# Electronic Supplementary Information (ESI)

## Reactivity of terminal phosphinidene versus Li/Cl phosphinidenoid complexes in cycloaddition chemistry. A case study

**Rainer Streubel,*[a] José Manuel Villalba Franco,[a] Gregor Schnakenburg,[a] and Arturo Espinosa Ferao[b]**

[a] *Institut für Anorganische Chemie der Reinischen Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str.1, 53121 Bonn, Germany. Fax: +49 228 739616; Tel: +49 228 735345; E-mail: r.streubel@uni-bonn.de.*
[b] *Departamento de Química Orgánica, Universidad de Murcia,Campus de Espinardo, 30100 – Murcia, Spain.*

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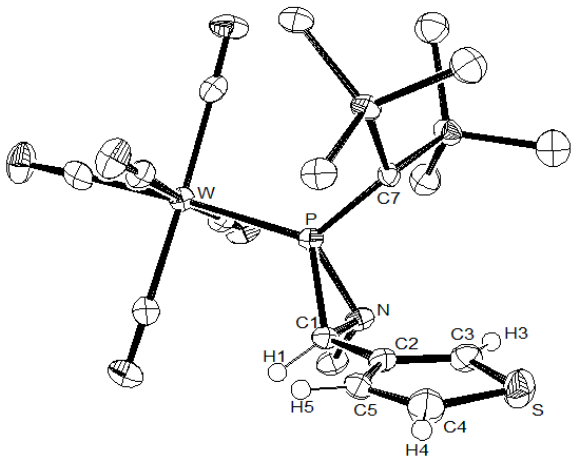
## Experimental data




Molecular structure of azaphosphiridine tungsten complex **4** in the crystal (50% probability level, hydrogen atoms except at C(1), C(3), C(4), C(5), are omitted for clarity). Selected bond lengths [Å] and angles [°]: W–P 2.4973(13), P–C1 1.833(5), P–N 1.734(4), P–C(7) 1.804(5), C(1)–N 1.483(6), C(1)–C(2) 1.481(7), P–C(1)–N 62.0(2), C(1)–P-N 49.0(2), C(1)-N-P 68.9(2).

§ X-ray crystallographic analysis of azaphosphiridine complex **4**: colorless single crystals were obtained from concentrated *n*-pentane solutions at 4 °C, $C_{18}H_{26}NO_5PSSi_2W$; crystal size 0.40 × 0.32 × 0.08 mm, triclinic, P-1, $a$ = 9.2854(4) Å, $b$ = 9.7913(5) Å, $c$ = 15.3748(7) Å; $\alpha$ = 72.585(2)°, $\beta$ = 74.551(3)°, $\gamma$ = 77.633(3)°; $V$ = 1271.75(10) Å$^3$, $Z$ = 2, $d_{calc}$ = 1.670 mg/m$^3$, $\mu$ = 4.807 mm$^{-1}$, collected reflections (unique) 16486 / 5984 [R(int) = 0.0913], 290 refined parameters, 52 restraints, $R_1$ (for $I > 2\sigma(I)$) = 0.0401, w$R_2$ (for all data) = 0.0832 max./min. largest diff. peak and hole 1.704 and -2.811e Å$^{-3}$

§ X-ray crystallographic analysis of azaphospholene complex **5**: colorless single crystals were obtained from concentrated *n*-pentane solutions at 4 °C, $C_{18}H_{26}NO_5PSSi_2W$; crystal size 0.60 × 0.24 × 0.20 mm, triclinic, P-1, $a$ = 8.7938(3) Å, $b$ = 10.6257(4) Å, $c$ = 14.0699(5); $\alpha$ = 107.3320(10)°, $\beta$ = 94.3980(10)°, $\gamma$ = 96.2240(10)°; $V$ = 1239.35(8) Å$^3$, $Z$ = 2, $d_{calc}$ = 1.714 mg/m$^3$, $\mu$ = 4.933 mm$^{-1}$, collected reflections (unique) 17237 / 5910, $R_{int}$ = 0.0307, 269 refined parameters, 0 restraints, $R_1$ (for $I > 2\sigma(I)$) = 0.0167, w$R_2$ (for all data) = 0.0391, max./min. largest diff. peak and hole 0.743/-1.157 e Å$^{-3}$.

CCDC 857934 (**4**) and 857935 (**5**) contain the supplementary crystallographic data

for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via “www.ccdc.cam.ac.uk/data_request/cif."

**Preparative methods**

All reactions and manipulations were carried out under an atmosphere of dry argon, using Schlenk and vacuum line techniques. Argon was cleaned over a BTS catalyst; the drying of the Ar gas occurred via silica gel and $P_2O_5$. Solvents were dried according to standard procedures and stored in brown glasses over sodium wire, and under inert gas atmosphere.

**Analytical methods**

*Melting point measurements* were determined with a Büchi (530) capillary apparatus.
*Elemental analyses were* performed using an Elementar VarioEL analytical gas chromatograph.
*Mass spectrometry:* Electron ionization (70eV) mass spectra were recorded on a Kratos MS 50 or on a MAT 95XL Finnigan spectrometer.
*NMR spectra* were recorded on a Bruker AX 300 spectrometer ($^{1}$H: 300.1 MHz, $^{13}$C: 75.0 MHz and $^{31}$P: 121.5 MHz,) using $CDCl_3$ as solvent; shifts are given relative to external tetramethylsilane ($^{1}$H, $^{13}$C,) and 85% $H_3PO_4$ ($^{31}$P).
*UV/vis spectra* were recorded on a Shimadzu UV-1650 PC spectrometer using dichloromethane as solvent and quartz glass cells.
*IR spectra* were recorded with a Thermo Nicolet 380 spectrometer; solid as KBr pellets and liquids as film in a KBr cell.
*Single-crystal structure analysis:* Crystal structures were recorded on a Nonius Kappa CCD diffractometer and a Nonius MACH3 diffractometer. The structures were solved by Patterson methods or Direct Methods (SHELXS-97) and refined by full-matrix least squares on F2 (SHELXL-97). All non-hydrogens were refined anisotropically. Hydrogen atoms were included isotropically using the riding model on the bound atoms; in some (denoted) cases hydrogen atoms were located in the Fourier difference electron density. Absorption corrections were carried out analytically or semi-empirically from equivalents. Additionally, some calculation of bond lengths and angles were obtained using the Ortep32 program.

Synthesis of complex **4**: A solution of 2 g (3.2 mmol) of 2*H*-azaphosphirene complex **1** and 0.5 mL (5.0 mmol) of *N*-[(thiophen-3-yl)methylene]methanamine **3** in 32.0 mL of toluene was stirred for 3h at 75 °C whereby the brown solution turned dark red. After removing all volatile components *in vacuo* ($10^{-2}$ mbar) the product was subsequently purified by column chromatography thus obtaining a white powder ($Al_2O_3$, h = 5 cm, ø = 3 cm, T = -30°C; eluent: petrolether 40/60).

