	-6.233525	-1.315488	1.174756
C	-5.128180	-2.083280	1.530546
C	-3.981181	-2.066108	0.744440
H	0.452494	5.083437	-1.507210
H	1.694487	3.887791	-1.969688
H	1.692776	4.594638	-0.330113
H	4.715474	-1.213537	-1.111106
H	4.193355	-2.205000	-2.489551
H	3.931828	-0.437773	-2.512008
H	0.792874	-4.383771	0.529672
H	-0.207643	-3.120762	1.299147
H	-0.677696	-3.794192	-0.290977
H	-3.041564	2.755804	1.471947
H	-3.611069	2.085163	-0.069344
H	-2.928902	0.997856	1.166337
H	3.924200	-1.186718	1.235169
H	2.713250	-2.730993	2.720343
H	0.713252	-1.940804	3.973855
H	-0.047570	0.402966	3.734336
H	1.161898	1.954785	2.225972
H	-4.992751	0.143023	-1.630053
H	-7.046647	0.073238	-0.251392
H	-7.127376	-1.334493	1.786586
H	-5.160074	-2.705674	2.417106
H	-3.125047	-2.673978	1.014159

3b' out/out

G(M06-2X/6-311+G**)= -7352.316883

E(M06-2X/6-311+G**)= -7352.657686

N	0.860277	-2.478356	0.252511
C	0.549389	-1.131786	0.139580
C	-0.753199	-1.055223	-0.263689
N	-1.210366	-2.358394	-0.399136
C	-0.220579	-3.248889	-0.084234
P	1.750005	0.150421	0.564129
Se	3.149253	0.054980	-1.268030
C	4.734737	-0.432704	-0.284007
C	5.404537	-1.608765	-0.617658
C	6.568279	-1.957132	0.062538
C	7.052737	-1.146281	1.082928
C	6.378570	0.024502	1.416932
C	5.226689	0.387985	0.729478
P	-1.805641	0.358424	-0.664711
Se	-3.094505	0.570688	1.238928
C	-4.710016	-0.153882	0.473878
C	-5.284937	-1.280332	1.059548
C	-6.450821	-1.818640	0.522845

C	-7.031903	-1.246344	-0.603650
C	-6.454583	-0.121991	-1.186303
C	-5.301023	0.433147	-0.643678
C	-2.562274	-2.778398	-0.729882
S	-0.313452	-4.916263	-0.110405
C	2.165259	-3.041546	0.555907
C	0.713136	1.566174	0.119088
C	-0.586184	1.644603	-0.297305
N	-0.883138	2.993598	-0.435669
C	0.196295	3.763786	-0.095428
N	1.176237	2.868410	0.244572
C	2.510777	3.256722	0.665212
S	0.283146	5.432193	-0.092610
C	-2.162519	3.562636	-0.824804
H	-2.503162	-3.638739	-1.394892
H	-3.089070	-1.959873	-1.221148
H	-3.099091	-3.064997	0.176098
H	-2.751720	3.814783	0.058538
H	-1.969404	4.466976	-1.399560
H	-2.700376	2.838812	-1.436630
H	2.474031	4.308628	0.941987
H	2.802760	2.656253	1.528821
H	3.225069	3.115347	-0.148594
H	2.018297	-3.950077	1.137786
H	2.691181	-3.288158	-0.368623
H	2.750033	-2.319773	1.127044
H	-4.817334	-1.738345	1.923400
H	-6.896612	-2.693480	0.980943
H	-7.933768	-1.673096	-1.025518
H	-6.907694	0.332015	-2.059523
H	-4.861507	1.318421	-1.087705
H	5.018814	-2.247091	-1.403996
H	7.089645	-2.869356	-0.201945
H	7.953995	-1.423925	1.615914
H	6.754469	0.663364	2.207144
H	4.714181	1.309391	0.977200

