

Supplementary Information

A homonuclear π -system with a singlet carbene-type α and a nucleophilic β phosphorus – first use in P-heterocyclic synthesis

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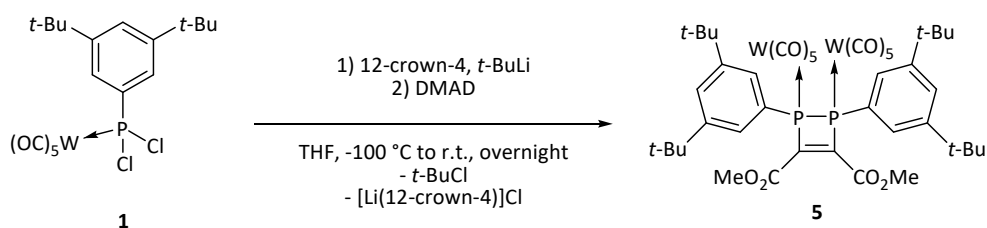
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1. Experimental details and devices

The syntheses of all compounds were performed under an argon atmosphere, using common Schlenk techniques and dry solvents. Tetrahydrofuran and petrol ether were dried over sodium wire and benzophenone. Dichloromethane was dried over CaH_2 . The solvents were freshly distilled before usage. The NMR spectra were recorded on a Bruker AVI-300 (300.1 MHz for ^1H NMR, 75.5 MHz for ^{13}C NMR, 59.6 MHz and 121.5 MHz for ^{31}P NMR) and Bruker AV III HD Prodigy 500 (500.2 MHz for ^1H NMR, 125.8 MHz for ^{13}C NMR, and 202.5 MHz for ^{31}P NMR) spectrometers at 25 °C. The ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were referenced to the residual proton resonances and the ^{13}C NMR signals of the deuterated solvents; the ^{31}P NMR spectra were referenced to 85 % H_3PO_4 as external standards, respectively. Melting points were determined in one-side melted off capillaries using a Büchi Type Sor a Carl Roth Type MPM-2 apparatus and are uncorrected. Elemental analyses were carried out on a Vario EL gas chromatograph. Mass spectrometric data were collected on a Thermo Finnigan MAT 90 and MAT 95 XL device using 70 eV voltage. For collecting MALDI spectra a Bruker Daltonik ultrafleXtreme TOF/TOF spectrometer was utilized while using DCTB (*trans*-2-[3-(4-*tert*-Butylphenyl)-2-methyl-2-propenylidene]malononitrile) as matrix material. The IR spectra were recorded on a Thermo Nicolet 380 FT-IR spectrometer with an attenuated total reflection (ATR) attachment or a Bruker Alpha Diamond ATR FTIR spectrometer. X-ray data were collected with a Bruker X8-KappaApexII diffractometer. CCDC 2000998, 2000999 and 2103740 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures

2. Experimental procedures

2.1. Experimental procedure for 5



Scheme S 1. Reaction of complex **1** with *t*-BuLi in presence of 12-crown-4 to yield complex **5**.

In a 250 mL Schlenk tube complex **1** (743 mg, 1.21 mmol, 1.00 eq.) was dissolved in 50 mL THF and 12-crown-4 (0.20 mL, 1.25 mmol, 1.03 eq.) was added. At -100 °C *t*-BuLi (1.7 M in *n*-hexane) (0.93 mL, 1.58 mmol, 1.31 eq.) was added dropwise to the reaction solution which turned red after complete addition of *t*-BuLi. Immediately afterwards DMAD (0.44 mL, 3.59 mmol, 2.97 eq.) was added and the reaction mixture was stirred overnight while warming up to room temperature. On the next day the solvent and all volatiles were removed under reduced pressure ($5 \cdot 10^{-2}$ mbar) and the residue was extracted with 80 mL of Et_2O . The red oil

was further purified via column chromatography (Al_2O_3 , $-20\text{ }^\circ\text{C}$, petrol ether and CH_2Cl_2 , $h=5\text{ cm}$, $\varnothing=6\text{ cm}$). After removal of the solvent under reduced pressure ($5\cdot 10^{-2}\text{ mbar}$) product **5** was obtained as an orange solid in 33 % yield (243 mg, 0.20 mmol).

Isomer 1: $^1\text{H NMR}$ (300.1 MHz, 298 K, CDCl_3) δ / ppm = 1.34 (s, 36H, tBu), 3.92 (s, 6H, OMe), 7.48 (m, $^4J_{\text{HH}} = 1.7\text{ Hz}$, $^3J_{\text{PH}} = 11.6\text{ Hz}$, 4H, *ortho*-H), 7.59 (t, $^4J_{\text{HH}} = 1.7\text{ Hz}$, 2H, *para*-H).

Isomer 2: $^1\text{H NMR}$ (300.1 MHz, 298 K, CDCl_3) δ / ppm = 1.12 (s, 36H, tBu), 3.92 (s, 6H, OMe), 7.03 (m, $^4J_{\text{HH}} = 1.7\text{ Hz}$, $^3J_{\text{PH}} = 12.2\text{ Hz}$, 4H, *ortho*-H), 7.28 (m, $^4J_{\text{HH}} = 1.7\text{ Hz}$, 2H, *para*-H).

Isomer 1: $^{31}\text{P}\{^1\text{H}\}$ NMR (121.5 MHz, 298 K, CDCl_3) δ / ppm = 43.1 (m, $^1J_{\text{WP}} = 246.5\text{ Hz}$, $^{2+4}J_{\text{WP}} = 3.0\text{ Hz}$, $^1J_{\text{PP}} = 35.5\text{ Hz}$).

Isomer 2: $^{31}\text{P}\{^1\text{H}\}$ NMR (121.5 MHz, 298 K, CDCl_3) δ / ppm = 45.3 (m).

Isomer 1: $^{13}\text{C}\{^1\text{H}\}$ NMR (125.8 MHz, 298 K, C_6D_6) δ / ppm = 31.3 (s, tBu), 35.4 (s, tBu), 53.3 (s, OMe), 126.1 (br s, *ortho*-C), 127.4 (s, *para*-C), 133.2 (dd, $^1J_{\text{PC}} = 12.2\text{ Hz}$, $^2J_{\text{PC}} = 12.2\text{ Hz}$, C=C), 147.7 (dd, $^1J_{\text{PC}} = 19.7\text{ Hz}$, $^2J_{\text{PC}} = 19.7\text{ Hz}$, *ipso*-C), 152.4 (dd, $^3J_{\text{PC}} = 4.1\text{ Hz}$, $^4J_{\text{PC}} = 4.1\text{ Hz}$, *meta*-C), 162.2 (dd, $^2J_{\text{PC}} = 12.7\text{ Hz}$, $^3J_{\text{PC}} = 12.7\text{ Hz}$, CO_2Me), 194.8 (dd_{sat}, $^2J_{\text{PC}} = 3.0\text{ Hz}$, $^3J_{\text{PC}} = 3.0\text{ Hz}$, $^1J_{\text{WC}} = 125.9\text{ Hz}$, *cis*-CO), 195.9 (dd_{sat}, $^2J_{\text{PC}} = 2.4\text{ Hz}$, $^3J_{\text{PC}} = 2.4\text{ Hz}$, *trans*-CO).

Isomer 2: $^{13}\text{C}\{^1\text{H}\}$ NMR (125.8 MHz, 298 K, C_6D_6) δ / ppm = 31.3 (s, tBu), 35.1 (s, tBu), 53.4 (s, OMe), 125.5 (dd, $^2J_{\text{PC}} = 7.2\text{ Hz}$, $^3J_{\text{PC}} = 7.2\text{ Hz}$, *ortho*-C), 126.0 (s, *para*-C), 133.0 (dd, $^1J_{\text{PC}} = 10.3\text{ Hz}$, $^2J_{\text{PC}} = 10.3\text{ Hz}$, C=C), 149.0 (dd, $^1J_{\text{PC}} = 18.1\text{ Hz}$, $^2J_{\text{PC}} = 18.1\text{ Hz}$, *ipso*-C), 151.5 (dd, $^3J_{\text{PC}} = 4.5\text{ Hz}$, $^4J_{\text{PC}} = 4.5\text{ Hz}$, *meta*-C), 162.4 (dd, $^2J_{\text{PC}} = 12.7\text{ Hz}$, $^3J_{\text{PC}} = 12.7\text{ Hz}$, CO_2Me), 197.3 (dd, $^2J_{\text{PC}} = 14.5\text{ Hz}$, $^3J_{\text{PC}} = 14.5\text{ Hz}$, *cis*-CO), 198.0 (dd_{sat}, $^2J_{\text{PC}} = 14.1\text{ Hz}$, $^3J_{\text{PC}} = 14.1\text{ Hz}$, *trans*-CO).

MS (MALDI TOF, Matrix DCTB) m/z (%) = 1230.155 (70) $[\text{M}]^+$.

IR (ATR Diamant) ν/cm^{-1} = 2067 (s, CO), 1989 (w, CO), 1919 (vs, CO), 1726 (s, CO ester), 1587 (m, C=C), 1240 (s, COC ester).

Melting point 148-150 $^\circ\text{C}$.

Elemental analysis cal. C 42.95, H 3.93; found C 43.56, H 4.15.

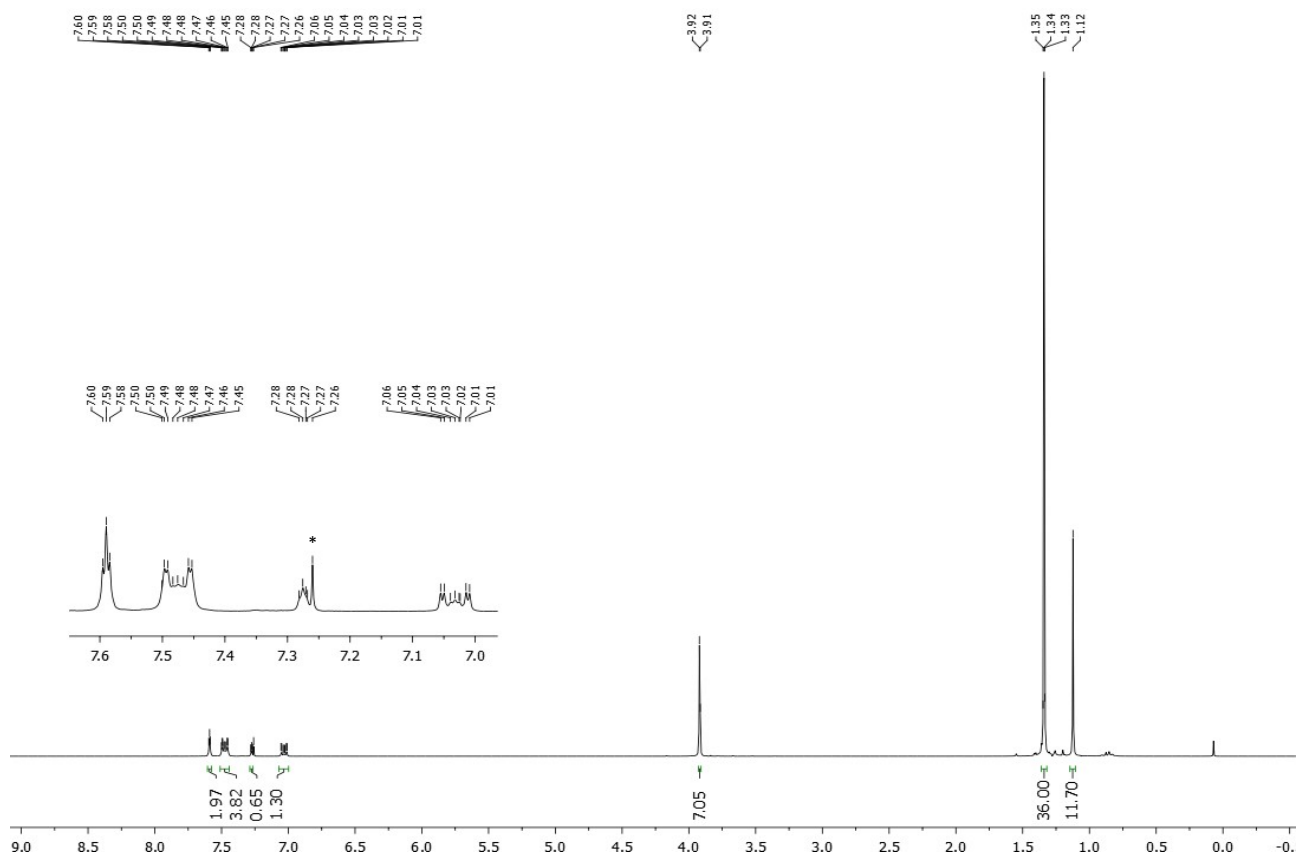


Figure S 1. ^1H NMR spectrum of **5** ($^*\text{CDCl}_3$).

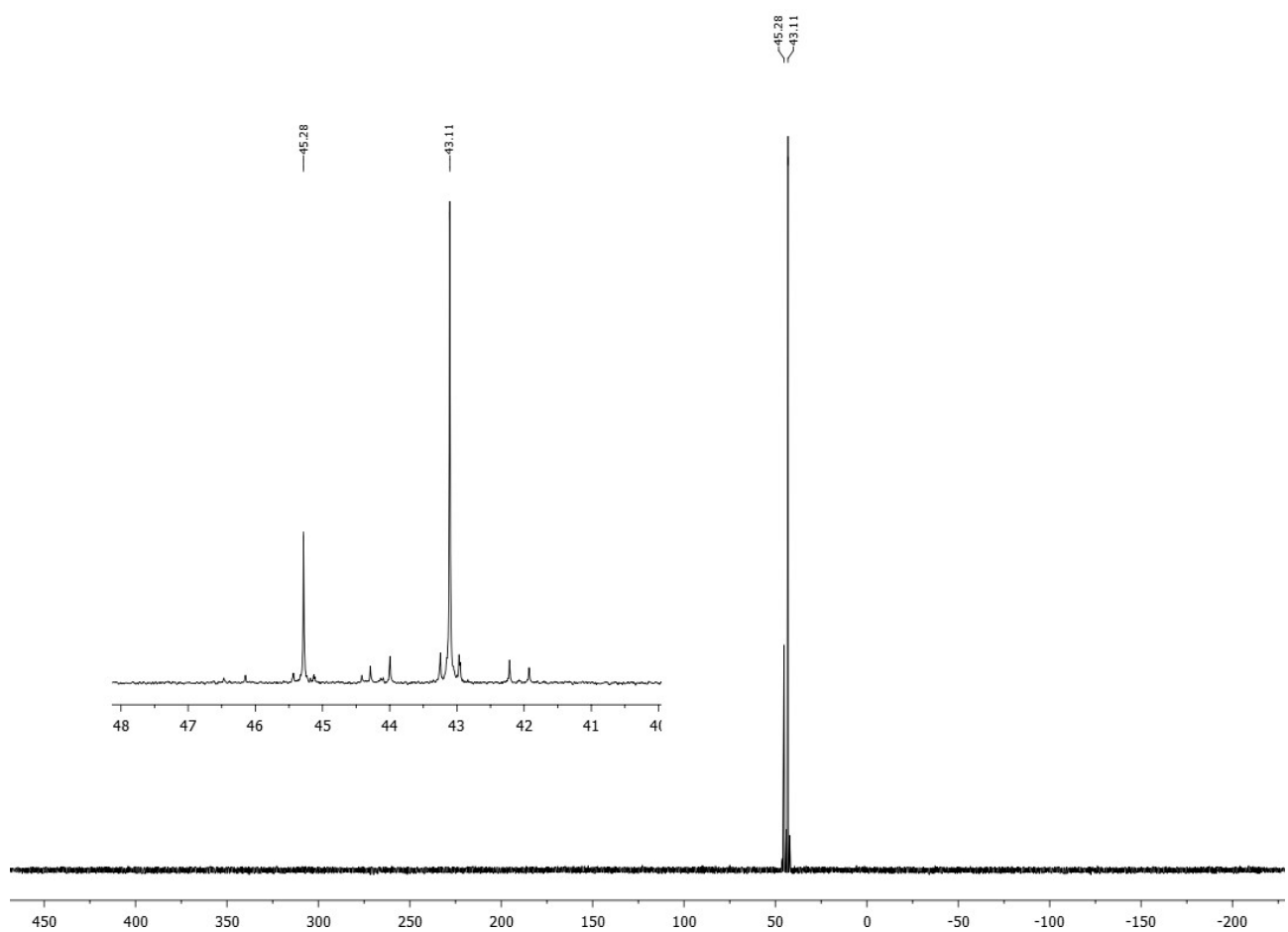
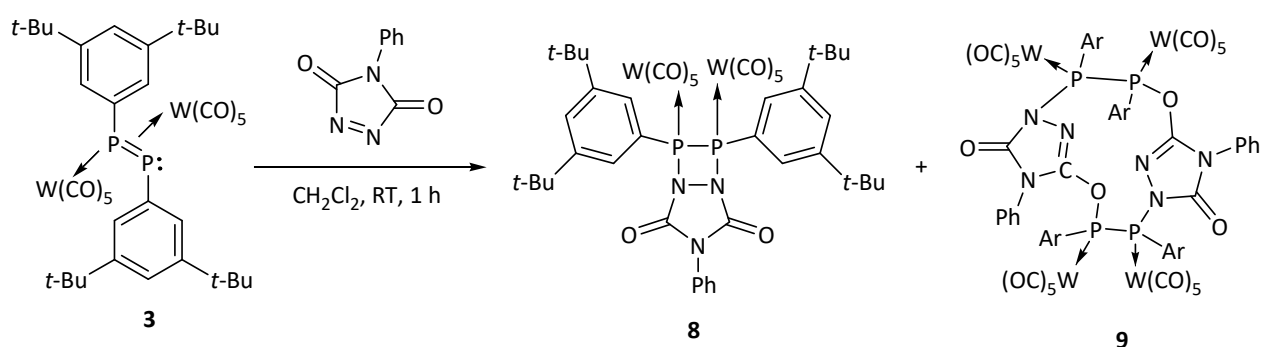


Figure S 2. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **5** in CDCl_3 .