Yield: 420 mg (21%); Found C 33.79 H 4.13, N 2.22, S 5.13, Calc(%): C 33.81, H 4.10, N 2.19, S 5.01, m.p. = 91-92 °C; $^{1}$H-NMR (300.1 MHz, 30 °C, $CDCl_3$): δ = 0.07 (s, 3H, Si(C*H*$_3$)$_3$), 0.41 (s, 3H, Si(C*H*$_3$)$_3$), 1.04 (d, $^{2}J_{P,H}$ = 17.5 Hz, 1H, C*H*(Si(Me$_3$)$_2$), 2.76 (d, $^{3}J_{P,H}$ = 15.77 Hz, 3H, NC*H*$_3$), 3.22 (d, $^{2}J_{P,H}$ = 6.6 Hz, 1H, P-*H*-N), 7.24 (d, $^{3}J_{H4,H3}$ = 4.9 Hz, 1H, *H4*), 7.36 (s, 1H, *H5*),7.44 (dd, $^{3}J_{H3,H4}$ = 4.9 Hz, $^{4}J_{P,H3}$ = 3.1 Hz, 1H, *H3*). $^{13}$C{$^{1}$H}-NMR (75.5 MHz, 30 °C, $CDCl_3$): δ = 0.02 (d, $^{3}J_{P,C}$ = 3.9 Hz, Si(*C*H$_3$)$_3$ ), 0.79 (d, $^{3}J_{P,C}$ = 3.5 Hz, Si(*C*H$_3$)$_3$), 17.4 (d, $^{1}J_{P,C}$ = 26.8 Hz, *C*H(SiMe$_3$)$_2$), 40.9 (d, 1$J_{P,C}$ = 2.3 Hz, P-*C*-N), 51.7 (d, $^{2}J_{P,C}$ = 2.26, N-*C*H$_3$), 120.1 (d, $^{2}J_{P,C}$ = 3.5 Hz, *C*3), 125.1 (s, *C*5), 126.7 (s, *C*4), 137.2 (d, $^{2}J_{P,C}$ = 4.5 Hz, *C*2), 196.7 (dSat, $^{2}J_{P,C}$ = 8.1 Hz, $^{1}J_{W,C}$ = 101.1 Hz, *cis*-*C*O), 199.9 (d, $^{2}J_{P,C}$ = 28.4 Hz, *trans*-*C*O). $^{31}$P-NMR (121.5 MHz, 30 °C, $CDCl_3$ ): δ = 37.70 (tdSat, $^{1}J_{W,P}$ = 270.1 Hz, $^{3}J_{P,H}$ = 15.77 Hz, $^{2}J_{P,H7}$ = 17.4 Hz, $^{2}J_{P,H1}$ = 6.6 Hz). MS (EI, $^{184}$W): m/z (%):639.0 ([M]+,19), 555.0 ([M-3CO]+, 10), 486.0 ([M-COArCHNMe]+, 100), 402.0 (M-4CO-ArCHNMe]+, 28), 358.0 ([M-5CO-$C_6H_7NSCH_3H$]+, 45), 73.1 ([SiMe$_3$]+, 79). IR (KBr): $\tilde{\nu}$ = (b, ν-CH), 2072 (s, ν-CO), 1947 (s, ν-CO), 1462 (s, ν-CO/Ar) cm$^{-1}$. UV/Vis ($CH_2Cl_2$): $\lambda_{max}$(abs.) = 234.6 (1.55), 215.5 (0.30). § X-ray crystallographic analysis (colorless single crystals were obtained from concentrated *n*-pentane solutions at 4 °C): $C_{18}H_{26}NO_5PSSi_2W$; crystal size 0.40 × 0.32 × 0.08 mm, monoclinic, P-1, *a* = 9.2854(4) Å, *b* = 9.7913(5) Å, *c* = 15.3748(7) Å; *β* = 74.551(3)°, *V* = 1271.75(10) Å$^3$, *Z* = 2, $d_{calc}$ = 1.670 mg/m$^3$, $\mu$ = 4.807 mm$^{-1}$, collected reflections (unique) 16486 / 5984 [R(int) = 0.0913], 290 refined parameters, 52 restraints, $R_1$ (for $I > 2\sigma(I)$) = 0.0401, w$R_2$ (for all data) = 0.0779 max./min. largest diff. peak and hole 1.704 and -2.811e Å$^{-3}$.

Synthesis of complex **5a**: To a solution of 380 mg (0.65 mmol) of dichlorophosphane complex **1** and 0.1 mL (0.65 mmol) of 12-crown-4 in 30 mL of THF 0.49 mL (0.78 mmol) of *tert*-butyl lithium (1.5 M in *n*-hexane) were slowly

added at -78 °C. After 15 min. 0.13 mL (1.3 mmol) of N-[(thienyl-3-yl)methylene]methanamine were slowly added. The color of the solution changed to orange. After warming to room temperature all volatile components were removed in *vacuo* (~$10^{-2}$ mbar). Complex **6** was purified by crystallization from *n*-pentane at -50 ºC and obtained as pale yellow solid.

Yield: 226 mg (55%); Found: C 33.91 H 4.14, N 2.19, S 4.90, Calc(%): C 33.81, H 4.10, N 2.19, S 5.01, m.p. = 129-130 °C; $^{1}$H-NMR (300.1 MHz, 30 °C, $CDCl_3$): δ = 0.21 (s, 3H, Si(C$H_3$)$_3$), 0.29 (s, 3H, Si(C$H_3$)$_3$), 1.61 (d, $^{2}J$P,H = 9.7 Hz, 1H, C$H$(Si(Me$_3$)$_2$), 2.64 (d, $^{3}J_{P,H}$ = 14.07 Hz, 3H, NC$H_3$), 5.29 (ft, $^{3}J_{P,H}$ = 3.6 Hz, 4$_{JH1,H5}$ = 3.6 Hz 1H, P-*H*-S), 5.84 (dd, $^{4}J_{H5,H3}$ = 3,47 Hz, $^{3}J_{P,H5}$ = 11.8 1H, H5), 6.06 (d, $^{3}J_{H3,H2}$ = 5.82 Hz 1H, H3), 6.21 (dd, 3$J_{H2,H3}$ = 5.82 Hz, $^{4}J_{P,H2}$ = 3.45 Hz, 1H, H2).$^{13}$C{$^{1}$H}-NMR (75.5 MHz, 30 °C, $CDCl_3$): δ = 2.89 (d, $^{3}J_{P,C}$ = 1.1 Hz, Si(*C*$H_3$)$_3$ ), 3.15 (d, $^{3}J_{P,C}$ = 4.2 Hz, Si(*C*$H_3$)$_3$), 27.2 (d, $^{1}J_{P,C}$ = 3.1 Hz, *C*H(SiMe$_3$)$_2$), 42.4 (d, $^{1}J_{P,C}$ = 3.6 Hz, N-*C*$H_3$), 62.7 (d, $^{1}J_{P,C}$ = 25.9 Hz, S-*C*-P), 117.1 (d, $^{2}J_{P,C}$ = 6.1 Hz, C3), 126.8 (s, C4), 127.1 (d, $^{3}J_{P,C}$ = 3.2 Hz, C2), 132.0 (d, $^{2}J_{P,C}$ = 7.4 Hz, C5), 198.0 (d$_{Sat}$, $^{2}J_{P,C}$ = 6.9 Hz, $^{1}J_{W,C}$ = 126.2 Hz, *cis*-CO), 198.7 (d, $^{2}J_{P,C}$ = 26.1 Hz, *trans*-CO). $^{31}$P-NMR (121.5 MHz, 30 °C, $CDCl_3$ ): δ = 166.1 (d$_{sat}$, $^{1}J_{W,P}$ = 256.4 Hz, $^{2}J_{P,H}$ = 9.7 Hz). MS (EI, $^{184}$W): m/z (%): 639.1 (14) ([M]+), 555.1 (5) ([M-3CO]+), 499.1 (20) ([M-5CO]+), 486.0 (44) ([M-CO-ArCHNMe]+), 358.0 (45) ([M-5CO-$C_6H_7$NS-$CH_3$]+), 73.1 (100) ([SiMe$_3$]+). IR (KBr): $\tilde{\nu}$ = 2924 (b, νCH), 2853 (s, νCH), 2067 (s, νCO), 1987 (s, νCO), 1937 (s, shoulder, νCO), 1461 (s, νC-C/Ar) cm$^{-1}$. UV/Vis ($CH_2Cl_2$): $\lambda_{max}$/nm 235 (ε/dm$^3$ mol$^{-1}$ cm$^{-1}$ 61410), § X-ray crystallographic analysis (colorless single crystals were obtained from concentrated *n*-pentane solutions at 4 °C): $C_{18}H_{26}NO_5PSSi_2W$; crystal size 0.60 × 0.24 × 0.20 mm, triclinic, P-1, $a$ = 8.7938(3) Å, $b$ = 10.6257(4) Å, $c$ = 14.0699(5); $\beta$ = 94.3980(10)°, $V$ = 1239.35(8) Å$^3$, $Z$ = 2, $d_{calc}$ = 1.714 mg/m$^3$, $\mu$ = 4.933 mm$^{-1}$, collected reflections (unique) 17237 / 5910, $R_{int}$ = 0.0307, 269 refined parameters, 0 restraints, $R_1$ (for $I > 2\sigma(I)$) = 0.0167, w$R_2$ (for all data) = 0.0386, max./min. largest diff. peak and hole 0.743/-1.157 e Å$^{-3}$.