PhTeTePh

G(M06-2X/6-311+G**)= -998.980237

E(M06-2X/6-311+G**)= -999.116604

C	-0.031069	0.230359	-0.018399
C	0.019398	0.004254	1.354024
C	1.254291	-0.158954	1.984150
C	2.429207	-0.097748	1.242237
C	2.380476	0.131846	-0.128874
C	1.149425	0.297233	-0.753726
Te	-1.705149	-0.176388	2.586822
Te	-3.613613	0.698734	0.933746
C	-4.014746	-1.084812	-0.150308

C	-3.050785	-2.067870	-0.362601
C	-3.363086	-3.190482	-1.123115
C	-4.628303	-3.331939	-1.684114
C	-5.587529	-2.346890	-1.476208
C	-5.286016	-1.227157	-0.706821
H	1.309810	-0.329691	3.054761
H	3.383444	-0.224903	1.740198
H	3.296206	0.183327	-0.705264
H	1.100749	0.477522	-1.821415
H	-0.983257	0.366048	-0.520354
H	-6.050225	-0.476111	-0.535638
H	-6.578025	-2.451695	-1.903327
H	-4.866350	-4.206085	-2.278025
H	-2.609222	-3.953257	-1.280123
H	-2.060305	-1.971014	0.069218

Trans product with PhTeTePh

G(M06-2X/6-311+G**)= -3085.109447

E(M06-2X/6-311+G**)= -3085.449212

C	0.306853	3.139221	-1.280055
C	-0.680958	3.316344	-0.310044
C	-2.022202	3.414448	-0.684839
C	-2.377566	3.304813	-2.023755
C	-1.395104	3.106206	-2.990994
C	-0.055241	3.035431	-2.619947
S	-0.261214	3.307094	1.420840
P	-0.261325	1.152284	1.823973
C	1.066302	0.572473	0.744179
N	2.402466	0.675094	1.111872
C	3.207372	0.165595	0.144307
N	2.366301	-0.258993	-0.837578
C	1.045070	-0.020882	-0.489041
C	2.897886	1.309339	2.326301
Te	5.270400	0.048216	0.155908
C	2.815064	-0.935807	-2.046030
P	-0.321437	-0.392403	-1.615886
Te	-0.604277	-2.882771	-1.226048
C	-1.257475	-2.616645	0.760559
C	-2.624298	-2.492150	1.021536
C	-3.060604	-2.169872	2.302671
C	-2.136026	-1.979830	3.326474
C	-0.774679	-2.118581	3.071308
C	-0.330757	-2.433622	1.788840
C	-1.622492	0.653746	0.752676
N	-2.940015	0.878601	1.121542
C	-3.786435	0.540312	0.104721
N	-2.973807	0.113996	-0.910074
C	-1.643490	0.181825	-0.530040
C	-3.387750	1.391172	2.405021

C	-3.479672	-0.344290	-2.191881
S	-5.459716	0.615715	0.096610
H	3.754166	-0.485304	-2.363233
H	2.060051	-0.813856	-2.822390
H	2.976835	-1.995983	-1.844250
H	-3.743773	-1.403100	-2.143928
H	-4.369262	0.235707	-2.432837
H	-2.713284	-0.187819	-2.951338
H	-4.396817	1.020593	2.578179
H	-2.715983	1.030199	3.184515
H	-3.398042	2.483622	2.399618
H	3.802816	0.790442	2.637550
H	3.131468	2.357572	2.133181
H	2.135360	1.235203	3.100989
H	-3.350907	-2.620789	0.226228
H	-4.122667	-2.055773	2.490392
H	-2.476393	-1.728976	4.324651
H	-0.053411	-1.976344	3.867944
H	0.730792	-2.529710	1.588952
H	-2.784022	3.551417	0.074650
H	-3.422840	3.364910	-2.305185
H	-1.672359	3.017414	-4.034888
H	0.711370	2.893697	-3.372991
H	1.347415	3.074179	-0.981165

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