2.2. Experimental procedure for 8



Scheme S 2. Reaction of complex **3** with 4-phenyl-1,2,4-triazoline-3,5-dione to yield complex **8**.

In a 25 mL Schlenk tube, μ^2 - (η^1 , η^2)-diphosphene complex **3** (119 mg, 0.11 mmol, 1.00 eq.) was dissolved in dichloromethane (4 mL). 4-phenyl-1,2,4-triazoline-3,5-dione (21.4 mg, 0.11 mmol, 1.00 eq.) was added to this solution and was allowed to stir for one hour. The solvent removed under reduced pressure ($5 \cdot 10^{-2}$ mbar) and the residue purified by column chromatography (Al_2O_3 , -20°C , petroleum ether/dichloromethane, $h = 3$ cm, $\varnothing = 1$ cm). The product was found as a yellow fraction collected at an eluent ratio of 1: 3. The solvent was removed under reduced pressure ($5 \cdot 10^{-2}$ mbar) and after drying for 2 h under vacuum ($5 \cdot 10^{-2}$ mbar), the crude product was obtained as a yellow powder.

$^1\text{H-NMR}$ (500.1 MHz, 298 K, CDCl_3): $\delta/\text{ppm} = 1.36$ (s, 36H, tBu), 7.33 (d, $^3J_{\text{PH}} = 13.3$ Hz, 2H, *ortho*-H), 7.45 (m, 5H, *ortho*-H, NPh), 7.53 (m, 2H, NPh), 7.82 (m, 2H, *ortho*-H), 7.69 (br s, 2H, *para*-H).

$^{31}\text{P}\{^1\text{H}\}$ -NMR (202.5 MHz, 298 K, CDCl_3): $\delta/\text{ppm} = 134.0$ (S_{sat}).

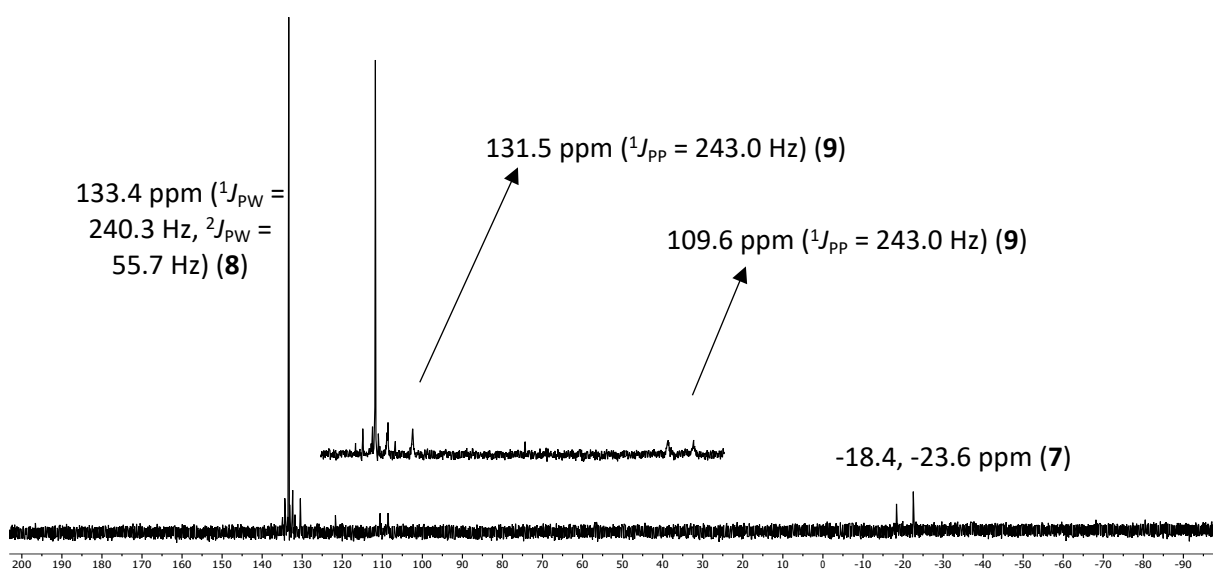
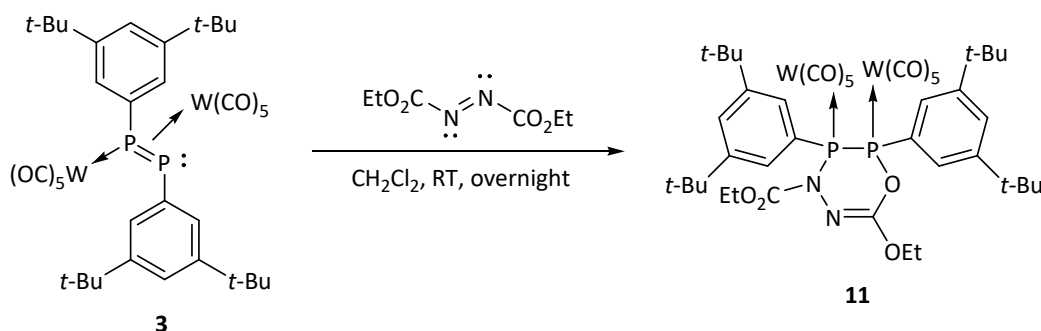


Figure S 3. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **8** in CDCl_3 .

2.3. Experimental procedure for 11



Scheme S 3. Reaction of complex **3** with DEAD to yield complex **11**.

In a 25 mL Schlenk tube, μ^2 - (η^1 , η^2)-diphosphene complex **3** (161 mg, 0.15 mmol, 1.00 eq.) was dissolved in dichloromethane (6 mL) and DEAD (0.03 mL, 0.19 mmol, 1.27 eq.) was added at room temperature and let the solution stir overnight. The next day the solvent was removed under reduced pressure ($5 \cdot 10^{-2}$ mbar) and the residue was purified by column chromatography (Al_2O_3 , -20°C , petroleum ether/diethylether, $h = 3$ cm, $\varnothing = 1$ cm). The product obtained as a light green fraction collected at an eluent ratio of 5:2. The solvent was removed under reduced pressure ($5 \cdot 10^{-2}$ mbar) and after drying for 2 h under vacuum ($5 \cdot 10^{-2}$ mbar) the product was obtained as a colorless powder in 33 % yield (62 mg, 0.05 mmol).

$^1\text{H-NMR}$ (500.1 MHz, 298 K, CDCl_3): δ / ppm = 1.09 (t, $^3J_{\text{HH}} = 7.1$ Hz, 3H, COCH_2CH_3), 1.31 (s, 18H, tBu), 1.35 (s, 18H, tBu), 1.45 (t, $^3J_{\text{HH}} = 7.1$ Hz, 3H, $\text{C}(\text{O})\text{OCH}_2\text{CH}_3$), 4.11 (dq, $^2J_{\text{HH}} = 10.7$ Hz, $^3J_{\text{HH}} = 7.1$ Hz, 1H, COCH_2CH_3), 4.23 (dq, $^2J_{\text{HH}} = 10.7$ Hz, $^3J_{\text{HH}} = 7.1$ Hz, 1H, COCH_2CH_3), 4.42 (q, $^3J_{\text{HH}} = 7.1$ Hz, 1H, $\text{C}(\text{O})\text{OCH}_2\text{CH}_3$), 4.43 (q, $^3J_{\text{HH}} = 7.1$ Hz, 1H, $\text{C}(\text{O})\text{OCH}_2\text{CH}_3$), 7.33 (d, $^3J_{\text{PH}} = 13.3$ Hz, 2H, *ortho*-H), 7.47 (d, $^3J_{\text{PH}} = 14.0$ Hz, 2H, *ortho*-H), 7.60 (br s, 1H, *para*-H), 7.64 (br s, 1H, *para*-H).

$^{13}\text{C}\{^1\text{H}\}$ -NMR (125.8 MHz, 298 K, C_6D_6): δ / ppm = 14.1 (s, CH_2CH_3), 31.4 (s, tBu), 31.5 (s, tBu), 35.5 (s, tBu), 63.9 (s, CH_2CH_3), 66.6 (s, CH_2CH_3), 124.4 (dd, $^2J_{\text{PC}} = 16.0$ Hz, $^3J_{\text{PC}} = 2.2$ Hz, *ortho*-C), 127.0 (dd, $^2J_{\text{PC}} = 17.1$ Hz, $^3J_{\text{PC}} = 2.7$ Hz, *ortho*-C), 127.8 (br s, *para*-C), 127.9 (br s, *para*-C), 130.3 (dd, $^1J_{\text{PC}} = 27.6$ Hz, $^2J_{\text{PC}} = 6.3$ Hz, *ipso*-C), 133.9 (dd, $^1J_{\text{PC}} = 35.8$ Hz, $^2J_{\text{PC}} = 8.7$ Hz, *ipso*-C), 142.5 (d, $^2J_{\text{PC}} = 3.4$ Hz, $\text{N}=\text{COO}$), 151.4 (d, $^3J_{\text{PC}} = 11.3$ Hz, *meta*-C), 152.1 (d, $^3J_{\text{PC}} = 10.3$ Hz, *meta*-C), 154.3 (dd, $^2J_{\text{PC}} = 5.2$ Hz, $^3J_{\text{PC}} = 5.2$ Hz, $\text{NC}(\text{O})\text{OEt}$), 194.5 (d_{sat} , $^2J_{\text{PC}} = 6.9$ Hz, $^1J_{\text{WC}} = 126.6$ Hz, *cis*-CO), 195.1 (d_{sat} , $^2J_{\text{PC}} = 7.1$ Hz, $^1J_{\text{WC}} = 126.6$ Hz, *cis*-CO), 197.1 (d, $^2J_{\text{PC}} = 6.3$ Hz, *trans*-CO), 197.3 (d, $^2J_{\text{PC}} = 6.6$ Hz, *trans*-CO).

^{31}P -NMR (202.5 MHz, 298 K, CDCl_3): δ / ppm = 68.0 (dt_{sat} , $^{1+5}J_{\text{PP}} = 139.4$ Hz, $^3J_{\text{PH}} = 14.0$ Hz, $^1J_{\text{WP}} = 278.6$ Hz, PN), 135.0 (dt_{sat} , $^{1+5}J_{\text{PP}} = 139.4$ Hz, $^3J_{\text{PH}} = 13.3$ Hz, $^1J_{\text{WP}} = 290.0$ Hz, PO).

MS (MALDI TOF, Matrix DCTB): m/z (%) = 982.2 (100) $[\text{M}-10\text{CO}]^+$.

IR (ATR Diamond): ν / cm^{-1} = 2069 (s, CO), 1997 (w, CO), 1988 (w, CO), 1936 (vs, CO), 1918 (vs, CO), 1705 (m, $\text{NC}(\text{O})\text{O}$), 1670 (w, $\text{C}=\text{N}$), 1296 (m, $\text{C}-\text{O}$), 1259 (s, $\text{C}-\text{O}$).

Melting point: 181-182 $^\circ\text{C}$

Elemental analysis: cal. C 41.86, H 4.15, N 2.22; found C 42.60, H 4.70, N 2.00.

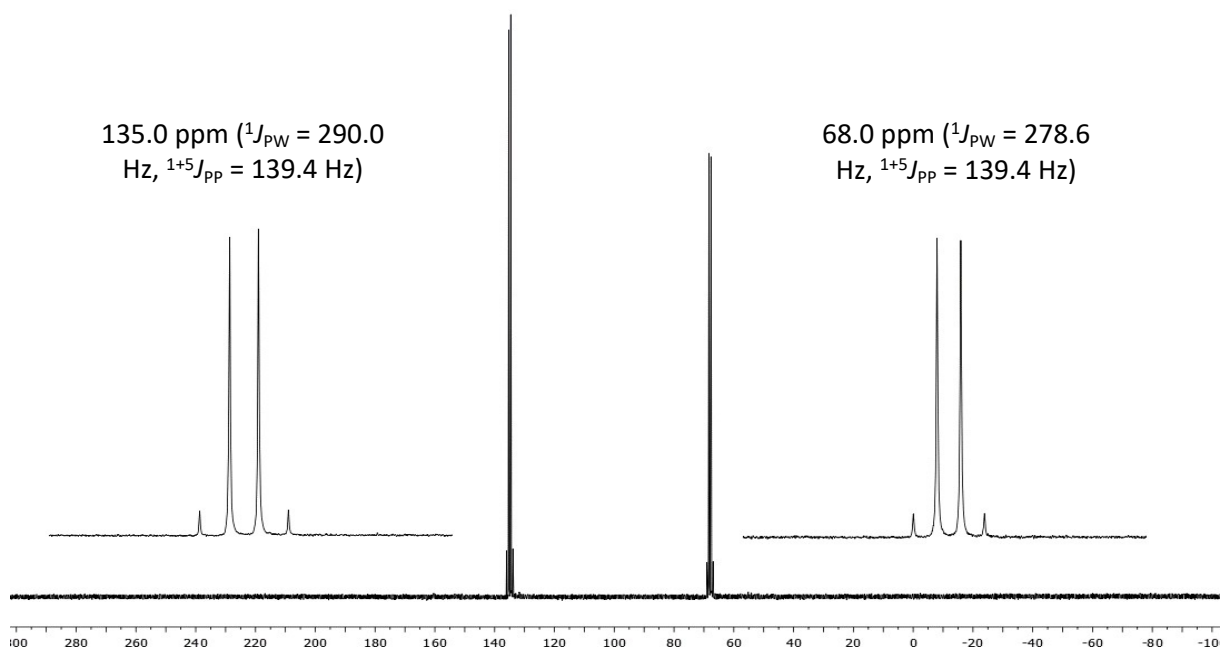


Figure S 4 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **11** in CDCl_3 .

3. Simulation of the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **5**

The $^{31}\text{P}\{^1\text{H}\}$ -NMR spectrum of **6** showed a complicated spectrum of higher order. An overlay of the three spin-system A_2 , ABX and $AA'XX'$ is caused by the natural abundance of the NMR-active ^{183}W nucleus (14.31 %). As the coupling constants were not available from the spectrum itself, we performed a simulation with gNMR.³ The simulation revealed for the ABX spin-system the following coupling constants: $^1J_{\text{PP}} = 35.5$ Hz, $^1J_{\text{WP}} = 246.5$ Hz, $^{2+4}J_{\text{WP}} = 3.3$ Hz. The same values are also valid for the $AA'XX'$ spin system (Figure S 6).