## Computational details

Quantum chemical calculations were performed with the ORCA electronic structure program package.[1] Unless otherwise stated all geometry optimizations were run in redundant internal coordinates with tight convergence criteria,[2] in the gas-phase and using the BP86[3] functional together with the def2-TZVP basis set.[4] In the case of intermediates **8a** and **9a** Grimme's semiempirical dispersion forces correction[5] (denoted as –D after the functional's name) was also included (*i.e.* BP86-D functional) and accounting for solvent effects (THF) via the COSMO solvation model.[6] Additionally, for checking purposes a second refinement for compound **8b** was also performed with the B3LYP functional[7] and dispersion correction (*i.e.* B3LYP-D functional) and COSMO salvation. For W atoms the [SD(60,MWB)] effective core potential[8] (ECP) was used. Harmonic frequency calculations verified the nature of ground states or transition states (TS) having all positive frequencies or only one imaginary frequency, respectively. For the later, the correct nature of the TS was checked by intrinsic reaction coordinate (IRC) calculations. The electron density at bond critical points, $\rho(r_c)$, derived from the topological analysis within the context of Bader's atoms-in-molecules (AIM) methodology,[9] was computed using the AIM2000 software[10] and wavefunctions

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[1] ORCA — an *ab initio*, density functional and semiempirical program package. Written by F. Neese. Version 2.8.0, Universität Bonn, 2010. Web page: http://www.thch.uni-bonn.de/tc/orca/.

[2] Energy change $1.0\cdot10^{-6}$ hartree; maximum gradient $1.0\cdot10^{-4}$ hartree/$a_0$; RMS gradient $3.0\cdot10^{-5}$ hartree/$a_0$; maximum displacement $1.0\cdot10^{-3}$ $a_0$; RMS displacement $6.0\cdot10^{-4}$ $a_0$.

[3] (a) Becke, A. D. *Phys. Rev. A.,* **1988**, *38*, 3098-3100; (b) Perdew, J. P. *Phys. Rev. B.* **1986**, *33*, 8822-8824.

[4] Weigend, F.; Ahlrichs, R. Phys. *Chem. Chem. Phys.*, **2005**, *7*, 3297-3305.

[5] a) Grimme, S. *J. Comput. Chem.*, **2004**, *25*, 1463-1476. b) Grimme, S. *J. Comput. Chem.*, **2006**, *27*, 1787-1799.

[6] Klamt, A.; Schüürmann, G. *J. Chem. Soc. Perkin Trans. 2* **1993**, *220*, 799-805. Klamt, A. *J. Phys. Chem.* **1995**, *99*, 2224-2235.

[7] Becke, A. D. *J. Chem. Phys.,* **1993**, *98*, 5648-5652. Lee, C. T.; Yang, W. T.; Parr, R. G. *Phys. Rev. B,* **1988**, *37*, 785-789.

[8] Andrae, D.; Haeussermann, U.; Dolg, M.; Stoll, H.; Preuss, H. *Theor. Chim. Acta*, **1990**, *77*, 123-141. ECP basis sets for W [SD(60,MWB)] have been obtained from Turbomole basis set library at ftp://ftp.chemie.uni-karlsruhe.de/pub/basen/.

[9] Bader, R. F. W. in *Atoms in Molecules: A Quantum Theory*, Oxford University Press, Oxford, **1990**.

[10] (a) AIM2000 v. 2.0, designed by Biegler-König, F. and Schönbohm, J. 2002. Home page http://www.aim2000.de/. Biegler-König, F.; Schönbohm, J.; Bayles, D. J. *Comp. Chem.* **2001**, *22*, 545-559. (b) Biegler-König, F.; Schönbohm, J. *J. Comp. Chem.* **2002**, *23*, 1489-1494.

(B3LYP/def2-TZVP) generated with the Gaussian 09 software.[11] From these optimized geometries all other reported data were obtained by means of single-point (SP) calculations using the more polarized def2-TZVPP[12] basis set. Reported energies were corrected for the zero-point vibrational term at the optimization level and computed at the RI-SCS-MP2 level of theory.[13] Mulliken charges were obtained using the B3LYP functional. The concept of softness[14] has been found to be intimately related to fundamental variables of DFT. Softness and philicity parameters were computed using Mulliken charges. Quadratic differences in philicity, $\Delta(\omega^2)_{kl}$, were obtained from group philicities.[15] These group quantities were obtained via the Fukui functions[16] adapted for reflecting changes in "group charges", that were in turn computed from the atomic charge of the atom involved in the bond under consideration, after adding the charges of all directly adjacent atoms. Every path was computed as the sum of the contributions of two nucleophilic attacks of the imine N atom to phosphorus and from the later to either the thiazole C2 ([4+1] path) or the imine C atom ([2+1] path).

[11] Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.
[12] Bergner, A.; Dolg, M.; Kuchle, W.; Stoll, H.; Preuss, H. *Mol. Phys.* **1993**, *80*, 1431−1441. Obtained from the EMSL Basis Set Library at https://bse.pnl.gov/bse/portal. D. Feller, *J. Comp. Chem.*, **1996**, *17*, 1571-1586.
[13] Gerenkamp, M; Grimme, S. *Chem. Phys Lett*, **2004**, *392*, 229-235. Grimme, S. *J. Chem. Phys.*, **2003**, *118*, 9095-9102.
[14] Yang, W.; Parr, R. G. *Proc. Natl. Acad. Sci. U.S.A.*, **1985**, *82*, 6723-6726.
[15] R. Parthasarathi, J. Padmanabhan, M. Elango, V. Subramanian and P. K. Chattaraj, *Chem. Phys. Lett.,* 2004, **394**, 225–230.
[16] Parr, R. G.; Yang, W. *J. Am. Chem. Soc.* **1984**, *106*, 4049-4050.

**Table SI 1:** Calculated (B3LYP/def2-TZVPPecp//BP86/def2-TZVPecp) quadratic difference in softness,[a] $\Delta(s^2)_{kl}$, for the reaction of **3** with either **2b** or **7b**.

| | [4+1] path | [2+1] path |
|---|---|---|
| **3** + **2b** | 4.09 | 5.65 |
| **3** + **7b** (without 12-crown-4) | 0.52 | 0.12 |
| **3** + **7b** | 1.81 | 2.83 |

[a] Computed at the "group" level using Mulliken charges.

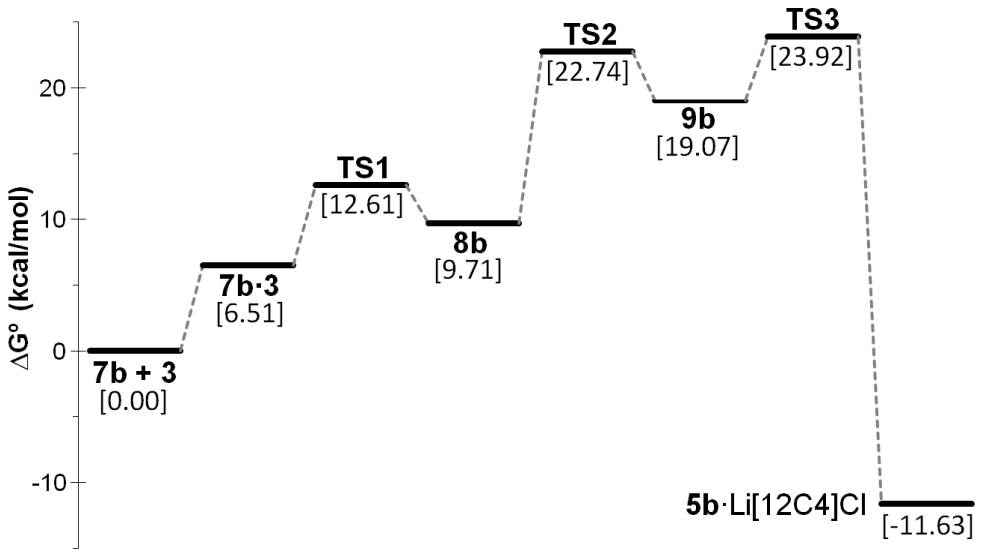



**Figure SI 1:** Calculated COSMO(THF)/RI-SCS-MP2/def2-TZVPP(ecp)] Gibbs free energy profile for the model conversion **7b**+**3**→**5b** (12C4 = 12-crown-4).

## Calculated structures.

Cartesian coordinates (in Å) and energies for all computed species.-

**2b**: E = -1015.82849991 au (BP86/def2-TZVP)

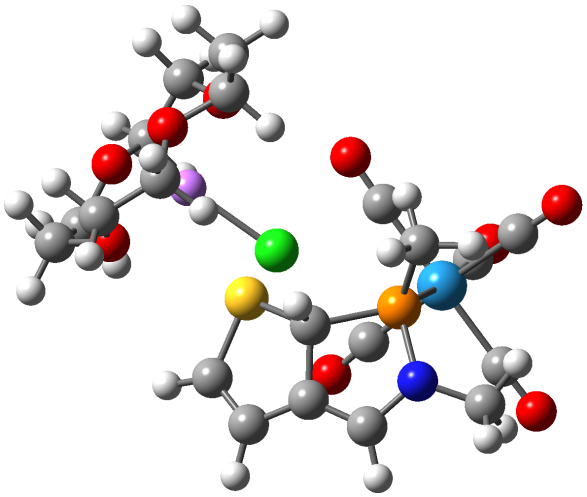
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 | O | 2.29271738 | 2.43547122 | -2.09644170 |
| W | 2.42228887 | 0.00000000 | 0.00000000 | O | 2.22726869 | 1.78476565 | 2.66457831 |
| C | 4.48413289 | 0.28430480 | 0.00000000 | O | 2.69511512 | -2.75009064 | 1.66200186 |
| C | 2.32128570 | 1.59965292 | -1.31196091 | O | 2.35312070 | -1.86285157 | -2.62666600 |
| C | 2.32155304 | 1.15484565 | 1.70966201 | C | -0.76144184 | -0.19734591 | 1.67975873 |
| C | 2.59382878 | -1.74686656 | 1.11637735 | H | -0.14319278 | 0.14601417 | 2.52059170 |
| C | 2.38967499 | -1.19822387 | -1.69314041 | H | -1.75351521 | 0.27875326 | 1.71273441 |
| O | 5.61139664 | 0.48830953 | 0.06175723 | H | -0.92438005 | -1.28611987 | 1.81236676 |

**3**: E = -685.92889927 au (BP86/def2-TZVP)

ZPE= 0.112278 au

E = -684.66429216 au (COSMO$_{THF}$/SCS-MP2/def2-TZVPP)

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 | C | 2.21337468 | -1.19647816 | 0.00000000 |
| C | 1.37645412 | 0.00000000 | 0.00000000 | H | 3.30611374 | -1.02079245 | 0.00000000 |
| C | 1.90792590 | 1.32571265 | 0.00000000 | N | 1.73360365 | -2.37857714 | 0.00000000 |
| C | 0.94474062 | 2.29101024 | 0.00000000 | C | 2.65901091 | -3.49775722 | 0.00000000 |
| S | -0.63445520 | 1.59012866 | 0.00000000 | H | 2.46431840 | -4.12346042 | 0.88538771 |
| H | -0.64280243 | -0.87240140 | -0.00000000 | H | 2.46433639 | -4.12344512 | -0.88540230 |
| H | 2.97297049 | 1.54360514 | -0.00000000 | **H** | **3.72356319** | **-3.18705304** | **0.00000000** |
| H | 1.06903936 | 3.36712785 | 0.00000000 | | | | |



**5b**·[(12-crown-4)LiCl]: E = -2785.01314219 au (BP86/def2-TZVP)

ZPE= 0.434008 au

E = -2779.35166256 au (COSMO$_{THF}$/SCS-MP2/def2-TZVPP)