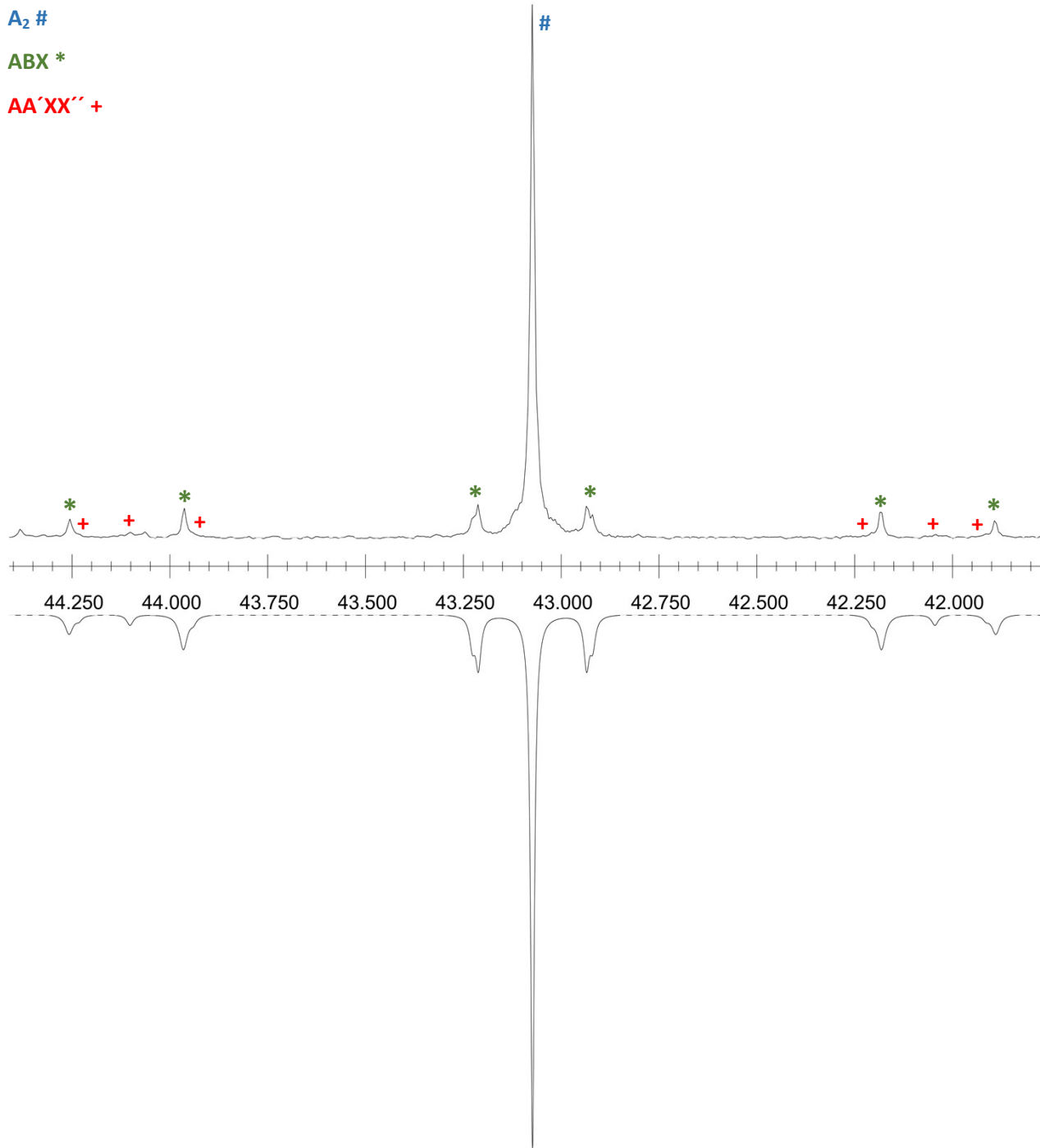


Figure S 5. Experimental $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (top) and simulated $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (bottom) of **5**.

4. Crystallographic Data

4.1. Crystallographic Data for 1 and 5

Data were collected with a Bruker X8-KappaApexII diffractometer equipped with a low-temperature device at 100 K by using graphite-monochromated Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$). Empirical formula: C₃₉H₄₇NO₁₀P₂W₂, formula weight M = 1119.42 g·mol⁻¹, crystal system triclinic, space group P-1, unit cell dimensions a = 9.8761(18) \AA , b = 10.9209(19) \AA , c = 12.138(2) \AA , $\alpha = 67.727(5)^\circ$, $\beta = 66.395(5)^\circ$, $\gamma = 70.170(5)^\circ$, volume V = 1082.7(3) \AA^3 , Z = 1, calculated density $\rho_{\text{calcd.}} = 1.717 \text{ g}\cdot\text{cm}^{-3}$, absorption coefficient $\mu = 5.435 \text{ mm}^{-1}$, crystal size 0.21 \times 0.06 \times 0.02 mm, transmission factors (min/max) 0.4878/ 0.7461, 2 θ range for data collection 4.98 to 56 $^\circ$, completeness to theta 0.998, reflections collected 30838, independent reflections 5213 [$R_{\text{int}} = 0.1006$, $R_{\text{sigma}} = 0.0675$], Goodness-of-fit on F² 1.044, final R indexes [$I \geq 2\sigma(I)$] $R_1 = 0.0420$, $wR_2 = 0.0880$, final R indexes [all data] $R_1 = 0.0561$, $wR_2 = 0.0944$, largest diff. peak and hole 2.25/-1.97 e \AA^{-3} . The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures (CCDC 2000999)

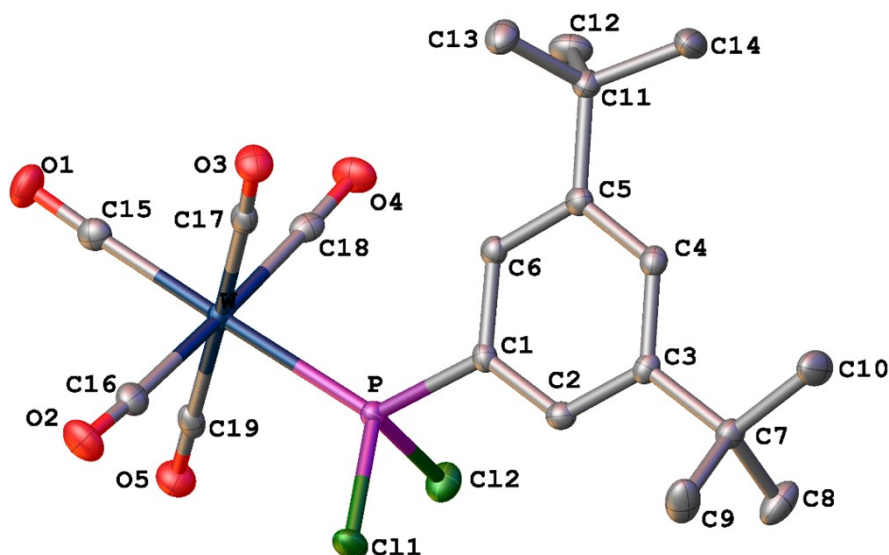


Figure S 6. Molecular structure of **1**. All hydrogen atoms are omitted for clarity. The thermal ellipsoids are set at 50 % probability.

Data were collected with a Bruker X8-KappaApexII diffractometer equipped with a low-temperature device at 100 K by using graphite-monochromated Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$). Empirical formula: C₄₄H₄₈O₁₄P₂W₂, formula weight M = 1230.46 g·mol⁻¹, crystal system triclinic, space group P-1, unit cell dimensions a = 9.838(3) \AA , b = 12.198(4) \AA , c = 21.758(7) \AA , $\alpha = 89.481(9)^\circ$, $\beta = 80.738(9)^\circ$, $\gamma = 67.861(9)^\circ$, volume V = 2383.2(13) \AA^3 , Z = 2, calculated density $\rho_{\text{calcd.}} = 1.715 \text{ g}\cdot\text{cm}^{-3}$, absorption coefficient $\mu = 4.952 \text{ mm}^{-1}$, crystal size 0.25 \times 0.09 \times 0.08 mm, transmission factors (min/max) 0.3084/ 0.7460, 2 θ range for data collection 4.536 to 55.998 $^\circ$, completeness to theta 0.999, reflections collected 84391, independent

reflections 11480 [$R_{\text{int}} = 0.2288$, $R_{\text{sigma}} = 0.1514$], Goodness-of-fit on F^2 1.067, final R indexes [$I \geq 2\sigma(I)$] $R_1 = 0.0907$, $wR_2 = 0.2022$, final R indexes [all data] $R_1 = 0.1688$, $wR_2 = 0.2510$, largest diff. peak and hole 5.79/-3.13 e \AA^{-3} . The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures (CCDC 2000998)

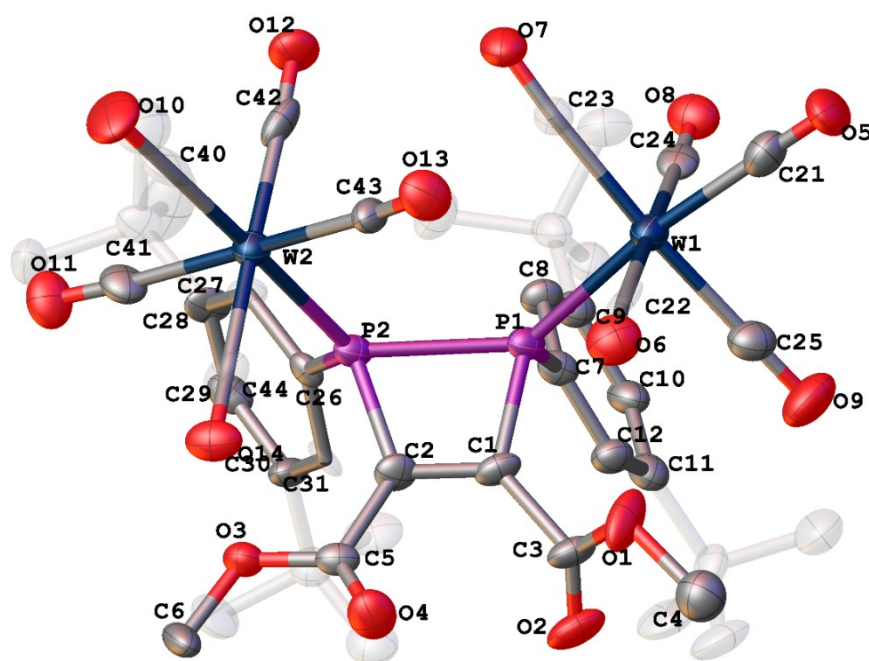


Figure S 7. Molecular structure of **5**. All hydrogen atoms are omitted for clarity and the *t*-Bu groups are presented transparently. The thermal ellipsoids are set at 50 % probability.

4.2. Crystallographic Data for **11**

Data were collected with a Bruker X8-KappaApexII diffractometer equipped with a low-temperature device at 100 K by using graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$). Empirical formula: $\text{C}_{44}\text{H}_{52}\text{N}_2\text{O}_{14}\text{P}_2\text{W}_2$, formula weight $M = 1262.51 \text{ g}\cdot\text{mol}^{-1}$, crystal system monoclinic, space group $P2_1$, unit cell dimensions $a = 11.4333(2) \text{ \AA}$, $b = 18.8510(3) \text{ \AA}$, $c = 11.5017(2) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90.5880(10)^\circ$, $\gamma = 90^\circ$, volume $V = 2476.42 \text{ \AA}^3$, $Z = 2$, calculated density $\rho_{\text{calcd.}} = 1.693 \text{ g}\cdot\text{cm}^{-3}$, absorption coefficient $\mu = 4.769 \text{ mm}^{-1}$, crystal size $0.398 \times 0.242 \times 0.108 \text{ mm}$, transmission factors (min/max) 0.2815/ 0.6205, 2θ range for data collection 3.273 to 33.217° , completeness to theta 0.988, reflections collected 17315, independent reflections 17315, Goodness-of-fit on F^2 1.006, final R indexes [$I \geq 2\sigma(I)$] $R_1 = 0.0354$, $wR_2 = 0.0808$, final R indexes [all data] $R_1 = 0.0420$, $wR_2 = 0.0837$, largest diff. peak and hole 1.683/-2.063 e \AA^{-3} . The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures (CCDC 2103740)

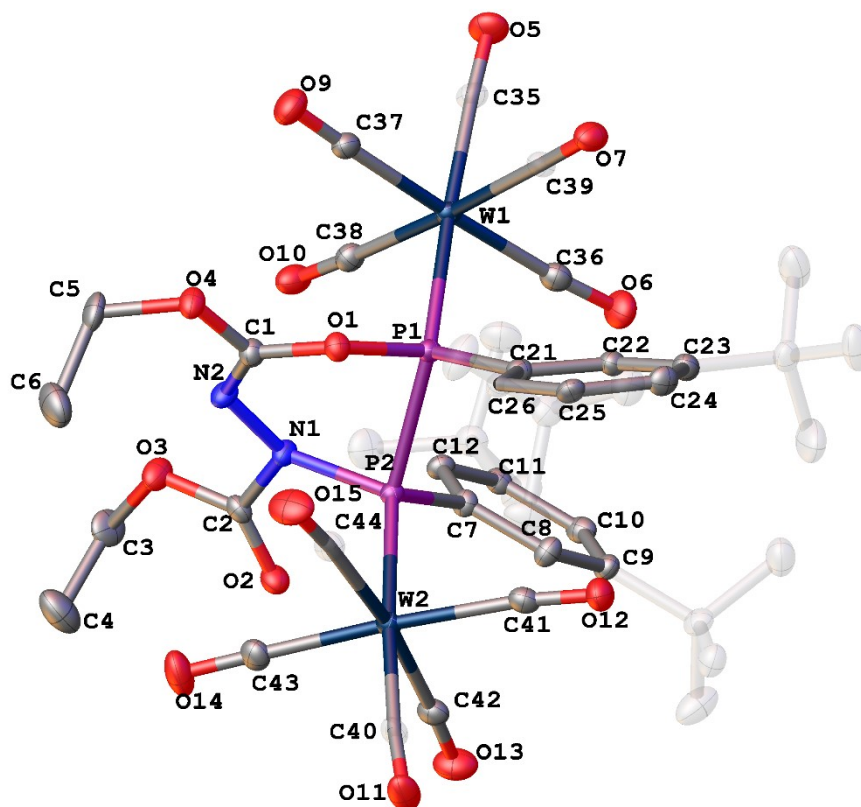
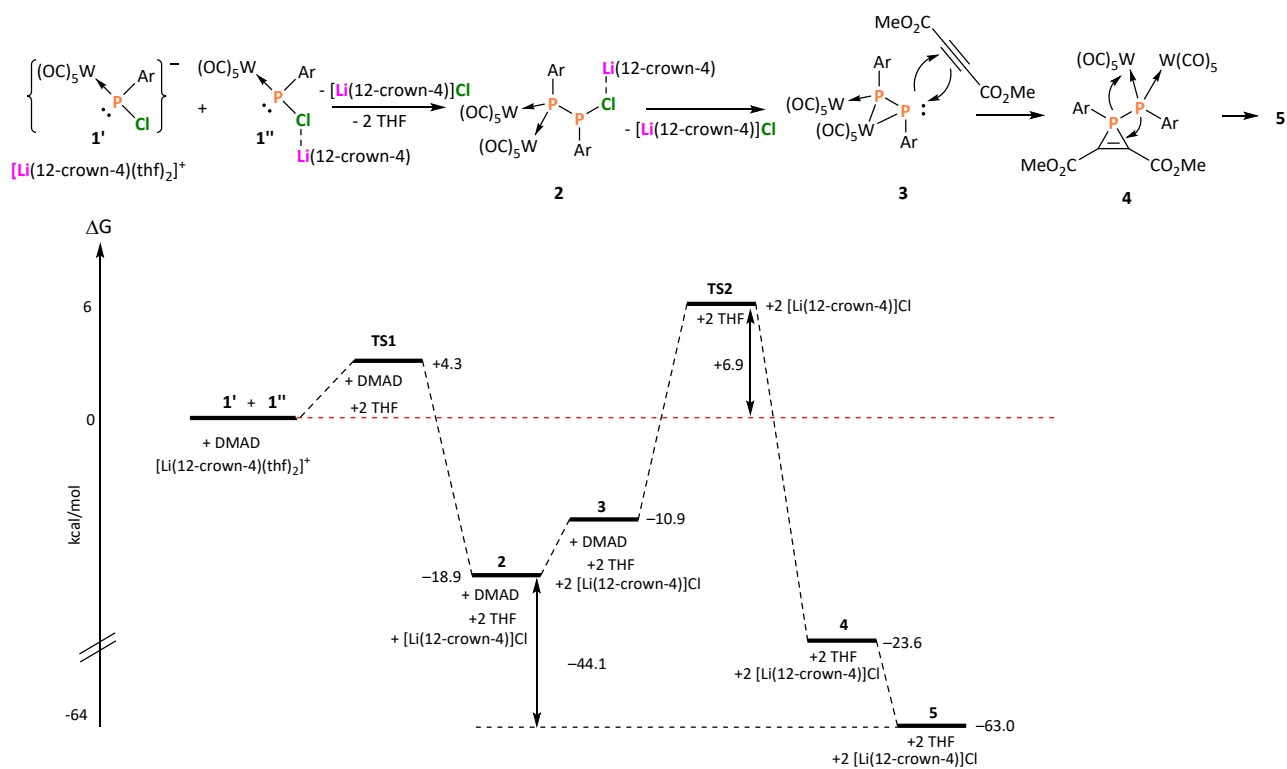


Figure S 8. Molecular structure of **11**. All hydrogen atoms are omitted for clarity and the *t*-Bu groups are presented transparently. The thermal ellipsoids are set at 50 % probability.