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 | Cl | 0.10560255 | 0.52147968 | -4.38120339 |
| N | 1.76764448 | 0.00000000 | 0.00000000 | Li | -1.52660308 | 1.66073041 | -5.40312467 |
| C | 2.22902801 | 1.32317495 | 0.00000000 | O | -1.90472722 | 0.98409064 | -7.33125122 |
| H | 3.23189934 | 1.52354494 | 0.37859908 | C | -2.25514313 | -0.36120336 | -6.96303307 |
| C | 1.33800583 | 2.24359726 | -0.45412516 | H | -1.45633303 | -0.79874195 | -6.33603111 |
| C | 0.05493762 | 1.60014306 | -0.95891406 | H | -2.41574477 | -0.99165529 | -7.85754949 |
| C | 1.24504682 | 3.67466303 | -0.40971704 | C | -3.55399906 | -0.24386359 | -6.17403208 |
| C | -0.02446886 | 4.13455627 | -0.56521491 | H | -4.33258316 | 0.21923106 | -6.80615679 |
| S | -1.24647378 | 2.87931784 | -0.80114966 | H | -3.89907097 | -1.24603275 | -5.86327611 |
| H | 0.14162539 | 1.33114540 | -2.03483335 | O | -3.30866691 | 0.58269379 | -5.02398249 |
| H | 2.08856491 | 4.32901833 | -0.18743884 | C | -4.35187736 | 1.48487972 | -4.62984145 |
| H | -0.35433068 | 5.16940204 | -0.49480899 | H | -4.99558623 | 1.71701405 | -5.49708916 |
| C | 2.52974879 | -1.02448849 | 0.70522165 | H | -4.97500596 | 1.04060971 | -3.83334852 |
| H | 2.06242072 | -2.00602180 | 0.55052784 | C | -3.69479843 | 2.76506424 | -4.12789562 |
| H | 3.54543194 | -1.07206354 | 0.28499696 | H | -3.05958175 | 2.57298325 | -3.24305471 |
| H | 2.60140949 | -0.83954201 | 1.79113246 | H | -4.46965236 | 3.50388018 | -3.85125713 |
| W | -1.31152024 | -0.14171665 | 2.19190200 | O | -2.89586542 | 3.23242372 | -5.22487797 |
| C | -2.50278351 | -0.28049122 | 3.82258275 | C | -1.99794944 | 4.32633768 | -4.99561947 |
| C | -1.48913223 | -2.16471886 | 1.89354970 | H | -1.35121917 | 4.11858924 | -4.12280503 |
| C | 0.31078013 | -0.48742421 | 3.41461976 | H | -2.54776458 | 5.26848783 | -4.81346560 |
| C | -1.05417658 | 1.87895773 | 2.56984310 | C | -1.17572567 | 4.43943703 | -6.27464289 |
| C | -2.99238402 | 0.21876368 | 1.05946542 | H | -1.84614574 | 4.66459870 | -7.12342087 |
| O | -3.20269377 | -0.36502357 | 4.74590059 | H | -0.43558951 | 5.25456088 | -6.18103150 |
| O | -1.58142279 | -3.31364833 | 1.75057658 | O | -0.52382894 | 3.18121933 | -6.48462413 |
| O | 1.18008445 | -0.67687384 | 4.15954261 | C | -0.39262295 | 2.72248957 | -7.83997585 |
| O | -0.90943261 | 2.98686763 | 2.87346442 | H | -1.16411887 | 3.19855049 | -8.47144426 |
| O | -3.95876921 | 0.40510605 | 0.44408096 | H | 0.60380260 | 2.98031640 | -8.24093361 |
| C | -0.41072158 | -1.27272437 | -1.24464179 | C | -0.58207270 | 1.21017072 | -7.84895847 |
| H | -0.07385381 | -2.25607743 | -0.88682349 | H | 0.16535364 | 0.72114212 | -7.19726542 |
| H | -1.50489946 | -1.31148773 | -1.34697744 | **H** | **-0.48636673** | **0.82625729** | **-8.88183192** |
| H | 0.03841060 | -1.03136038 | -2.22010783 | | | | |

**7b** without 12-crown-4: E = -1483.45624230 au (BP86/def2-TZVP)

ZPE= 0.080143 au

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 | O | 2.93766212 | -1.42707124 | -2.86842852 |
| W | 2.61502361 | 0.00000000 | 0.00000000 | O | 1.64108014 | 2.63451282 | -1.42246775 |
| C | 4.64844820 | 0.11931267 | 0.00000000 | O | 2.85616661 | 1.61261933 | 2.76252967 |
| C | 2.29377782 | -1.79194309 | 1.00463162 | C | -0.85569058 | -0.67887194 | 1.49892064 |
| C | 2.76997832 | -0.95540704 | -1.83623245 | H | -0.41344136 | -0.17723473 | 2.37737876 |
| C | 2.20075748 | 1.71058465 | -0.93134143 | H | -1.93728592 | -0.48016369 | 1.47230446 |
| C | 2.71819596 | 1.01524139 | 1.78752206 | H | -0.67859068 | -1.75795548 | 1.58608845 |
| O | 5.79839357 | 0.18392274 | 0.01387104 | Li | -0.26376818 | 2.08870595 | -1.11067061 |
| O | 1.95463630 | -2.74279174 | 1.55181261 | Cl | -0.82410294 | -1.28132217 | -1.52146035 |

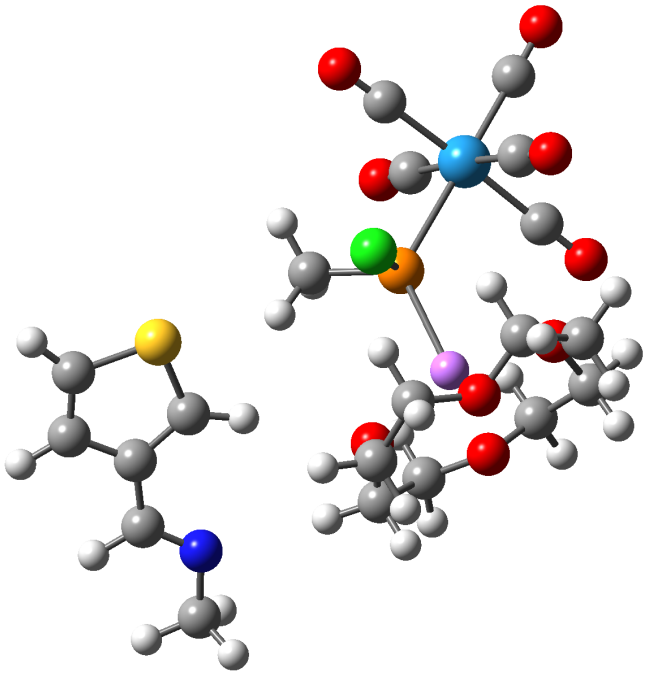
**7b**: E = -2099.06089610 au (BP86/def2-TZVP)

ZPE= 0.319076 au

E = -2094.64687595 au ($COSMO_{THF}$/SCS-MP2/def2-TZVPP)

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 | O | 2.46105426 | 1.00651706 | -3.06102230 |
| W | 2.58880456 | 0.00000000 | 0.00000000 | O | 2.49186821 | 3.04015143 | 1.04790671 |
| C | 4.61273346 | 0.03428819 | 0.00000000 | O | 2.58337043 | -1.03095858 | 3.04048855 |
| C | 2.51463170 | 0.64074377 | -1.96287757 | O | 2.55126197 | -3.08835255 | -0.91136687 |
| C | 2.53116937 | 1.94582109 | 0.65886687 | C | -0.64356853 | 1.64320275 | -0.59219545 |
| C | 2.58558484 | -0.64945580 | 1.93811580 | H | -0.17386136 | 1.96850964 | -1.53062366 |
| C | 2.56647303 | -1.96991437 | -0.60043348 | H | -1.73471661 | 1.61008865 | -0.72245213 |
| O | 5.77650942 | 0.06401078 | -0.01504730 | H | -0.40118314 | 2.38303650 | 0.18822779 |

| | | | |
|---|---|---|---|
| Cl | -0.70582967 | -1.16725240 | -1.73807695 |
| Li | -1.75652815 | -1.76108726 | 0.79789842 |
| O | -2.84419371 | -3.44244360 | 0.25401383 |
| C | -1.78369826 | -4.30871254 | -0.18344157 |
| H | -1.21164989 | -3.82916368 | -0.99744675 |
| H | -2.17787456 | -5.27800261 | -0.53970375 |
| C | -0.91030682 | -4.52635225 | 1.04695120 |
| H | -1.48784623 | -5.06151542 | 1.82099953 |
| H | -0.02409905 | -5.12813668 | 0.78159822 |
| O | -0.51482436 | -3.23795069 | 1.54903916 |
| C | -0.43536835 | -3.10422055 | 2.98142262 |
| H | -1.08389606 | -3.86107764 | 3.45648689 |
| H | 0.60189395 | -3.25042947 | 3.32655383 |
| C | -0.91330650 | -1.70840638 | 3.35977548 |
| H | -0.25337802 | -0.93696646 | 2.92664614 |
| H | -0.92183591 | -1.60089910 | 4.45965708 |
| O | -2.23801148 | -1.58499988 | 2.81271100 |
| C | -2.81621251 | -0.27431572 | 2.77359064 |
| H | -2.09685551 | 0.44161665 | 2.33317522 |
| H | -3.10009825 | 0.07452899 | 3.78398473 |
| C | -4.06047312 | -0.40023662 | 1.90288160 |
| H | -4.76956440 | -1.10254534 | 2.37436149 |
| H | -4.55262666 | 0.58244441 | 1.79705409 |
| O | -3.66625360 | -0.90743017 | 0.61396301 |
| C | -4.56122633 | -1.85440490 | 0.00033671 |
| H | -5.16504420 | -2.34786197 | 0.78165302 |
| H | -5.24057068 | -1.34447534 | -0.70507645 |
| C | -3.72907164 | -2.89857816 | -0.73493190 |
| H | -3.14940503 | -2.43873167 | -1.55502436 |
| **H** | **-4.39426160** | **-3.67674508** | **-1.15304186** |