5. Computational details

The energies of all complexes included in this study were fully optimized at the B3LYP-D3/def2-TZVP level of theory. The calculations have been performed by using the program TURBOMOLE version 7.0.⁴ For the calculations we have used the DFT-D functional with the latest available correction for dispersion (D3).⁵ This level of theory is a good compromise between the accuracy of the results and the size of the systems (> 100 atoms). In order to reproduce solvent effects, we have used the conductor-like screening model COSMO,⁶ which is a variant of the dielectric continuum solvation models.⁷ We have used THF as solvent. The minimum or transition state nature of the compounds has been confirmed by doing frequency calculations. Due to the size of the systems, IRC have not been computed. However, we have checked that the negative frequency corresponds to the transition from the starting points to the products.

Scheme S1 shows the species that are used to compute the relative energies of each point of Scheme 1 discussed the main text, in order to be stoichiometrically consistent.



Scheme S4. Energetic profile and equations used to evaluate the mechanism analysed in this work.

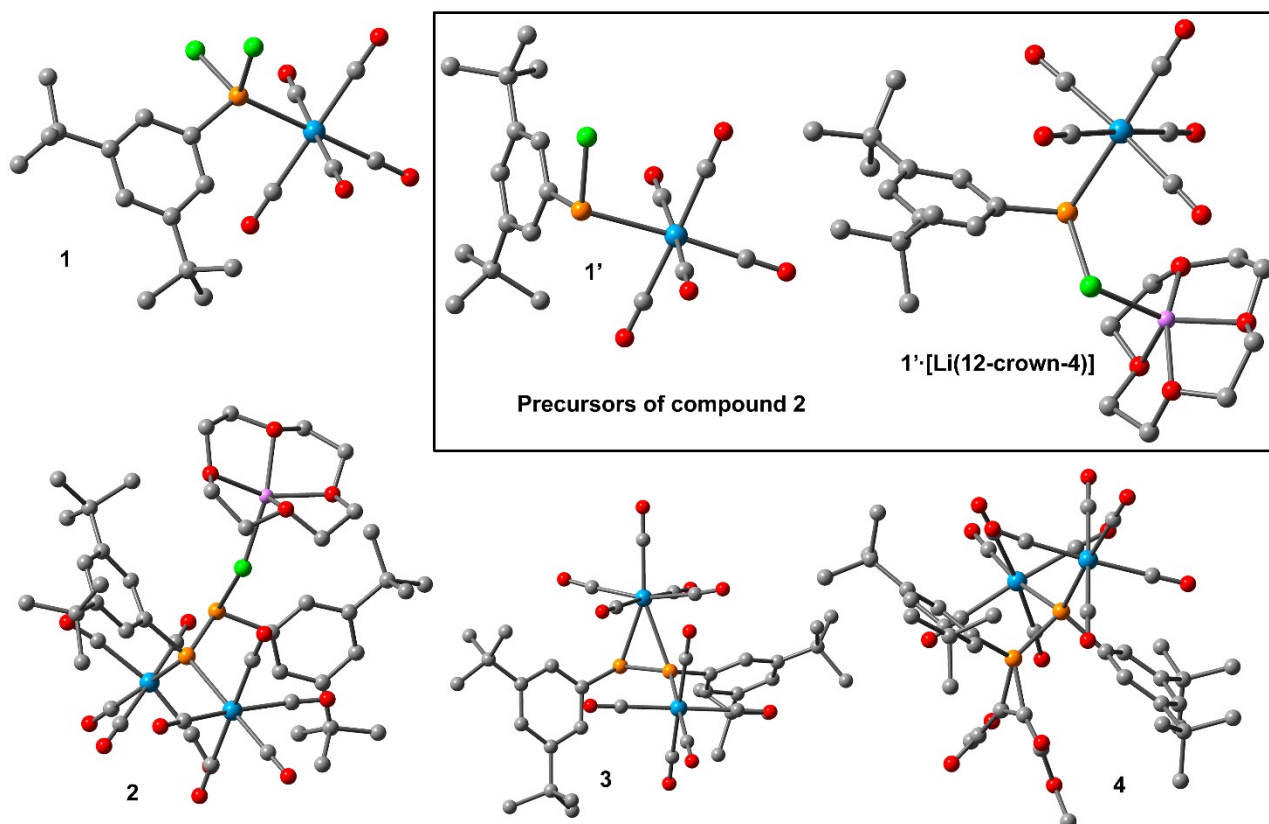


Figure S9. Optimized structures of several compounds (see main text for discussion).

HOMO-LUMO pictures of compound 3 are given in Figure S13, showing that the HOMO is composed by a lone pair type atomic orbital of the P-atom in combination with d-orbitals of the W atoms. The LUMO is composed by the π -antibonding type orbital localized at P=P bond with some additional participation of the W-CO ligands

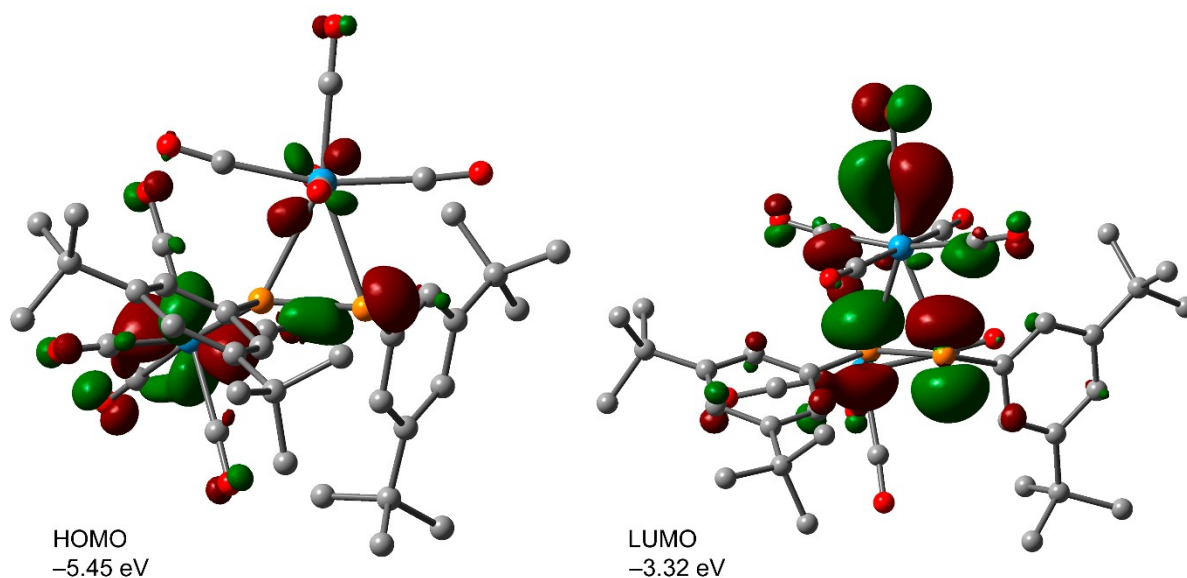


Figure S10. HOMO-LUMO representation for compound 3 (isovalue 0.02 a.u.) at the B3LYP-D3/def2-TZVP level of theory

6. Cartesian coordinates

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1.
E (THF): -2441.59879622459 Ha
NIMAG=0
W   -3.6238394    2.2162704   -1.3355967
P   -2.8674156    0.4162141    0.2498156
O   -4.5584938    4.4946738   -3.3607455
O   -1.5226458    1.1767128   -3.5314004
O   -1.4556740    4.2493418   -0.1185003
O   -5.7850749    3.2457962    0.8216333
O   -5.8414741    0.2400653   -2.5837175
C   -1.1370069   -0.1365456    0.3222163
C   -0.1712159    0.6976019   -0.2227559
H   -0.4695602    1.6180203   -0.6994561
C   1.1862048     0.3620458   -0.1607683
C   1.5203523   -0.8376355    0.4546487
H   2.5595920   -1.1243991    0.5075930
C   0.5668317   -1.7044149    1.0150124
C   -0.7671602   -1.3328313    0.9482802
H   -1.5342035   -1.9622103    1.3708818
C   1.0285741   -3.0143402    1.6680315
C   1.7631702   -3.8737397    0.6177050
H   1.1035350   -4.1091203   -0.2199195
H   2.0952506   -4.8134009    1.0651288
H   2.6433148   -3.3665469    0.2200870
C   1.9873871   -2.6944473    2.8336621
H   2.8732339   -2.1554005    2.4951154
H   2.3226921   -3.6187546    3.3097936
H   1.4896899   -2.0829400    3.5891903
C   -0.1459340   -3.8341045    2.2225026
H   -0.6918974   -3.2888786    2.9949470
H   0.2316004   -4.7537579    2.6728086
H   -0.8500448   -4.1165174    1.4371336
C   -4.2254535    3.6768210   -2.6320596
C   -2.2677447    1.5442580   -2.7450525
C   -2.2284574    3.5199217   -0.5437905

```

| | | | |
|----|------------|------------|------------|
| C | -5.0161717 | 2.8764636 | 0.0642761 |
| C | -5.0541622 | 0.9342188 | -2.1374703 |
| C | 2.2237500 | 1.3203349 | -0.7597575 |
| C | 3.6559780 | 0.7824770 | -0.6323039 |
| H | 4.3539442 | 1.4960320 | -1.0733921 |
| H | 3.9465529 | 0.6415705 | 0.4109854 |
| H | 3.7799306 | -0.1672910 | -1.1571346 |
| C | 2.1441415 | 2.6726825 | -0.0199753 |
| H | 1.1594597 | 3.1324897 | -0.1129060 |
| H | 2.3561097 | 2.5458661 | 1.0436173 |
| H | 2.8763406 | 3.3703968 | -0.4330275 |
| C | 1.9190365 | 1.5359567 | -2.2562987 |
| H | 1.9557061 | 0.5917338 | -2.8026282 |
| H | 0.9327737 | 1.9720617 | -2.4151508 |
| H | 2.6549260 | 2.2140207 | -2.6942987 |
| Cl | -3.2285943 | 0.8261943 | 2.2586694 |
| Cl | -3.8878543 | -1.3829655 | 0.0543713 |

1'

E (THF) : -1981.5248860565 Ha

NIMAG=0

| | | | |
|----|------------|------------|------------|
| W | -3.6118437 | 1.5412749 | -1.4124995 |
| P | -2.7137251 | 1.3805554 | 1.1176497 |
| O | -4.6446753 | 1.8951102 | -4.3868718 |
| O | -1.4824803 | -0.7176080 | -2.2480535 |
| O | -1.3907670 | 3.8121774 | -1.8428073 |
| O | -5.6784225 | 3.7291447 | -0.2905398 |
| O | -5.7795686 | -0.7778486 | -0.8800728 |
| C | -1.0969125 | 0.5195574 | 0.9343052 |
| C | -0.0337120 | 1.3139571 | 0.4976064 |
| H | -0.2142645 | 2.3673151 | 0.3142659 |
| C | 1.2360663 | 0.7860503 | 0.2660982 |
| C | 1.4339659 | -0.5723038 | 0.5100928 |
| H | 2.4070136 | -1.0077311 | 0.3373814 |
| C | 0.3987260 | -1.3984544 | 0.9637341 |
| C | -0.8568685 | -0.8383547 | 1.1717313 |
| H | -1.6817786 | -1.4495756 | 1.5011733 |
| C | 0.6716626 | -2.8959023 | 1.1771682 |
| C | 1.0888473 | -3.5305324 | -0.1661589 |
| H | 0.3023503 | -3.3963811 | -0.9114430 |
| H | 1.2723001 | -4.6024497 | -0.0433840 |
| H | 1.9989760 | -3.0752264 | -0.5591175 |
| C | 1.8072485 | -3.0789766 | 2.2047527 |
| H | 2.7317367 | -2.6038336 | 1.8736020 |
| H | 2.0132603 | -4.1421682 | 2.3619363 |
| H | 1.5303733 | -2.6379004 | 3.1649644 |
| C | -0.5624933 | -3.6499705 | 1.6955161 |
| H | -0.9059628 | -3.2510297 | 2.6516419 |
| H | -0.3141305 | -4.7048671 | 1.8401796 |
| H | -1.3932589 | -3.5961825 | 0.9901582 |
| C | -4.2681238 | 1.7673165 | -3.2976177 |
| C | -2.2424247 | 0.0934550 | -1.9596835 |
| C | -2.1933036 | 2.9982378 | -1.6901966 |
| C | -4.9400580 | 2.9468751 | -0.6980361 |
| C | -5.0061897 | 0.0495756 | -1.0606241 |
| C | 2.3478511 | 1.7022849 | -0.2688949 |
| C | 3.6923008 | 0.9736582 | -0.4171569 |
| H | 4.4476356 | 1.6698588 | -0.7903437 |
| H | 4.0449419 | 0.5783953 | 0.5381356 |
| H | 3.6263868 | 0.1455102 | -1.1261132 |
| C | 2.5549455 | 2.8893068 | 0.6935376 |
| H | 1.6462233 | 3.4813738 | 0.8025069 |
| H | 2.8449218 | 2.5353297 | 1.6856412 |
| H | 3.3431064 | 3.5503476 | 0.3203745 |
| C | 1.9350267 | 2.2364611 | -1.6563598 |
| H | 1.7708556 | 1.4101385 | -2.3514283 |
| H | 1.0134976 | 2.8155233 | -1.6084845 |
| H | 2.7191802 | 2.8809548 | -2.0660422 |
| Cl | -3.8684363 | -0.1424491 | 2.1177758 |

[Li (12-crown-4) (THF)₂]

E (THF) : -1087.5662691371 Ha

Nimag: 0

| | | | |
|----|------------|------------|------------|
| Li | -0.0051335 | -0.4513968 | -0.6329326 |
| O | -1.1365938 | -1.5448775 | 0.6600502 |
| C | -0.2791052 | -1.9369261 | 1.7401448 |
| H | -0.5546741 | -2.9290879 | 2.1091262 |
| H | -0.3641719 | -1.2180021 | 2.5600944 |
| C | 1.1522138 | -1.9369110 | 1.2224320 |
| H | 1.8470983 | -2.1791719 | 2.0331491 |
| H | 1.2792067 | -2.6735012 | 0.4194906 |

| | | | |
|---|------------|------------|------------|
| O | 1.3709584 | -0.6196409 | 0.7266567 |
| C | 2.5569539 | -0.3270953 | -0.0135238 |
| H | 2.7040510 | -1.0755306 | -0.8018944 |
| H | 3.4381270 | -0.3257929 | 0.6359507 |
| C | 2.3412023 | 1.0584193 | -0.6034497 |
| H | 2.2357212 | 1.7844340 | 0.2045740 |
| H | 3.1881404 | 1.3328510 | -1.2382631 |
| O | 1.1296761 | 1.0224941 | -1.3760952 |
| C | 0.3250287 | 2.2135966 | -1.3822167 |
| H | 0.5015598 | 2.7773372 | -0.4649386 |
| H | 0.5710205 | 2.8336361 | -2.2488408 |
| C | -1.1332432 | 1.7856840 | -1.4416384 |
| H | -1.7852469 | 2.6638553 | -1.4002090 |
| H | -1.3474726 | 1.2328123 | -2.3651462 |
| O | -1.3303292 | 0.9400383 | -0.3069471 |
| C | -2.5393277 | 0.1982986 | -0.1735403 |
| H | -3.3867369 | 0.8530310 | 0.0537039 |
| H | -2.7589719 | -0.3484669 | -1.0988220 |
| C | -2.2937436 | -0.7622404 | 0.9810136 |
| H | -3.1633896 | -1.4069898 | 1.1370576 |
| H | -2.1100324 | -0.1869885 | 1.8930190 |
| C | -0.9212432 | -2.8005483 | -2.2862553 |
| C | -0.4656415 | -3.5053990 | -3.5575687 |
| H | -0.8224065 | -3.3999260 | -1.3827915 |
| C | 0.0357511 | -2.3368352 | -4.4133975 |
| H | -1.2704869 | -4.0697661 | -4.0261812 |
| H | -0.8035453 | -1.8136449 | -4.8769556 |
| C | 0.7069415 | -1.4511347 | -3.3746051 |
| H | 1.7362794 | -1.7684610 | -3.1820914 |
| O | -0.0651204 | -1.6321828 | -2.1555553 |
| H | 0.7106813 | -0.3898932 | -3.6166719 |
| H | 0.7219380 | -2.6428440 | -5.2018956 |
| H | 0.3511467 | -4.1967862 | -3.3398743 |
| H | -1.9574790 | -2.4590280 | -2.3646944 |
| C | 1.3363330 | 1.8913991 | 3.0776745 |
| C | -0.8730492 | 2.4844555 | 3.7044938 |
| C | 0.5345481 | 2.3440582 | 4.2944481 |
| H | 2.3825212 | 2.2028240 | 3.1081490 |
| H | 1.3015751 | 0.8028887 | 2.9546436 |
| H | -1.5219460 | 3.1413478 | 4.2828776 |
| H | -1.3565230 | 1.5053818 | 3.6392117 |
| H | 0.8937357 | 3.3121879 | 4.6487593 |
| H | 0.5904114 | 1.6375570 | 5.1224310 |
| O | 0.7102834 | 2.5047041 | 1.9384734 |
| C | -0.5766555 | 3.0299370 | 2.3088962 |
| H | -1.3038872 | 2.7121263 | 1.5590239 |
| H | -0.5269475 | 4.1237141 | 2.3114507 |

1''

E (THF) = -2604.2753771179 Ha

NImag: 0

| | | | |
|---|------------|------------|------------|
| W | 1.2838596 | 1.5982717 | -2.5793165 |
| P | -0.3018345 | 0.3545029 | -0.8966173 |
| O | 3.0712097 | 3.2110013 | -4.6559104 |
| O | 2.7434699 | -1.1653036 | -3.2675717 |
| O | 3.4195814 | 2.0665237 | -0.2133905 |
| O | -0.3073513 | 4.2639665 | -1.7200089 |
| O | -0.9182825 | 1.0166064 | -4.8312206 |
| C | -0.0535589 | 1.1313428 | 0.7491776 |
| C | -0.9536578 | 2.1549456 | 1.0599373 |
| H | -1.7421656 | 2.3887092 | 0.3535802 |
| C | -0.8556398 | 2.8786185 | 2.2473139 |
| C | 0.1550330 | 2.5265354 | 3.1463034 |
| H | 0.2360398 | 3.0645667 | 4.0756879 |
| C | 1.0599099 | 1.4962686 | 2.8791695 |
| C | 0.9462180 | 0.8160931 | 1.6672879 |
| H | 1.6506005 | 0.0329248 | 1.4264647 |
| C | 2.1747398 | 1.0985653 | 3.8594690 |
| C | 3.5461083 | 1.2940587 | 3.1808419 |
| H | 3.6436688 | 0.6872952 | 2.2810002 |
| H | 4.3508928 | 1.0158650 | 3.8666608 |
| H | 3.6889091 | 2.3358819 | 2.8880576 |
| C | 2.1554930 | 1.9359501 | 5.1471457 |
| H | 2.3070477 | 2.9973626 | 4.9408373 |
| H | 2.9617725 | 1.6099372 | 5.8075711 |
| H | 1.2152311 | 1.8226753 | 5.6909334 |
| C | 2.0046335 | -0.3841574 | 4.2503557 |
| H | 1.0393845 | -0.5475212 | 4.7352848 |
| H | 2.7923231 | -0.6863337 | 4.9455799 |
| H | 2.0566359 | -1.0379928 | 3.3791955 |

| | | | |
|----|------------|------------|------------|
| C | 2.4204117 | 2.6294182 | -3.9036129 |
| C | 2.2340726 | -0.1574992 | -3.0296410 |
| C | 2.6571850 | 1.9089347 | -1.0518292 |
| C | 0.2668007 | 3.3215474 | -2.0281541 |
| C | -0.1250667 | 1.2311742 | -4.0228290 |
| C | -1.8531358 | 4.0137744 | 2.5264613 |
| C | -1.6166958 | 4.6846214 | 3.8881260 |
| H | -2.3488848 | 5.4813056 | 4.0348729 |
| H | -1.7263985 | 3.9779118 | 4.7135294 |
| H | -0.6234166 | 5.1335526 | 3.9503548 |
| C | -3.2902540 | 3.4523345 | 2.5158079 |
| H | -3.5423437 | 3.0061853 | 1.5529892 |
| H | -3.4115511 | 2.6847018 | 3.2834833 |
| H | -4.0112658 | 4.2500609 | 2.7129668 |
| C | -1.7167405 | 5.0905026 | 1.4307133 |
| H | -0.7066470 | 5.5047918 | 1.4195705 |
| H | -1.9147581 | 4.6881520 | 0.4376069 |
| H | -2.4202091 | 5.9075649 | 1.6120926 |
| Cl | 0.6633969 | -1.6191476 | -0.4753389 |
| Li | -0.2918294 | -3.0222416 | -2.1407377 |
| O | -1.4355167 | -1.8702002 | -3.2818080 |
| C | -1.2529080 | -2.2208802 | -4.6568466 |
| H | -1.3704467 | -1.3424191 | -5.2948152 |
| H | -1.9878462 | -2.9807169 | -4.9425940 |
| C | 0.1445615 | -2.7970352 | -4.7962780 |
| H | 0.3029582 | -3.1602837 | -5.8171877 |
| H | 0.9050972 | -2.0487073 | -4.5659041 |
| O | 0.2006203 | -3.8744698 | -3.8566879 |
| C | 1.4557115 | -4.4679645 | -3.5294738 |
| H | 2.1642032 | -3.7033184 | -3.1931667 |
| H | 1.8860857 | -4.9929850 | -4.3894031 |
| C | 1.1375173 | -5.4595995 | -2.4192348 |
| H | 0.4765138 | -6.2388425 | -2.8116663 |
| H | 2.0546120 | -5.9257083 | -2.0466706 |
| O | 0.4770476 | -4.7471056 | -1.3695445 |
| C | -0.5867319 | -5.4107466 | -0.6801829 |
| H | -1.0662006 | -6.1326855 | -1.3493569 |
| H | -0.2036427 | -5.9405098 | 0.1976591 |
| C | -1.6060400 | -4.3632288 | -0.2575648 |
| H | -2.4537143 | -4.8499962 | 0.2376340 |
| H | -1.1568675 | -3.6396392 | 0.4302849 |
| O | -2.0167492 | -3.7147580 | -1.4599001 |
| C | -2.7382859 | -2.4800920 | -1.3619370 |
| H | -3.7595230 | -2.6506913 | -1.0044191 |
| H | -2.2279097 | -1.7903529 | -0.6835543 |
| C | -2.7732169 | -1.9054064 | -2.7718393 |
| H | -3.1914012 | -0.8960802 | -2.7518241 |
| H | -3.3908697 | -2.5403820 | -3.4139699 |

TS 1-2

E(THF): -2604.2753771179 Ha

NImag=1 (-127 cm-1)

| | | | |
|---|------------|------------|------------|
| W | -1.5942949 | 2.9933757 | -2.1787842 |
| W | -0.6870588 | -2.9114930 | 1.3702068 |
| P | -0.2834077 | 0.8545832 | -1.1604679 |
| P | 0.2772424 | -0.5014804 | 1.7590606 |
| O | -2.7518254 | 5.6091644 | -3.5286170 |
| O | -3.9576383 | 3.3426938 | -0.0595001 |
| O | -3.6069643 | 1.1591493 | -3.8834995 |
| O | 0.5010410 | 2.7408256 | -4.6206028 |
| O | 0.3650416 | 4.7211407 | -0.3136649 |
| O | -1.8136053 | -3.0214059 | 4.3718870 |
| O | -1.9784487 | -5.7857188 | 0.9996347 |
| O | -3.4271109 | -1.4428734 | 0.6345632 |
| O | 0.5271504 | -3.4610270 | -1.5540412 |
| O | 2.1091257 | -4.0480333 | 2.4931485 |
| C | -0.5207166 | -0.4449763 | -2.4398996 |
| C | -1.7485208 | -1.1212938 | -2.4078266 |
| H | -2.4746662 | -0.8403277 | -1.6588582 |
| C | -2.0524762 | -2.1216703 | -3.3231634 |
| C | -1.0888066 | -2.4420353 | -4.2879657 |
| H | -1.3058212 | -3.2230572 | -4.9974193 |
| C | 0.1379206 | -1.7887392 | -4.3526423 |
| C | 0.4089793 | -0.7907280 | -3.4138730 |
| H | 1.3538840 | -0.2691331 | -3.4409980 |
| C | 1.2026049 | -2.1298534 | -5.4059683 |
| C | 2.4765475 | -2.6249763 | -4.6930866 |
| H | 2.8835362 | -1.8626308 | -4.0307057 |
| H | 3.2492605 | -2.8826689 | -5.4232967 |
| H | 2.2622373 | -3.5070316 | -4.0873388 |

| | | | |
|----|------------|------------|------------|
| C | 0.7428224 | -3.2265966 | -6.3783804 |
| H | 0.5324375 | -4.1638746 | -5.8588052 |
| H | 1.5313188 | -3.4216066 | -7.1091185 |
| H | -0.1540333 | -2.9300994 | -6.9269641 |
| C | 1.5321029 | -0.8673066 | -6.2289204 |
| H | 0.6427581 | -0.5021220 | -6.7471921 |
| H | 2.2993581 | -1.0900508 | -6.9760607 |
| H | 1.8998525 | -0.0577549 | -5.5982610 |
| C | 2.0140804 | -0.2379232 | 1.2513978 |
| C | 2.6050998 | 0.9611219 | 1.6384918 |
| H | 2.0202276 | 1.6540914 | 2.2269033 |
| C | 3.9133478 | 1.2811790 | 1.2844911 |
| C | 4.6192089 | 0.3590350 | 0.5155415 |
| H | 5.6309938 | 0.5878897 | 0.2139113 |
| C | 4.0562103 | -0.8519350 | 0.0943494 |
| C | 2.7522435 | -1.1365629 | 0.4814051 |
| H | 2.2816565 | -2.0549723 | 0.1748614 |
| C | 4.4822424 | 2.6470574 | 1.6924231 |
| C | 4.3311206 | 2.8430293 | 3.2153177 |
| H | 3.2858464 | 2.7966898 | 3.5218327 |
| H | 4.7288309 | 3.8176770 | 3.5135330 |