**7b·3**: E = -2784.99251379 au (BP86/def2-TZVP)

ZPE= 0.432069 au

E = -2779.31686924 au ($COSMO_{THF}$/SCS-MP2/def2-TZVPP)

| | | | |
|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 6.63225426 | 0.00000000 | 0.00000000 |
| C | 6.93106274 | 1.24628584 | 0.00000000 |
| H | 7.91461315 | 1.59299760 | 0.38191582 |
| C | 6.04778809 | 2.30852827 | -0.47912278 |
| C | 4.75708372 | 2.13987063 | -0.96175963 |
| C | 6.44008893 | 3.68757887 | -0.48887714 |
| C | 5.46133837 | 4.52010369 | -0.97049894 |
| S | 4.04881391 | 3.63224407 | -1.41026870 |
| H | 4.19679867 | 1.21333575 | -1.06406618 |
| H | 7.41409538 | 4.03908094 | -0.14705499 |
| H | 5.48670007 | 5.60025235 | -1.08520860 |
| C | 7.62172932 | -0.92433275 | 0.52263068 |
| H | 8.55373852 | -0.43146959 | 0.86400786 |
| H | 7.18961904 | -1.48472638 | 1.36803106 |
| H | 7.87791454 | -1.66672289 | -0.25120038 |
| W | -2.48560910 | -0.01368840 | 0.73465995 |
| C | -4.42167220 | -0.01607778 | 1.32413214 |
| C | -2.43372205 | -2.05487569 | 0.84287512 |
| C | -1.86236377 | 0.09487810 | 2.69118177 |
| C | -2.46398855 | 2.04774846 | 0.59821810 |
| C | -3.02621430 | -0.18292376 | -1.24231167 |
| O | -5.53491308 | -0.00003762 | 1.66530589 |
| O | -2.40764852 | -3.21967125 | 0.89576774 |
| O | -1.50475052 | 0.13979764 | 3.79565437 |
| O | -2.43848135 | 3.20401710 | 0.52719063 |
| O | -3.32661859 | -0.30564935 | -2.35836316 |
| C | 0.99147563 | 1.09575739 | 1.13044529 |
| H | 0.53291515 | 2.08378626 | 1.27361203 |
| H | 1.03073942 | 0.58942706 | 2.10881421 |
| H | 2.01862540 | 1.22089177 | 0.75963768 |
| Cl | 0.18054509 | 1.27927772 | -1.79745525 |
| Li | 1.14806687 | -1.31082374 | -1.99261087 |
| O | 1.36914765 | -1.39824545 | -4.05296741 |
| C | 2.26352010 | -0.30416909 | -4.29525646 |
| H | 1.81805271 | 0.64062240 | -3.93661798 |

| | | | |
|---|---|---|---|
| H | 2.49876557 | -0.20696639 | -5.37147951 |
| C | 3.53273596 | -0.64135059 | -3.52224320 |
| H | 3.97517372 | -1.56699994 | -3.92900597 |
| H | 4.26874341 | 0.17571944 | -3.62121406 |
| O | 3.18730798 | -0.84600600 | -2.13836468 |
| C | 3.93300216 | -1.87648896 | -1.44356231 |
| H | 4.36152704 | -2.57227795 | -2.18526318 |
| H | 4.75147348 | -1.41767027 | -0.86063251 |
| C | 2.97019593 | -2.63435015 | -0.54070306 |
| H | 2.53314093 | -1.96788337 | 0.22682526 |
| H | 3.50406848 | -3.46071770 | -0.03574678 |
| O | 1.93408569 | -3.12869267 | -1.40253020 |
| C | 0.76598404 | -3.69547241 | -0.78564263 |
| H | 0.40114670 | -3.02900846 | 0.01543952 |
| H | 0.98106318 | -4.69203820 | -0.35857881 |
| C | -0.26880639 | -3.82266969 | -1.89608818 |
| H | 0.10123805 | -4.51788069 | -2.67014862 |
| H | -1.21509556 | -4.21107352 | -1.48380748 |
| O | -0.46771929 | -2.52056219 | -2.47975982 |
| C | -0.71350133 | -2.48435501 | -3.89644629 |
| H | -0.31325808 | -3.40165207 | -4.36265425 |
| H | -1.79603227 | -2.42032038 | -4.09950993 |
| C | 0.00030341 | -1.26536089 | -4.47019349 |
| H | -0.43041172 | -0.32879715 | -4.07348352 |
| **H** | **-0.08612598** | **-1.26397506** | **-5.57221726** |

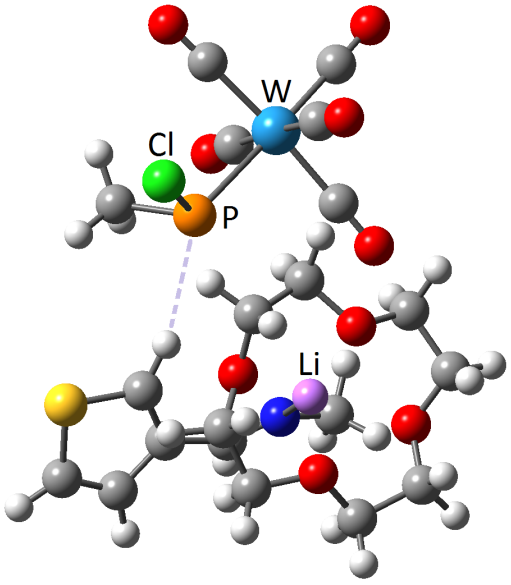
**TS1(7b·3→8b)**: E = -2784.98001440 au (BP86/def2-TZVP)
ZPE= 0.432406 au
E = -2779.31329282 au (COSMO$_{THF}$/SCS-MP2/def2-TZVPP)