| H | 4.8729508 | 2.0676315 | 3.7615736 |
| C | 3.6911026 | 3.7479003 | 0.9560220 |
| H | 3.7741027 | 3.6292082 | -0.1254416 |
| H | 4.0669935 | 4.7388483 | 1.2277021 |
| H | 2.6294266 | 3.7079511 | 1.1978017 |
| C | 5.9684922 | 2.7968163 | 1.3362985 |
| H | 6.5767197 | 2.0293526 | 1.8208374 |
| H | 6.3305763 | 3.7724838 | 1.6691913 |
| H | 6.1340047 | 2.7354614 | 0.2587095 |
| C | 4.8692488 | -1.7958925 | -0.8015215 |
| C | 5.2166799 | -1.0603724 | -2.1127510 |
| H | 4.3095916 | -0.7098353 | -2.6070261 |
| H | 5.7488254 | -1.7269977 | -2.7972242 |
| H | 5.8490577 | -0.1900316 | -1.9293909 |
| C | 6.1696345 | -2.2090768 | -0.0834736 |
| H | 6.7903474 | -1.3451488 | 0.1610342 |
| H | 6.7595492 | -2.8759055 | -0.7188885 |
| H | 5.9434727 | -2.7335578 | 0.8474725 |
| C | 4.0913324 | -3.0721745 | -1.1555200 |
| H | 3.8347025 | -3.6463106 | -0.2625773 |
| H | 4.7041475 | -3.7093826 | -1.7975474 |
| H | 3.1690803 | -2.8518819 | -1.6928033 |
| C | -2.3397167 | 4.6473611 | -3.0341162 |
| C | -3.0730955 | 3.1696837 | -0.7830292 |
| C | -2.8762986 | 1.7960851 | -3.2705555 |
| C | -0.2134410 | 2.8306889 | -3.7319495 |
| C | -0.3181468 | 4.1053119 | -1.0056227 |
| C | -1.3953226 | -2.9251551 | 3.3053439 |
| C | -1.5093025 | -4.7384127 | 1.1400134 |
| C | -2.4288237 | -1.9848342 | 0.8399454 |
| C | 0.0695546 | -3.1698631 | -0.5451040 |
| C | 1.1141537 | -3.6525779 | 2.0869591 |
| C | -3.3672791 | -2.9137197 | -3.2313232 |
| C | -3.8031119 | -3.4539836 | -4.6063262 |
| H | -4.7763608 | -3.9430333 | -4.5175431 |
| H | -3.8922517 | -2.6464089 | -5.3364350 |
| H | -3.1060581 | -4.1950511 | -5.0004375 |
| C | -4.5180679 | -2.0446468 | -2.6914631 |
| H | -4.3450868 | -1.7210747 | -1.6669009 |
| H | -4.6614022 | -1.1572878 | -3.3095485 |
| H | -5.4464023 | -2.6221363 | -2.6939179 |
| C | -3.1416293 | -4.1046696 | -2.2771314 |
| H | -2.3403771 | -4.7507953 | -2.6423901 |
| H | -2.8572374 | -3.7619613 | -1.2824029 |
| H | -4.0523210 | -4.7037517 | -2.1844037 |
| Cl | 1.7366774 | 1.4298714 | -1.5365635 |
| Cl | 1.0287627 | -0.7882072 | 4.0759267 |
| Li | -0.6180479 | 0.9713867 | 3.7761803 |
| O | 0.4901981 | 2.7626459 | 3.8946615 |
| C | -0.1273636 | 3.7463551 | 3.0504509 |
| H | 0.6309346 | 4.2886071 | 2.4793381 |
| H | -0.6816407 | 4.4566509 | 3.6712152 |
| C | -1.0882217 | 3.0511311 | 2.1058322 |
| H | -1.6410488 | 3.7989057 | 1.5316062 |
| H | -0.5574633 | 2.3973135 | 1.4087932 |
| O | -1.9592272 | 2.2841812 | 2.9335669 |
| C | -2.8430634 | 1.3630896 | 2.2898445 |
| H | -2.2879145 | 0.7524042 | 1.5756506 |
| H | -3.6412105 | 1.8841113 | 1.7589416 |

| | | | |
|---|------------|------------|-----------|
| C | -3.4365673 | 0.5198526 | 3.4003078 |
| H | -4.0741938 | 1.1492415 | 4.0296686 |
| H | -4.0384679 | -0.2874854 | 2.9741302 |
| O | -2.3716242 | -0.0141716 | 4.1916930 |
| C | -2.6054482 | -0.1145497 | 5.5925868 |
| H | -3.3827777 | 0.6001600 | 5.8839419 |
| H | -2.9323055 | -1.1262922 | 5.8516805 |
| C | -1.3179937 | 0.2150062 | 6.3323951 |
| H | -1.5193621 | 0.2770861 | 7.4098951 |
| H | -0.5620285 | -0.5518813 | 6.1484722 |
| O | -0.8834680 | 1.4730212 | 5.8212232 |
| C | 0.4290716 | 1.9153109 | 6.1418159 |
| H | 0.5013059 | 2.2116988 | 7.1969990 |
| H | 1.1577094 | 1.1255724 | 5.9387987 |
| C | 0.6871377 | 3.1260695 | 5.2593749 |
| H | 1.7093488 | 3.4897648 | 5.4142386 |
| H | -0.0133167 | 3.9225208 | 5.5310254 |

2 (Scheme 2).

E (THF) : -3502.7830046803 Ha

NImag=0

| | | | |
|---|------------|------------|------------|
| W | -0.1424282 | 0.6276204 | -4.5418988 |
| W | 0.2871437 | -2.9787818 | -1.6258109 |
| P | 0.5690949 | 1.2731148 | -1.9884124 |
| P | -0.4748979 | -0.5705891 | -2.1130581 |
| O | -0.3967827 | 1.0832682 | -7.6810387 |
| O | 2.3629411 | -1.3285351 | -4.9958561 |
| O | 1.6056155 | 3.3266300 | -4.7640538 |
| O | -2.7724873 | 2.4037353 | -3.9747348 |
| O | -1.9900529 | -1.8951205 | -5.2720014 |
| O | 0.3628746 | -3.9060678 | -4.7041676 |
| O | 1.0902218 | -5.9259748 | -0.7795916 |
| O | 3.4566454 | -2.4690992 | -1.8861865 |
| O | 0.1534935 | -2.3791882 | 1.5209120 |
| O | -2.7613230 | -3.9604155 | -1.4582606 |
| C | 2.3150078 | 0.7868671 | -1.6966113 |
| C | 3.3314310 | 0.9446889 | -2.6364963 |
| H | 3.0857593 | 1.2414069 | -3.6444427 |
| C | 4.6665042 | 0.7227974 | -2.3032454 |
| C | 4.9548171 | 0.3438151 | -0.9918533 |
| H | 5.9808777 | 0.1608465 | -0.7207040 |
| C | 3.9648239 | 0.1916815 | -0.0194785 |
| C | 2.6401129 | 0.4224280 | -0.3862685 |
| H | 1.8502774 | 0.3481181 | 0.3502546 |
| C | 4.2897258 | -0.1951978 | 1.4294203 |
| C | 3.4136868 | -1.3905860 | 1.8515827 |
| H | 2.3595087 | -1.1217981 | 1.8690636 |
| H | 3.6916916 | -1.7170100 | 2.8564907 |
| H | 3.5480341 | -2.2344243 | 1.1717785 |
| C | 5.7622005 | -0.5883480 | 1.6154198 |
| H | 6.0372884 | -1.4336929 | 0.9805487 |
| H | 5.9331761 | -0.8814678 | 2.6536284 |
| H | 6.4382086 | 0.2403767 | 1.3957859 |
| C | 3.9769571 | 1.0069816 | 2.3448417 |
| H | 4.5786057 | 1.8733598 | 2.0602247 |
| H | 4.2089624 | 0.7536697 | 3.3829683 |
| H | 2.9223064 | 1.2786944 | 2.2918885 |
| C | -2.1916006 | -0.1309619 | -1.6503914 |
| C | -2.4518778 | 0.8454194 | -0.6953264 |
| H | -1.6301155 | 1.2937936 | -0.1578589 |
| C | -3.7675925 | 1.2268771 | -0.4073621 |
| C | -4.7972962 | 0.5746144 | -1.0775633 |
| H | -5.8186555 | 0.8590639 | -0.8734260 |
| C | -4.5686503 | -0.4491117 | -2.0079333 |
| C | -3.2526602 | -0.7890234 | -2.2835566 |
| H | -3.0387451 | -1.5678492 | -2.9958834 |
| C | -4.0319044 | 2.3036680 | 0.6535141 |
| C | -3.0201859 | 3.4596130 | 0.5139864 |
| H | -2.0004770 | 3.1359155 | 0.7212987 |
| H | -3.2639521 | 4.2507139 | 1.2275200 |
| H | -3.0511527 | 3.8868259 | -0.4906682 |
| C | -3.8637649 | 1.6601289 | 2.0442951 |
| H | -4.5847505 | 0.8515842 | 2.1885905 |
| H | -4.0348538 | 2.4114863 | 2.8216169 |
| H | -2.8607584 | 1.2513518 | 2.1695067 |
| C | -5.4480567 | 2.8903660 | 0.5407363 |
| H | -5.6297699 | 3.3091792 | -0.4516536 |
| H | -5.5711185 | 3.6920821 | 1.2718493 |
| H | -6.2204200 | 2.1465542 | 0.7453239 |
| C | -5.7572619 | -1.1361303 | -2.6935218 |

| | | | |
|----|------------|------------|------------|
| C | -6.6716911 | -1.7659142 | -1.6224300 |
| H | -6.1247537 | -2.5095943 | -1.0395764 |
| H | -7.5232872 | -2.2609973 | -2.0957835 |
| H | -7.0637886 | -1.0174688 | -0.9322523 |
| C | -6.5523992 | -0.0881592 | -3.4992437 |
| H | -6.9393325 | 0.7063314 | -2.8594718 |
| H | -7.4021229 | -0.5597261 | -3.9989981 |
| H | -5.9210856 | 0.3742208 | -4.2608804 |
| C | -5.3129779 | -2.2493721 | -3.6543804 |
| H | -4.6913445 | -1.8645342 | -4.4650224 |
| H | -6.1922208 | -2.7129826 | -4.1058098 |
| H | -4.7539984 | -3.0308430 | -3.1364534 |
| C | -0.3091253 | 0.9206403 | -6.5518977 |
| C | 1.4959324 | -0.6091791 | -4.8171775 |
| C | 1.0025295 | 2.3661713 | -4.6376717 |
| C | -1.8388640 | 1.7799840 | -4.1670166 |
| C | -1.3395034 | -1.0138829 | -4.9505560 |
| C | 0.3305421 | -3.5511427 | -3.6174607 |
| C | 0.8035438 | -4.8597835 | -1.1018135 |
| C | 2.3235923 | -2.5620079 | -1.7788624 |
| C | 0.2171850 | -2.5304094 | 0.3868245 |
| C | -1.6848683 | -3.5730591 | -1.5232193 |
| C | 5.7541329 | 0.9015465 | -3.3726126 |
| C | 7.1630345 | 0.6236329 | -2.8282148 |
| H | 7.8967649 | 0.7701043 | -3.6234138 |
| H | 7.4229200 | 1.2993476 | -2.0108269 |
| H | 7.2635409 | -0.4035187 | -2.4715124 |
| C | 5.7189237 | 2.3517213 | -3.8982904 |
| H | 4.7534275 | 2.5993627 | -4.3415902 |
| H | 5.9071591 | 3.0622679 | -3.0906687 |
| H | 6.4843868 | 2.4950039 | -4.6650867 |
| C | 5.4899402 | -0.0715796 | -4.5389628 |
| H | 5.4662058 | -1.1043600 | -4.1869508 |
| H | 4.5377391 | 0.1306629 | -5.0281811 |
| H | 6.2765190 | 0.0196065 | -5.2924632 |
| Cl | -0.0054947 | 1.0343617 | 2.0101472 |
| Li | -0.1438717 | 0.0482476 | 4.0047026 |
| O | -2.2096969 | -0.1273570 | 4.4378005 |
| C | -2.4948281 | -1.4238232 | 4.9532428 |
| H | -3.4424087 | -1.7999275 | 4.5534450 |
| H | -2.5621973 | -1.3864206 | 6.0457039 |
| C | -1.3505006 | -2.3434515 | 4.5571286 |
| H | -1.4847711 | -3.3308304 | 5.0145683 |
| H | -1.2951346 | -2.4606203 | 3.4713242 |
| O | -0.1804168 | -1.6990581 | 5.0518028 |
| C | 1.1027565 | -2.2661088 | 4.8044341 |
| H | 1.2610046 | -2.4118370 | 3.7328655 |
| H | 1.2156149 | -3.2295894 | 5.3152613 |
| C | 2.0879449 | -1.2571915 | 5.3713624 |
| H | 1.9363728 | -1.1771885 | 6.4531126 |
| H | 3.1165707 | -1.5828280 | 5.1830004 |
| O | 1.8312836 | -0.0034346 | 4.7489693 |
| C | 2.0346164 | 1.1737690 | 5.5306855 |
| H | 1.9966261 | 0.9214562 | 6.5953286 |
| H | 3.0108163 | 1.6149244 | 5.3060767 |
| C | 0.9275424 | 2.1648185 | 5.2079591 |
| H | 1.0214403 | 3.0477751 | 5.8515685 |
| H | 0.9710079 | 2.4678124 | 4.1574251 |
| O | -0.2914182 | 1.4689806 | 5.4674242 |
| C | -1.5195359 | 2.0726555 | 5.0624638 |
| H | -1.7601348 | 2.9372548 | 5.6930474 |
| H | -1.4581563 | 2.3871241 | 4.0162877 |
| C | -2.5754608 | 0.9953514 | 5.2406871 |
| H | -3.5572654 | 1.3732451 | 4.9419174 |
| H | -2.6133629 | 0.6998361 | 6.2944552 |

3.

E (THF) : -3042.4375376366 Ha
NImag=0

| | | | |
|---|------------|------------|------------|
| W | -0.2184476 | 1.5967996 | -2.6953490 |
| W | 0.5635100 | -2.6475878 | -0.9109316 |
| P | 0.3585211 | 1.5060127 | -0.0532708 |
| P | -0.4780892 | -0.3089563 | -0.7875152 |
| O | -0.4991581 | 2.9331353 | -5.5744919 |
| O | 2.4847019 | 0.1037514 | -3.5838056 |
| O | 1.2791469 | 4.3822686 | -2.0576642 |
| O | -3.0216118 | 2.8661274 | -1.7409461 |
| O | -1.8111135 | -0.7564098 | -4.1929521 |
| O | 0.6689151 | -2.6936235 | -4.1248080 |
| O | 1.7321978 | -5.5951090 | -0.7614505 |

| | | | |
|---|------------|------------|------------|
| O | 3.6480546 | -1.7440827 | -1.0638440 |
| O | 0.3762705 | -2.5590561 | 2.2942913 |
| O | -2.3245959 | -4.0374786 | -1.0399387 |
| C | 2.1246548 | 1.0859143 | 0.2070197 |
| C | 3.1623794 | 1.6158649 | -0.5505408 |
| H | 2.9369273 | 2.2148765 | -1.4197588 |
| C | 4.4970075 | 1.3809543 | -0.2135812 |
| C | 4.7546378 | 0.6072460 | 0.9152880 |
| H | 5.7785534 | 0.4068036 | 1.1830525 |
| C | 3.7394909 | 0.0726383 | 1.7169788 |
| C | 2.4227215 | 0.3257246 | 1.3458921 |
| H | 1.6086306 | -0.0687360 | 1.9366218 |
| C | 4.0718306 | -0.8289828 | 2.9151352 |
| C | 4.1700132 | -2.2829088 | 2.4055175 |
| H | 3.2258091 | -2.6094114 | 1.9681344 |
| H | 4.4146926 | -2.9595197 | 3.2280584 |
| H | 4.9424829 | -2.3774695 | 1.6401061 |
| C | 5.4125760 | -0.4361779 | 3.5626695 |
| H | 6.2604208 | -0.6040988 | 2.8977544 |
| H | 5.5808980 | -1.0430179 | 4.4543843 |
| H | 5.4154117 | 0.6142966 | 3.8612270 |
| C | 2.9846305 | -0.7485444 | 4.0021305 |
| H | 2.8378140 | 0.2808744 | 4.3360695 |
| H | 3.2842901 | -1.3455874 | 4.8657789 |
| H | 2.0270796 | -1.1399765 | 3.6618825 |
| C | -2.2357590 | -0.2325245 | -0.2788629 |
| C | -2.6324812 | 0.3974814 | 0.8943625 |
| H | -1.8891476 | 0.8754575 | 1.5157277 |
| C | -3.9777812 | 0.4227209 | 1.2797309 |
| C | -4.8996324 | -0.2136414 | 0.4565305 |
| H | -5.9417854 | -0.2125471 | 0.7367223 |
| C | -4.5323892 | -0.8721627 | -0.7266490 |
| C | -3.1909130 | -0.8715765 | -1.0779873 |
| H | -2.8717894 | -1.3793321 | -1.9730484 |
| C | -4.3706711 | 1.1430028 | 2.5765372 |
| C | -3.9567411 | 2.6261559 | 2.4761600 |
| H | -2.8805201 | 2.7390413 | 2.3389425 |
| H | -4.2339103 | 3.1579119 | 3.3895274 |
| H | -4.4534252 | 3.1105614 | 1.6331262 |
| C | -3.6416960 | 0.4842750 | 3.7660749 |
| H | -3.9167763 | -0.5686764 | 3.8547744 |
| H | -3.9096737 | 0.9873930 | 4.6981592 |
| H | -2.5577467 | 0.5385045 | 3.6585067 |
| C | -5.8810997 | 1.0830455 | 2.8456826 |
| H | -6.4541847 | 1.5606743 | 2.0481268 |
| H | -6.1077324 | 1.6095864 | 3.7746541 |
| H | -6.2331094 | 0.0551473 | 2.9554969 |
| C | -5.6023420 | -1.5770224 | -1.5704947 |
| C | -6.2279948 | -2.7138238 | -0.7352343 |
| H | -5.4673485 | -3.4410443 | -0.4453280 |
| H | -6.9933864 | -3.2325381 | -1.3173953 |
| H | -6.6983989 | -2.3350809 | 0.1734577 |
| C | -6.6954105 | -0.5642356 | -1.9685153 |
| H | -7.1899296 | -0.1330086 | -1.0973156 |
| H | -7.4604027 | -1.0551784 | -2.5746714 |
| H | -6.2708677 | 0.2546096 | -2.5533843 |
| C | -5.0229723 | -2.1874973 | -2.8557470 |
| H | -4.5698022 | -1.4288167 | -3.4971507 |
| H | -5.8232141 | -2.6649195 | -3.4241682 |
| H | -4.2726986 | -2.9495208 | -2.6402255 |
| C | -0.3994900 | 2.4535244 | -4.5422380 |
| C | 1.5442143 | 0.6517833 | -3.2462252 |
| C | 0.7622764 | 3.3829910 | -2.2418561 |
| C | -2.0260615 | 2.4236590 | -2.0735031 |
| C | -1.2474888 | 0.0480777 | -3.6132959 |
| C | 0.6243094 | -2.6734760 | -2.9822148 |
| C | 1.3123012 | -4.5289177 | -0.8281573 |
| C | 2.5362747 | -1.9871383 | -0.9661031 |
| C | 0.4603687 | -2.5929572 | 1.1524710 |
| C | -1.3123280 | -3.5051755 | -0.9815717 |
| C | 5.6112382 | 1.9731729 | -1.0876757 |
| C | 7.0126866 | 1.6062880 | -0.5783700 |
| H | 7.7656671 | 2.0538638 | -1.2295860 |
| H | 7.1886838 | 1.9788271 | 0.4330919 |
| H | 7.1736674 | 0.5264172 | -0.5815405 |
| C | 5.4873502 | 3.5111013 | -1.0953175 |
| H | 4.5247372 | 3.8399516 | -1.4896040 |
| H | 5.5898917 | 3.9141051 | -0.0854159 |
| H | 6.2699015 | 3.9496436 | -1.7192118 |
| C | 5.4677273 | 1.4393349 | -2.5273381 |

| | | | |
|---|-----------|-----------|------------|
| H | 5.5101243 | 0.3490339 | -2.5453055 |
| H | 4.5226991 | 1.7392704 | -2.9796557 |
| H | 6.2737286 | 1.8276443 | -3.1546433 |

4

E (THF) : -3575.5030149871 Ha
NImag=0

| | | | |
|---|------------|------------|------------|
| C | 0.1163124 | -1.8133348 | -1.0188771 |
| C | 1.4150442 | -1.5741553 | -1.0458000 |
| C | 2.7285335 | -2.2235473 | -1.2509076 |
| C | -0.8830709 | -2.8771127 | -1.2407686 |
| O | -1.9394242 | -2.6641902 | -1.7787499 |
| O | 2.9897641 | -2.8932599 | -2.2141010 |
| O | 3.5404258 | -1.9290418 | -0.2402306 |
| O | -0.4490316 | -4.0601439 | -0.8092235 |
| C | 4.8903301 | -2.4365170 | -0.3308320 |
| H | 5.3673120 | -2.1346719 | 0.5958182 |
| H | 4.8783474 | -3.5207858 | -0.4329411 |
| H | 5.3892172 | -1.9913115 | -1.1908799 |
| C | -1.3231000 | -5.1818805 | -1.0722497 |
| H | -0.8299840 | -6.0402562 | -0.6270054 |
| H | -2.2975152 | -5.0145683 | -0.6163308 |
| H | -1.4405757 | -5.3138965 | -2.1471938 |
| P | 0.4567616 | -0.0964666 | -0.8064249 |
| C | 0.1012598 | 0.8815060 | -2.2665319 |
| C | 0.9660883 | 1.8806312 | -2.7192264 |
| C | -1.1095298 | 0.6305867 | -2.9068153 |
| C | 0.6321200 | 2.6315393 | -3.8370478 |
| H | 1.8861355 | 2.0670948 | -2.1958922 |
| C | -1.4811868 | 1.3871728 | -4.0206749 |
| H | -1.7638130 | -0.1451445 | -2.5317900 |
| C | -0.5944808 | 2.3660383 | -4.4600797 |
| H | -0.8652538 | 2.9646184 | -5.3163955 |
| C | -2.8451446 | 1.1372158 | -4.6753044 |
| C | -3.0506392 | 1.9879827 | -5.9364295 |
| H | -4.0241297 | 1.7603357 | -6.3744843 |
| H | -3.0351916 | 3.0566493 | -5.7133546 |
| H | -2.2908262 | 1.7808274 | -6.6932571 |
| C | -3.9489699 | 1.4958327 | -3.6573917 |
| H | -3.8949756 | 0.8706966 | -2.7666030 |
| H | -3.8637578 | 2.5384251 | -3.3439209 |
| H | -4.9344080 | 1.3531238 | -4.1069514 |
| C | -2.9692385 | -0.3497504 | -5.0659035 |
| H | -2.1924305 | -0.6295735 | -5.7808303 |
| H | -2.8873231 | -1.0094381 | -4.2015419 |
| H | -3.9410162 | -0.5328228 | -5.5299662 |
| C | 1.5373980 | 3.7459816 | -4.3748667 |
| C | 2.8790286 | 3.8149684 | -3.6291927 |
| H | 2.7450945 | 4.0610313 | -2.5757085 |
| H | 3.4319722 | 2.8764664 | -3.6995172 |
| H | 3.4979766 | 4.5991653 | -4.0683995 |
| C | 1.8310385 | 3.4997041 | -5.8685678 |
| H | 0.9217260 | 3.4964735 | -6.4703891 |
| H | 2.4800641 | 4.2881011 | -6.2557396 |
| H | 2.3355796 | 2.5419816 | -6.0134661 |
| C | 0.8125613 | 5.0974203 | -4.2021374 |
| H | 1.4405594 | 5.9096271 | -4.5757233 |
| H | -0.1298360 | 5.1208964 | -4.7511873 |
| H | 0.5920367 | 5.2869143 | -3.1507629 |
| P | 0.4069427 | 0.9724558 | 1.1161771 |
| C | 0.1656795 | -0.4972392 | 2.2110469 |
| C | -0.9494493 | -1.3276780 | 2.0507871 |
| C | 1.0022262 | -0.6810584 | 3.3079074 |
| C | -1.2259252 | -2.3424005 | 2.9614800 |
| H | -1.6276450 | -1.1462268 | 1.2320568 |
| C | 0.7549149 | -1.6832885 | 4.2475101 |
| H | 1.8395329 | -0.0194446 | 3.4405243 |
| C | -0.3512270 | -2.5043472 | 4.0397403 |
| H | -0.5547849 | -3.2884616 | 4.7556916 |
| C | -2.4556673 | -3.2527503 | 2.8397392 |
| C | 1.6479650 | -1.8961696 | 5.4780024 |
| C | 2.3076257 | -3.2874639 | 5.3840453 |
| H | 2.9449430 | -3.4641271 | 6.2538650 |
| H | 1.5633973 | -4.0849226 | 5.3466246 |
| H | 2.9261778 | -3.3615710 | 4.4872395 |
| C | 0.7886291 | -1.8165660 | 6.7565866 |
| H | 0.0129773 | -2.5835796 | 6.7784926 |
| H | 1.4164463 | -1.9556055 | 7.6396205 |
| H | 0.2996719 | -0.8436694 | 6.8338629 |
| C | 2.7591789 | -0.8405237 | 5.5836383 |

| | | | |
|---|------------|------------|------------|
| H | 3.4412238 | -0.8829670 | 4.7338090 |
| H | 2.3525485 | 0.1707691 | 5.6513774 |
| H | 3.3470448 | -1.0204356 | 6.4853389 |
| C | -1.9830533 | -4.7082242 | 2.6486246 |
| H | -1.4027013 | -5.0579879 | 3.5037663 |
| H | -2.8407358 | -5.3753914 | 2.5312943 |
| H | -1.3518908 | -4.7949726 | 1.7628314 |
| C | -3.2998036 | -3.1472437 | 4.1270986 |
| H | -4.1876872 | -3.7789763 | 4.0477159 |
| H | -2.7434530 | -3.4672200 | 5.0087707 |
| H | -3.6246061 | -2.1181093 | 4.2911302 |
| C | -3.3561924 | -2.8670669 | 1.6571398 |
| H | -3.7365824 | -1.8488250 | 1.7521233 |
| H | -2.8456098 | -2.9406689 | 0.6972363 |
| H | -4.2174828 | -3.5367235 | 1.6212002 |
| W | -1.8043152 | 2.4094396 | 1.1415955 |
| W | 2.8319289 | 2.0495817 | 1.1919057 |
| C | -2.8584693 | 0.9320908 | 0.1803615 |
| C | -1.4738709 | 3.3628766 | -0.6644880 |
| C | -3.4964604 | 3.4977354 | 1.3187124 |
| C | -2.2287915 | 1.5364496 | 2.9735796 |
| C | -0.7616948 | 3.9247232 | 2.1030405 |
| C | 1.9843627 | 3.6944007 | 0.2564629 |
| C | 3.5605244 | 1.3115344 | -0.5744544 |
| C | 3.7953883 | 0.4110147 | 1.9863175 |
| C | 4.5427391 | 3.1038352 | 1.3954434 |
| C | 2.2730904 | 2.6696521 | 3.1028334 |
| O | -4.4648940 | 4.1091695 | 1.4179258 |
| O | -3.4547486 | 0.1068385 | -0.3524580 |
| O | -1.3667602 | 3.9439402 | -1.6446607 |
| O | -2.4902669 | 1.0660725 | 3.9828828 |
| O | -0.2128826 | 4.7789230 | 2.6284694 |
| O | 5.5094035 | 3.7128249 | 1.5164186 |
| O | 2.0145941 | 2.9694619 | 4.1739219 |
| O | 4.4081141 | -0.4771390 | 2.3762472 |
| O | 4.0353561 | 0.8638837 | -1.5221169 |
| O | 1.5571898 | 4.6042337 | -0.2892871 |

5.

E (THF): -3575.5657996221 Ha

NImag=0

| | | | |
|---|------------|------------|------------|
| C | -0.5830493 | -2.4142872 | -0.4508213 |
| C | 0.5853979 | -2.4625943 | 0.2120799 |
| P | -0.8426794 | -0.6336585 | -0.8039000 |
| P | 0.8902251 | -0.7113064 | 0.6843682 |
| C | 2.3934110 | -0.0997670 | -0.1169321 |
| C | 3.2923633 | -0.9372246 | -0.7742563 |
| C | 2.6345607 | 1.2719808 | -0.0193523 |
| C | 4.4566620 | -0.4103799 | -1.3328260 |
| H | 3.0858302 | -1.9928520 | -0.8474095 |
| C | 3.7783029 | 1.8308197 | -0.5788296 |
| H | 1.9214614 | 1.8976803 | 0.4974355 |
| C | 4.6672782 | 0.9647102 | -1.2217901 |
| H | 5.5679162 | 1.3820193 | -1.6512096 |
| C | -2.2835121 | -0.0040226 | 0.0958849 |
| C | -3.1799307 | -0.8108294 | 0.7833257 |
| C | -2.4956238 | 1.3765038 | 0.0137987 |
| C | -4.3324648 | -0.2597778 | 1.3572999 |
| H | -3.0030705 | -1.8743275 | 0.8459700 |
| C | -3.6062835 | 1.9612086 | 0.5999182 |
| H | -1.7833682 | 1.9804209 | -0.5289966 |
| C | -4.5144257 | 1.1155653 | 1.2523922 |
| H | -5.3966018 | 1.5594218 | 1.6871434 |
| C | 1.3872830 | -3.6686515 | 0.5771136 |
| C | -1.3702932 | -3.5977766 | -0.8739540 |
| O | 2.3285864 | -4.0492763 | -0.0701388 |
| O | -0.9880968 | -4.7375382 | -0.7815834 |
| O | -2.5619215 | -3.2253740 | -1.3631276 |
| O | 0.9641671 | -4.2014081 | 1.7202643 |
| C | 1.6947273 | -5.3546418 | 2.1909122 |
| H | 1.2073162 | -5.6425614 | 3.1174407 |
| H | 1.6365668 | -6.1548948 | 1.4546076 |
| H | 2.7358644 | -5.0874445 | 2.3674397 |
| C | -3.4115962 | -4.2809741 | -1.8510804 |
| H | -2.9194564 | -4.8079920 | -2.6670959 |
| H | -3.6383434 | -4.9819786 | -1.0482365 |
| H | -4.3122235 | -3.7872009 | -2.2031515 |
| W | 0.6382985 | -0.3963407 | 3.1951197 |
| W | -0.5610322 | 0.1092830 | -3.2256145 |
| C | 2.2152932 | -1.7250506 | 3.3481681 |

| | | | |
|---|------------|------------|------------|
| C | 1.9747765 | 1.1856783 | 3.2057396 |
| C | 0.5687785 | -0.3182775 | 5.2254018 |
| C | -0.9384870 | 0.9574142 | 3.1572696 |
| C | -0.6985284 | -1.9762389 | 3.2193359 |
| C | 1.1726847 | -1.0096461 | -3.4308129 |
| C | -1.6532635 | -1.5334532 | -3.8621294 |
| C | -2.3242146 | 1.1886177 | -3.1619161 |
| C | 0.4583145 | 1.8213581 | -2.6662706 |
| C | -0.3565123 | 0.6700047 | -5.1691412 |
| O | 3.0848167 | -2.4629836 | 3.4482510 |
| O | 2.7116530 | 2.0599321 | 3.2478932 |
| O | -1.4302341 | -2.8544109 | 3.2492368 |
| O | -1.7895202 | 1.7161936 | 3.2346093 |
| O | 0.5371173 | -0.2886374 | 6.3714939 |
| O | -0.2393748 | 0.9868805 | -6.2650583 |
| O | -2.2610409 | -2.4171196 | -4.2604130 |
| O | 2.1028608 | -1.6442633 | -3.6279883 |
| O | 0.9705867 | 2.8096258 | -2.3992074 |
| O | -3.2961966 | 1.7923462 | -3.1702921 |
| C | 5.4903299 | -1.2870205 | -2.0531717 |
| C | 6.8522116 | -1.1534556 | -1.3407925 |
| H | 7.5981049 | -1.7785198 | -1.8373667 |
| H | 7.2203903 | -0.1263263 | -1.3507755 |
| H | 6.7774506 | -1.4741342 | -0.2998209 |
| C | 5.6255926 | -0.8146541 | -3.5157258 |
| H | 4.6736152 | -0.9058110 | -4.0405491 |
| H | 5.9491648 | 0.2256241 | -3.5780263 |
| H | 6.3646333 | -1.4251259 | -4.0398655 |
| C | 5.0928036 | -2.7706013 | -2.0581394 |
| H | 4.9967414 | -3.1719350 | -1.0477627 |
| H | 4.1490202 | -2.9359432 | -2.5780238 |
| H | 5.8617275 | -3.3496074 | -2.5732887 |
| C | 4.1010135 | 3.3280532 | -0.4833617 |
| C | 4.3123702 | 3.9052326 | -1.8979242 |
| H | 4.5453154 | 4.9707091 | -1.8353826 |
| H | 5.1377974 | 3.4171532 | -2.4177465 |
| H | 3.4128493 | 3.7867675 | -2.5029026 |
| C | 5.3910522 | 3.5044752 | 0.3450150 |
| H | 5.2616874 | 3.1025599 | 1.3519055 |
| H | 6.2394905 | 2.9955507 | -0.1153726 |
| H | 5.6426529 | 4.5643567 | 0.4294012 |
| C | 2.9781542 | 4.1244786 | 0.1990370 |
| H | 2.0374090 | 4.0402432 | -0.3471062 |
| H | 2.8197183 | 3.7987551 | 1.2285879 |
| H | 3.2495205 | 5.1813833 | 0.2286389 |
| C | -5.3520243 | -1.1807847 | 2.0420350 |
| C | -6.5685790 | -0.4122217 | 2.5779127 |
| H | -6.2830129 | 0.3240570 | 3.3318007 |
| H | -7.1086747 | 0.1019964 | 1.7803592 |
| H | -7.2618848 | -1.1118048 | 3.0482178 |
| C | -4.6793887 | -1.9066013 | 3.2231065 |
| H | -3.8512702 | -2.5334125 | 2.8975145 |
| H | -4.2909786 | -1.1893407 | 3.9492093 |
| H | -5.4022998 | -2.5485459 | 3.7321710 |
| C | -5.8525700 | -2.2230322 | 1.0194579 |
| H | -6.5841187 | -2.8875705 | 1.4854073 |
| H | -6.3290082 | -1.7341256 | 0.1670339 |
| H | -5.0366227 | -2.8392922 | 0.6400583 |
| C | -3.8851291 | 3.4667149 | 0.5163526 |
| C | -5.1689306 | 3.6876253 | -0.3112514 |
| H | -5.0529128 | 3.2854425 | -1.3193786 |
| H | -6.0317968 | 3.2033826 | 0.1491231 |
| H | -5.3878587 | 4.7552092 | -0.3898169 |
| C | -2.7370017 | 4.2311956 | -0.1599683 |
| H | -1.7958829 | 4.1054638 | 0.3799763 |
| H | -2.5901220 | 3.9139931 | -1.1941011 |
| H | -2.9679435 | 5.2976903 | -0.1758584 |
| C | -4.0770873 | 4.0416116 | 1.9341986 |
| H | -4.2755357 | 5.1142738 | 1.8777736 |
| H | -4.9173919 | 3.5770459 | 2.4515726 |
| H | -3.1845471 | 3.8863183 | 2.5412351 |

TS 3-4

E (THF) : -3575.454179349 Ha

NImag = 1 (-301 cm⁻¹)

| | | | |
|---|-----------|------------|-----------|
| C | 3.5133113 | 0.1866469 | 0.2798980 |
| C | 3.1804883 | 1.4029943 | 0.0436024 |
| C | 3.5879686 | 2.8158291 | 0.0510174 |
| C | 4.4384204 | -0.8323985 | 0.7973310 |
| O | 4.3224620 | -2.0149737 | 0.6210718 |

| | | | |
|---|------------|------------|------------|
| O | 4.3068495 | 3.2892925 | -0.7887628 |
| O | 3.0293060 | 3.4566031 | 1.0752215 |
| O | 5.4182430 | -0.2292643 | 1.4786729 |
| C | 3.2987864 | 4.8748207 | 1.1606821 |
| C | 6.4307300 | -1.1005249 | 2.0305672 |
| H | 2.7526024 | 5.2115692 | 2.0359380 |
| H | 4.3683083 | 5.0457494 | 1.2754076 |
| H | 2.9409374 | 5.3706061 | 0.2597133 |
| H | 7.1603916 | -0.4380768 | 2.4862670 |
| H | 5.9888964 | -1.7606113 | 2.7758564 |
| H | 6.8847439 | -1.6966528 | 1.2399256 |
| P | 1.5619606 | 0.1394183 | -0.5815081 |
| P | -0.3184151 | 0.3618057 | 0.6200138 |
| W | -1.1394928 | 2.8512971 | 0.7356273 |
| C | -2.3127953 | 2.4831556 | -0.9368239 |
| C | 0.2599827 | 3.6856552 | -0.4993673 |
| C | 0.0762786 | 3.4556148 | 2.2834259 |
| C | -2.0540694 | 4.6493289 | 0.8812063 |
| C | -2.5350472 | 2.0793988 | 2.0811367 |
| O | -2.5802445 | 5.6660412 | 0.9749370 |
| O | -3.2824753 | 1.6814902 | 2.8467978 |
| O | 0.7374369 | 3.9008497 | 3.1088705 |
| O | 1.0424813 | 4.1969065 | -1.1699659 |
| O | -2.9416385 | 2.3616716 | -1.8832540 |
| W | -1.8322039 | -1.4884881 | -0.5263036 |
| C | -0.3035568 | -2.7891627 | -0.9725307 |
| C | -1.7121712 | -0.6382429 | -2.4102506 |
| C | -3.1161601 | -2.8550434 | -1.2768159 |
| C | -2.0197043 | -2.3812680 | 1.3360131 |
| C | -3.5007251 | -0.3347182 | -0.0848186 |
| O | -3.8427916 | -3.6346005 | -1.7064453 |
| O | 0.5050036 | -3.5655305 | -1.2233796 |
| O | -1.6968772 | -0.2170303 | -3.4739575 |
| O | -2.1440751 | -2.8963970 | 2.3487142 |
| O | -4.4605491 | 0.2404468 | 0.1469651 |
| C | 0.4085627 | -0.3549349 | 2.1621161 |
| C | 0.9706592 | -1.6401822 | 2.1450652 |
| C | 0.2823418 | 0.3120047 | 3.3712175 |
| C | 1.3893551 | -2.2580964 | 3.3112505 |
| H | 1.0533374 | -2.1627282 | 1.2061291 |
| C | 0.6893619 | -0.2791979 | 4.5759713 |
| H | -0.1564684 | 1.2959259 | 3.3865199 |
| C | 1.2410821 | -1.5519342 | 4.5157992 |
| H | 1.5579626 | -2.0306829 | 5.4297795 |
| C | 1.5481532 | 0.1733813 | -2.3742757 |
| C | 1.1865170 | 1.3257587 | -3.0605871 |
| C | 1.7912426 | -1.0285823 | -3.0525309 |
| C | 1.0333106 | 1.3003036 | -4.4479052 |
| H | 1.0186797 | 2.2401038 | -2.5182633 |