| | | | |
|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 3.79972957 | 0.00000000 | 0.00000000 |
| C | 4.33057482 | 1.16945782 | 0.00000000 |
| H | 4.91831178 | 1.51791783 | 0.87384091 |
| C | 4.20894367 | 2.14161620 | -1.08609270 |
| C | 3.18434937 | 2.18104673 | -2.02213245 |
| C | 5.12766779 | 3.23038596 | -1.25710481 |
| C | 4.80293598 | 4.04357059 | -2.31268034 |
| S | 3.35331423 | 3.51333110 | -3.08600394 |
| H | 2.31102676 | 1.53537652 | -2.09404719 |
| H | 5.99864736 | 3.39034155 | -0.62100445 |
| H | 5.32515679 | 4.92551273 | -2.67329874 |
| C | 3.94040340 | -0.77783408 | 1.22382036 |
| H | 4.45183722 | -1.73096558 | 1.01312546 |
| H | 4.49667546 | -0.24687622 | 2.01915995 |
| H | 2.93924576 | -1.03831910 | 1.60049972 |
| W | -2.03345706 | -0.86581788 | 1.43749319 |
| C | -3.61320329 | -1.44996991 | 2.54866995 |
| C | -1.24852595 | -2.74279584 | 1.62179834 |
| C | -1.00176381 | -0.34789721 | 3.13730742 |
| C | -2.79910626 | 1.05201166 | 1.31526784 |
| C | -3.00269796 | -1.41614285 | -0.28900503 |
| O | -4.53048140 | -1.77060307 | 3.19155243 |
| O | -0.82022144 | -3.81995605 | 1.76390011 |
| O | -0.41439321 | -0.07619027 | 4.10267962 |
| O | -3.22507928 | 2.12780596 | 1.27387193 |
| O | -3.54960199 | -1.75412313 | -1.25895211 |
| C | 0.80523779 | 1.35339571 | 0.99742699 |
| H | 0.06667253 | 2.07701453 | 1.36770776 |
| H | 1.29430132 | 0.88549779 | 1.86595587 |
| H | 1.56311896 | 1.88222002 | 0.40445164 |
| Cl | -0.79822553 | 1.32402052 | -1.53304368 |
| Li | 1.80444580 | -1.55087237 | -1.77190716 |
| O | 0.43443441 | -2.75716628 | -2.78706088 |
| C | -0.40775197 | -1.74687354 | -3.36513263 |
| H | -0.80589111 | -1.07785927 | -2.58413348 |
| H | -1.25806271 | -2.19606340 | -3.91019235 |
| C | 0.47009653 | -0.97431443 | -4.33894770 |
| H | 0.76644872 | -1.62890933 | -5.17611668 |
| H | -0.08707795 | -0.11023802 | -4.73801432 |
| O | 1.66045200 | -0.52481040 | -3.65220716 |
| C | 2.88091887 | -0.61138958 | -4.40813543 |
| H | 2.75560517 | -1.34273742 | -5.22470974 |
| H | 3.13661406 | 0.36883138 | -4.84793956 |
| C | 3.99614346 | -1.07572435 | -3.48130674 |
| H | 4.21233999 | -0.32557926 | -2.69934593 |
| H | 4.91706320 | -1.25329549 | -4.06829980 |
| O | 3.51225222 | -2.28347993 | -2.88446452 |
| C | 4.31408581 | -2.87513494 | -1.86046552 |
| H | 4.57566198 | -2.11368526 | -1.10584454 |
| H | 5.24840278 | -3.30212510 | -2.27233100 |
| C | 3.46234002 | -3.99188529 | -1.26973687 |
| H | 3.30515188 | -4.76998971 | -2.03625513 |
| H | 3.97940899 | -4.45070289 | -0.40767943 |
| O | 2.19260883 | -3.45056947 | -0.87101066 |
| C | 1.05054404 | -4.30709819 | -1.11424547 |
| H | 1.32934721 | -5.07333984 | -1.85715098 |
| H | 0.74272313 | -4.80266306 | -0.17957355 |
| C | -0.09407268 | -3.46342166 | -1.65404485 |
| H | -0.45615269 | -2.74531853 | -0.89628146 |
| **H** | **-0.93494046** | **-4.12061711** | **-1.94148370** |

**8a**: E = -3602.705706650 au (COSMO$_{THF}$/BP86-D/def2-TZVP)

| | | | |
|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 4.34895625 | 0.00000000 | 0.00000000 |
| C | 4.48787389 | 1.27926644 | 0.00000000 |
| H | 5.00086086 | 1.77758373 | 0.84345945 |
| C | 4.01684405 | 2.16137266 | -1.05975274 |
| C | 2.82018373 | 2.00628231 | -1.73791284 |
| C | 4.73392080 | 3.33139323 | -1.47637541 |
| C | 4.09759977 | 4.00831563 | -2.48524262 |
| S | 2.59363138 | 3.25293734 | -2.88908583 |
| H | 2.05300589 | 1.25570394 | -1.54496314 |
| H | 5.69099186 | 3.63572998 | -1.05238952 |
| H | 4.41679899 | 4.90766935 | -3.00582953 |

| | | | |
|---|---|---|---|
| C | 4.79324947 | -0.69826435 | 1.20439429 |
| H | 5.54761045 | -1.45184550 | 0.93786218 |
| H | 5.19950086 | -0.01179203 | 1.96920897 |
| H | 3.93740413 | -1.24394752 | 1.63054946 |
| W | -0.86646720 | -2.20420620 | 1.21091150 |
| C | -1.60080461 | -3.84393966 | 2.10051447 |
| C | 1.04991066 | -2.64711327 | 1.75328542 |
| C | -1.07230184 | -1.14983354 | 2.95431483 |
| C | -2.70703763 | -1.51678197 | 0.59280959 |
| C | -0.65276378 | -3.24185403 | -0.54631521 |
| O | -2.05273262 | -4.79353115 | 2.61580827 |
| O | 2.14919646 | -2.88440595 | 2.06730432 |
| O | -1.19780828 | -0.56405731 | 3.95182695 |
| O | -3.72606597 | -1.08804043 | 0.24273961 |
| O | -0.54925718 | -3.86167322 | -1.52627586 |
| Cl | -1.00953941 | -0.08397539 | -1.96604072 |
| Li | 4.10870164 | -1.32797271 | -1.70312065 |
| O | 2.89660738 | -2.83376369 | -2.53739881 |
| C | 1.78329630 | -1.95561281 | -2.78458907 |
| H | 1.50544731 | -1.43033533 | -1.84943411 |
| H | 0.90189183 | -2.50949458 | -3.14309924 |
| C | 2.25804882 | -0.95938256 | -3.82157615 |
| H | 2.58272381 | -1.48131546 | -4.73800515 |
| H | 1.44504205 | -0.25558621 | -4.06731038 |
| O | 3.37021908 | -0.26515501 | -3.23547870 |
| C | 4.43588499 | 0.15295499 | -4.09605535 |
| H | 4.47532855 | -0.49697615 | -4.98693274 |
| H | 4.28735293 | 1.19982308 | -4.41416046 |
| C | 5.72359781 | 0.02833686 | -3.29928079 |
| H | 5.67750185 | 0.66626962 | -2.39859610 |
| H | 6.58904340 | 0.33269891 | -3.91276338 |
| O | 5.81957857 | -1.35152352 | -2.90923678 |
| C | 6.73957081 | -1.64146672 | -1.84704007 |
| H | 6.62178414 | -0.89403486 | -1.04023082 |
| H | 7.78427519 | -1.62059915 | -2.20315370 |
| C | 6.38285148 | -3.03066880 | -1.34846658 |
| H | 6.43928629 | -3.74911381 | -2.18369787 |
| H | 7.08624107 | -3.34385742 | -0.55826834 |
| O | 5.03954280 | -2.97905756 | -0.83671658 |
| C | 4.20491222 | -4.13045765 | -1.06231844 |
| H | 4.57641808 | -4.69831570 | -1.93208221 |
| H | 4.20548811 | -4.78617961 | -0.17588257 |
| C | 2.80419920 | -3.62380932 | -1.34324835 |
| H | 2.44257802 | -2.99511448 | -0.50827422 |
| H | 2.10587312 | -4.46757303 | -1.47135638 |
| H | 0.47722434 | 3.16409542 | 4.33361894 |
| C | -0.28929512 | 2.78986779 | 3.63391094 |
| Si | 0.53872774 | 2.15592723 | 2.06024888 |
| H | -0.83968002 | 1.97830724 | 4.13477528 |
| H | -0.99350256 | 3.60814550 | 3.42476526 |
| C | -0.81148731 | 1.42787540 | 0.90719370 |
| C | 1.48186275 | 3.56734574 | 1.23259345 |
| C | 1.83079466 | 0.86732718 | 2.56460070 |
| H | -1.60836413 | 1.04643733 | 1.57135309 |
| Si | -1.71308635 | 2.79218413 | -0.07053977 |
| H | 2.28558035 | 3.90569460 | 1.90850407 |
| H | 1.94929317 | 3.23985465 | 0.29195989 |
| H | 0.83673566 | 4.43040559 | 1.01169929 |
| H | 1.39572813 | 0.04899901 | 3.15679812 |
| H | 2.32461008 | 0.42963030 | 1.68379081 |
| H | 2.60496924 | 1.35994922 | 3.17770569 |
| C | -3.38689219 | 2.16107577 | -0.67104916 |
| C | -2.11361928 | 4.24041181 | 1.08570686 |
| C | -0.68403356 | 3.44380400 | -1.50692370 |
| H | -3.99503750 | 1.81831759 | 0.18183161 |
| H | -3.93247746 | 2.98041512 | -1.17008897 |
| H | -3.28501665 | 1.32198271 | -1.37287949 |
| H | -2.71098757 | 4.98218891 | 0.52827809 |
| H | -2.71413256 | 3.90407204 | 1.94631710 |
| H | -1.21875255 | 4.74799017 | 1.47452647 |
| H | -0.43326566 | 2.63428487 | -2.20839718 |
| H | -1.24839150 | 4.21635445 | -2.05605185 |
| H | 0.25340488 | 3.89390920 | -1.14974139 |