| C | 1.6478504 | -1.0831285 | -4.4320879 |
| H | 2.0693174 | -1.9049398 | -2.4882310 |
| C | 1.2638392 | 0.0913293 | -5.0970970 |
| H | 1.1302394 | 0.0447612 | -6.1669907 |
| C | 0.6037733 | 2.5807003 | -5.1742621 |
| C | 1.6772505 | 3.6674487 | -4.9581683 |
| H | 1.3823737 | 4.5900039 | -5.4637377 |
| H | 1.8147722 | 3.8972788 | -3.9011040 |
| H | 2.6407798 | 3.3496055 | -5.3622383 |
| C | -0.7416255 | 3.0631374 | -4.5916954 |
| H | -1.0800324 | 3.9561865 | -5.1214849 |
| H | -1.5089282 | 2.2935599 | -4.6852009 |
| H | -0.6570522 | 3.3212745 | -3.5362766 |
| C | 0.4259941 | 2.3613598 | -6.6829885 |
| H | 1.3560063 | 2.0451119 | -7.1606138 |
| H | -0.3440083 | 1.6167660 | -6.8958296 |
| H | 0.1176251 | 3.2971298 | -7.1523448 |
| C | 1.8386883 | -2.3805839 | -5.2277705 |
| C | 2.3726313 | -3.5254243 | -4.3542251 |
| H | 3.3380109 | -3.2755456 | -3.9081457 |
| H | 1.6815822 | -3.7867647 | -3.5521564 |
| H | 2.5131513 | -4.4164633 | -4.9687255 |
| C | 0.4709095 | -2.8032883 | -5.8047091 |
| H | 0.0599190 | -2.0400241 | -6.4672995 |
| H | 0.5727713 | -3.7278884 | -6.3774934 |
| H | -0.2513022 | -2.9749825 | -5.0043448 |
| C | 2.8371097 | -2.1482908 | -6.3794953 |
| H | 2.4902627 | -1.3870808 | -7.0794214 |
| H | 3.8088928 | -1.8334087 | -5.9937168 |
| H | 2.9779832 | -3.0732461 | -6.9430704 |
| C | 1.9633391 | -3.6813003 | 3.3273382 |

| | | | |
|---|------------|------------|-----------|
| C | 0.5208001 | 0.4947266 | 5.8905656 |
| C | 3.4178917 | -3.6375387 | 3.8373514 |
| H | 3.8304455 | -4.6478832 | 3.8931938 |
| H | 4.0396064 | -3.0572865 | 3.1534255 |
| H | 3.4857508 | -3.1910040 | 4.8307528 |
| C | 1.9601886 | -4.3270529 | 1.9335251 |
| H | 2.3731560 | -5.3353828 | 2.0004881 |
| H | 0.9486426 | -4.4133937 | 1.5324426 |
| H | 2.5687807 | -3.7672806 | 1.2231878 |
| C | 1.1101153 | -4.5602029 | 4.2655311 |
| H | 1.1291665 | -4.2004350 | 5.2951372 |
| H | 0.0699012 | -4.5788713 | 3.9350560 |
| H | 1.4887424 | -5.5848675 | 4.2651000 |
| C | -0.9380912 | 0.9771171 | 6.0274365 |
| H | -1.0692395 | 1.5097774 | 6.9719545 |
| H | -1.2238806 | 1.6579651 | 5.2257364 |
| H | -1.6305258 | 0.1330215 | 6.0115261 |
| C | 0.8547188 | -0.3638679 | 7.1195397 |
| H | 0.2190388 | -1.2498043 | 7.1774310 |
| H | 1.8978220 | -0.6870801 | 7.1202695 |
| H | 0.6947594 | 0.2209298 | 8.0272697 |
| C | 1.4662209 | 1.7137971 | 5.8759144 |
| H | 1.2528842 | 2.3793705 | 5.0405597 |
| H | 1.3583453 | 2.2869913 | 6.7999375 |
| H | 2.5073541 | 1.3932345 | 5.7935313 |

10'

E(THF): -3687.43281062658 Ha

NImag = 0

| | | | |
|---|-------------|-------------|-------------|
| C | 1.79477900 | -1.60001540 | -1.83777640 |
| C | -1.00069400 | -2.48312850 | 0.00682130 |
| O | -2.19400750 | -2.51000540 | 0.15284320 |
| O | 1.43088770 | -2.42707790 | -2.62573890 |
| O | 2.90253340 | -0.86923390 | -1.87709590 |
| O | -0.10979910 | -3.37236840 | 0.41869580 |
| C | 3.71496390 | -0.97229660 | -3.07960560 |
| H | 4.67677510 | -0.56680140 | -2.77405870 |
| H | 3.82475620 | -2.02624570 | -3.33460410 |
| C | -0.60310510 | -4.53251720 | 1.13703520 |
| H | -1.51679410 | -4.88136310 | 0.65547960 |
| P | 0.10731270 | 0.11555430 | -0.49791920 |
| C | -0.08592230 | 0.99834340 | -2.04102010 |
| C | 0.47522270 | 2.26977000 | -2.22931560 |
| C | -0.72782670 | 0.33404870 | -3.08463150 |
| C | 0.42595390 | 2.86730920 | -3.48129420 |
| H | 0.96020460 | 2.76488500 | -1.40465300 |
| C | -0.82608460 | 0.92991750 | -4.34201300 |
| H | -1.13663540 | -0.64966390 | -2.91247370 |
| C | -0.24039120 | 2.18042470 | -4.50765700 |
| H | -0.29095460 | 2.65130420 | -5.47727660 |
| C | -1.53394070 | 0.17358450 | -5.47312220 |
| C | -1.62276850 | 1.00301730 | -6.76189330 |
| H | -2.14535370 | 0.42884430 | -7.52873560 |
| H | -2.17713350 | 1.93164270 | -6.60900370 |
| H | -0.63514230 | 1.25141770 | -7.15600320 |
| C | -2.96675260 | -0.18717690 | -5.03012250 |
| H | -2.97396550 | -0.83205830 | -4.15099460 |
| H | -3.53863950 | 0.71169100 | -4.79075950 |
| H | -3.48381170 | -0.71695420 | -5.83307820 |
| C | -0.74589630 | -1.11836800 | -5.77501550 |
| H | 0.26219040 | -0.88449650 | -6.12472040 |
| H | -0.65260940 | -1.75663330 | -4.89530700 |
| H | -1.24997990 | -1.69185600 | -6.55618840 |
| C | 1.08722840 | 4.21720700 | -3.79535780 |
| C | 1.82880220 | 4.80832520 | -2.58885750 |
| H | 1.16253180 | 5.00531660 | -1.75217860 |
| H | 2.63343960 | 4.15451500 | -2.25294050 |
| H | 2.28044650 | 5.75999900 | -2.87412960 |
| C | 2.11603110 | 4.01544610 | -4.92908120 |
| H | 1.65439550 | 3.64305860 | -5.84446250 |
| H | 2.59922730 | 4.96609870 | -5.16497250 |
| H | 2.89088740 | 3.30787570 | -4.62771520 |
| C | 0.00698920 | 5.22068550 | -4.24979540 |
| H | 0.46859930 | 6.18219150 | -4.48532360 |
| H | -0.51677120 | 4.87742410 | -5.14381450 |
| H | -0.72971000 | 5.37894560 | -3.46223360 |
| P | 0.16308320 | 1.18994700 | 1.39638960 |
| C | -0.20794620 | -0.28642270 | 2.45788860 |
| C | -1.52899170 | -0.73152710 | 2.53755910 |

| | | | |
|---|-------------|-------------|-------------|
| C | 0.76143750 | -0.87566160 | 3.26545110 |
| C | -1.90720020 | -1.72925630 | 3.42868880 |
| H | -2.27198690 | -0.28176400 | 1.90185770 |
| C | 0.42872600 | -1.89072660 | 4.16196960 |
| H | 1.77586230 | -0.52638790 | 3.20795910 |
| C | -0.90664890 | -2.29203530 | 4.22401870 |
| H | -1.18233760 | -3.06495590 | 4.92912430 |
| C | -3.36879430 | -2.17365260 | 3.58918560 |
| C | 1.46961220 | -2.54689890 | 5.07956280 |
| C | 1.53432800 | -4.05724970 | 4.77503390 |
| H | 2.26061440 | -4.54528430 | 5.42908600 |
| H | 0.56955880 | -4.54420330 | 4.92707300 |
| H | 1.84006280 | -4.22890540 | 3.74132990 |
| C | 1.05830410 | -2.33427420 | 6.55083160 |
| H | 0.08786370 | -2.78102050 | 6.77128560 |
| H | 1.79402510 | -2.78993760 | 7.21763310 |
| H | 0.99856720 | -1.26975590 | 6.78496950 |
| C | 2.87425590 | -1.95747870 | 4.88293480 |
| H | 3.23704160 | -2.10124710 | 3.86389360 |
| H | 2.90068620 | -0.89014320 | 5.11182620 |
| H | 3.57555120 | -2.45407590 | 5.55602350 |
| C | -3.50000490 | -3.67807170 | 3.27951860 |
| H | -2.84326990 | -4.28300930 | 3.90775500 |
| H | -4.52586150 | -4.00690460 | 3.46103490 |
| H | -3.25996880 | -3.87330460 | 2.23435760 |
| C | -3.80767070 | -1.90437330 | 5.04407700 |
| H | -4.85390480 | -2.18931170 | 5.17816070 |
| H | -3.21417410 | -2.47497760 | 5.76046350 |
| H | -3.70730760 | -0.84545450 | 5.28768460 |
| C | -4.31613570 | -1.41098500 | 2.64958930 |
| H | -4.31787260 | -0.34054140 | 2.86187130 |
| H | -4.05332760 | -1.56343290 | 1.60268500 |
| H | -5.33610050 | -1.77222310 | 2.79453960 |
| W | -1.81620990 | 2.93741260 | 1.54897690 |
| W | 2.72127500 | 1.91862790 | 1.37822290 |
| C | -2.99517120 | 1.74422400 | 0.33998550 |
| C | -1.30350230 | 4.07098550 | -0.08831120 |
| C | -3.31416620 | 4.26748810 | 1.79053300 |
| C | -2.53152400 | 2.05655460 | 3.28380660 |
| C | -0.58826500 | 4.07777590 | 2.76576650 |
| C | 2.12079090 | 3.87141950 | 1.06894640 |
| C | 3.29968590 | 1.89087310 | -0.59317740 |
| C | 3.40145770 | -0.03799190 | 1.45975570 |
| C | 4.59434940 | 2.56712720 | 1.75166340 |
| C | 2.41483810 | 2.06672360 | 3.43409810 |
| O | -4.17000670 | 5.02215280 | 1.92329250 |
| O | -3.62898220 | 1.07480220 | -0.33999150 |
| O | -1.12557580 | 4.78545160 | -0.96718900 |
| O | -2.97479650 | 1.65611780 | 4.25925530 |
| O | 0.07050170 | 4.70331850 | 3.45984320 |
| O | 5.65742610 | 2.93240140 | 1.98633730 |
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| N | 1.09203090 | -1.26782090 | -0.64535420 |
| N | -0.37623530 | -1.48491680 | -0.76573290 |
| C | 3.10062180 | -0.17459600 | -4.21206490 |
| H | 3.76066750 | -0.20594280 | -5.08126100 |
| H | 2.13525030 | -0.59072960 | -4.49797950 |
| H | 2.96485180 | 0.86464590 | -3.91508920 |
| C | 0.49500360 | -5.56882620 | 1.11165340 |
| H | 0.18152130 | -6.44750200 | 1.67849700 |
| H | 0.71718480 | -5.87473540 | 0.08875170 |
| H | 1.40706130 | -5.17577110 | 1.56134200 |
| H | -0.84338630 | -4.21302240 | 2.15021440 |

10'

E(THF): -3687.4525675787 Ha

NImag = 0

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| C | 0.0805746 | 1.2928401 | -2.0822676 |
| C | 0.7205215 | 2.5316331 | -2.2376836 |
| C | -0.8455722 | 0.8473774 | -3.0195940 |
| C | 0.4719891 | 3.3028633 | -3.3660745 |
| H | 1.4107077 | 2.8736320 | -1.4850277 |
| C | -1.1728597 | 1.6363476 | -4.1215044 |
| H | -1.3471388 | -0.0951108 | -2.8774608 |

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| C | -2.2724681 | 1.1596075 | -5.0788737 |
| C | -2.4836731 | 2.1278021 | -6.2511032 |
| H | -3.2738529 | 1.7474407 | -6.9008230 |
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| H | -1.5812184 | 2.2361682 | -6.8569787 |
| C | -3.5953957 | 1.0480969 | -4.2909934 |
| H | -3.5191403 | 0.3480297 | -3.4579613 |
| H | -3.8826288 | 2.0147072 | -3.8743246 |
| H | -4.3958883 | 0.7053526 | -4.9507927 |
| C | -1.8961313 | -0.2210219 | -5.6541297 |
| H | -0.9551792 | -0.1716649 | -6.2062082 |
| H | -1.7878027 | -0.9730391 | -4.8708690 |
| H | -2.6751670 | -0.5672531 | -6.3369531 |
| C | 1.2218690 | 4.6074216 | -3.6722487 |
| C | 2.2479119 | 4.9661447 | -2.5872989 |
| H | 1.7814502 | 5.1182610 | -1.6156542 |
| H | 3.0170674 | 4.1992617 | -2.4945198 |
| H | 2.7464325 | 5.8986660 | -2.8575096 |
| C | 1.9830671 | 4.4287425 | -5.0044136 |
| H | 1.3084362 | 4.2235097 | -5.8369757 |
| H | 2.5363294 | 5.3402067 | -5.2413599 |
| H | 2.6974647 | 3.6056050 | -4.9358820 |
| C | 0.2172006 | 5.7697725 | -3.8091503 |
| H | 0.7515536 | 6.6947123 | -4.0370507 |
| H | -0.4982476 | 5.5959846 | -4.6142735 |
| H | -0.3380453 | 5.9167919 | -2.8837292 |
| P | 0.4631330 | 1.2889643 | 1.3064745 |
| C | 0.1508008 | -0.2841838 | 2.2586572 |
| C | -1.1466630 | -0.8053246 | 2.3071011 |
| C | 1.1666005 | -0.9248321 | 2.9657943 |
| C | -1.4334030 | -1.9667633 | 3.0184748 |
| H | -1.9313757 | -0.2907179 | 1.7790046 |
| C | 0.9165933 | -2.0796775 | 3.7083436 |
| H | 2.1557380 | -0.5063686 | 2.9527132 |
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| H | -0.5888869 | -3.4888461 | 4.2561298 |
| C | -2.8467495 | -2.5616686 | 3.1095172 |
| C | 2.0136787 | -2.7949522 | 4.5112355 |
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| H | 2.7167337 | -3.9722653 | 2.8153265 |
| C | 1.5261104 | -3.0584065 | 5.9505770 |
| H | 0.6521235 | -3.7094577 | 5.9793175 |
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| C | 3.3068824 | -1.9700501 | 4.5959762 |
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| H | 3.1297002 | -0.9896816 | 5.0433753 |
| H | 4.0332338 | -2.4933939 | 5.2207271 |
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| H | -3.2935124 | -1.5847033 | 5.0081218 |
| C | -3.8859161 | -1.7459185 | 2.3257530 |
| H | -3.9707939 | -0.7302658 | 2.7124635 |
| H | -3.6558938 | -1.6925661 | 1.2625436 |
| H | -4.8652364 | -2.2179550 | 2.4283325 |
| W | -1.4817380 | 3.0657041 | 1.5792891 |
| W | 3.0276260 | 2.1192648 | 1.4784888 |
| C | -2.4764653 | 1.9308517 | 2.9976588 |
| C | -2.6859385 | 2.4317876 | 0.0034719 |
| C | -2.8622587 | 4.4796729 | 1.9603881 |
| C | -0.3224848 | 3.8629572 | 3.0908548 |
| C | -0.6950789 | 4.4086722 | 0.2395381 |
| C | 2.4199823 | 4.0967103 | 1.3186824 |
| C | 3.5785844 | 2.0863819 | -0.5016638 |
| C | 3.8705836 | 0.2440059 | 1.4992073 |
| C | 4.8543027 | 2.8477514 | 1.9045740 |
| C | 2.6559494 | 2.0646712 | 3.5263323 |
| O | -3.6491999 | 5.2896093 | 2.1784008 |
| O | -3.0718543 | 1.3955984 | 3.8165056 |
| O | -3.3783990 | 2.2299869 | -0.8822876 |
| O | 0.2948682 | 4.3437942 | 3.9263436 |

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| O | -0.3684555 | 5.2329924 | -0.4876977 |
| O | 5.8959741 | 3.2599047 | 2.1620857 |
| O | 2.5069182 | 2.0073986 | 4.6573729 |
| O | 4.4289807 | -0.7585947 | 1.4612628 |
| O | 3.9704239 | 2.0348123 | -1.5786339 |
| O | 2.1932412 | 5.2122299 | 1.2170141 |
| C | 1.7993570 | -1.7924469 | -0.7828499 |
| P | 0.4281857 | 0.2820145 | -0.6520428 |
| N | -0.3021600 | -1.2794741 | -0.8151610 |
| N | 0.6381366 | -2.3252999 | -0.7387395 |
| O | 1.9049559 | -0.4431550 | -0.8806494 |
| O | 2.9537249 | -2.3975630 | -0.7175557 |
| C | 2.9389256 | -3.8178252 | -0.3956675 |
| H | 2.2662334 | -3.9631542 | 0.4511411 |
| H | 2.5370440 | -4.3573051 | -1.2560094 |
| C | 4.3595584 | -4.2106140 | -0.0735493 |
| H | 4.7324958 | -3.6316499 | 0.7713163 |
| H | 4.3925455 | -5.2705515 | 0.1847682 |
| H | 5.0143898 | -4.0409551 | -0.9286439 |
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| O | -2.3572805 | -0.4529081 | -0.5847344 |
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| C | -1.6401287 | -3.8597787 | -1.3184091 |
| H | -1.0784448 | -3.6030191 | -2.2163037 |
| H | -0.9531302 | -4.2879456 | -0.5920714 |
| C | -2.7990954 | -4.7812463 | -1.6212168 |
| H | -2.4203660 | -5.7196924 | -2.0311161 |
| H | -3.3617954 | -5.0022481 | -0.7135970 |
| H | -3.4765904 | -4.3306872 | -2.3473143 |

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