**8b**: E = -2784.98200352 au (BP86/def2-TZVP)

ZPE= 0.432558 au

E = -2779.31512249 au ($COSMO_{THF}$/SCS-MP2/def2-TZVPP)

| | | | |
|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 4.47533966 | 0.00000000 | 0.00000000 |
| C | 4.55464817 | 1.28705901 | 0.00000000 |
| H | 5.06945920 | 1.79588997 | 0.83800594 |
| C | 3.98388505 | 2.17718073 | -1.00469132 |
| C | 2.78727247 | 1.94543450 | -1.66994940 |
| C | 4.54528650 | 3.45842136 | -1.33185072 |
| C | 3.79421944 | 4.14702201 | -2.24909044 |
| S | 2.37271515 | 3.26245133 | -2.68377377 |
| H | 2.09585515 | 1.11220814 | -1.51681501 |
| H | 5.47489598 | 3.83976645 | -0.90807794 |
| H | 3.98705891 | 5.12436195 | -2.68320721 |
| C | 4.96575388 | -0.66747233 | 1.20933758 |
| H | 5.68614514 | -1.45168228 | 0.93873961 |
| H | 5.42955675 | 0.03729259 | 1.92219545 |
| H | 4.11810039 | -1.16309375 | 1.70828862 |
| W | -0.92375140 | -1.68981883 | 1.79456234 |
| C | -1.65576694 | -2.94313104 | 3.19693268 |
| C | 0.98445167 | -2.29818219 | 2.13112118 |
| C | -0.67317143 | -0.22260094 | 3.21322537 |
| C | -2.78652062 | -0.93140618 | 1.30528438 |
| C | -1.09245792 | -3.14818858 | 0.35919793 |
| O | -2.09407966 | -3.65819685 | 4.00731667 |
| O | 2.09573775 | -2.63464377 | 2.29355650 |
| O | -0.50954323 | 0.59709743 | 4.02126936 |
| O | -3.81051400 | -0.47499128 | 1.01389937 |
| O | -1.15346551 | -3.99377494 | -0.43930678 |
| C | -0.63434726 | 1.70144226 | 0.42772639 |
| H | -1.72085976 | 1.73095515 | 0.58979954 |
| H | -0.13228199 | 2.00985459 | 1.35883636 |
| H | -0.36991009 | 2.41694391 | -0.36515465 |
| Cl | -1.17054947 | -0.23872891 | -1.82283614 |
| Li | 4.09949795 | -1.40347994 | -1.61736578 |
| O | 3.10948934 | -3.13810949 | -1.91324916 |
| C | 1.75906695 | -2.65128526 | -2.06815957 |
| H | 1.45803929 | -2.04679498 | -1.19121734 |
| H | 1.04052922 | -3.47914269 | -2.18813332 |
| C | 1.79294060 | -1.79522445 | -3.32349226 |
| H | 2.02816821 | -2.41948167 | -4.20249973 |
| H | 0.81908307 | -1.29880230 | -3.46054574 |
| O | 2.84132073 | -0.80766890 | -3.15265756 |
| C | 3.59706173 | -0.46454759 | -4.32112660 |
| H | 3.55155057 | -1.29252182 | -5.04980789 |
| H | 3.19599824 | 0.44830620 | -4.79602091 |
| C | 5.04585808 | -0.24097200 | -3.89743421 |
| H | 5.13279827 | 0.63212288 | -3.22412302 |
| H | 5.68013252 | -0.06942738 | -4.78616952 |
| O | 5.42164776 | -1.44352975 | -3.21051393 |
| C | 6.70133251 | -1.50964480 | -2.57767375 |
| H | 6.82339670 | -0.67520868 | -1.86080148 |
| H | 7.52381647 | -1.46119342 | -3.31533032 |
| C | 6.72436030 | -2.85903969 | -1.86657133 |
| H | 6.64728898 | -3.66426721 | -2.61714040 |
| H | 7.67272144 | -2.98257232 | -1.31338183 |
| O | 5.60183860 | -2.92064932 | -0.97325079 |
| C | 4.92554944 | -4.19325582 | -0.87229953 |
| H | 5.13402790 | -4.78769850 | -1.77799338 |
| H | 5.28385166 | -4.74952105 | 0.01085149 |
| C | 3.42714231 | -3.93617869 | -0.76730640 |
| H | 3.16610459 | -3.40945971 | 0.16829297 |
| **H** | **2.88388778** | **-4.89849852** | **-0.78054319** |

**8b COSMO$_{THF}$/B3LYP-D**: E = -2783.876143823 au (COSMO$_{THF}$/B3LYPD/def2-TZVP)

| | | | |
|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 3.70818907 | 0.00000000 | 0.00000000 |
| C | 3.73377362 | 1.27219403 | 0.00000000 |
| H | 4.02775578 | 1.81537692 | 0.90601644 |
| C | 3.36048723 | 2.11267045 | -1.13204634 |
| C | 2.35040119 | 1.82098690 | -2.01580148 |
| C | 3.95103318 | 3.39111499 | -1.38576136 |
| C | 3.40518151 | 4.01769130 | -2.46558201 |
| S | 2.13565494 | 3.07530134 | -3.15578048 |
| H | 1.72260224 | 0.94504893 | -2.01530075 |
| H | 4.75243799 | 3.80857016 | -0.79095174 |
| H | 3.66577330 | 4.97737958 | -2.88435492 |
| C | 3.97307261 | -0.66368009 | 1.27115496 |
| H | 4.80744356 | -1.35478480 | 1.15174068 |
| H | 4.19445865 | 0.04316131 | 2.07967684 |
| H | 3.09171668 | -1.24717210 | 1.54997644 |
| W | -1.45605886 | -1.59923711 | 1.51497082 |
| C | -2.58396673 | -2.81401365 | 2.66399525 |
| C | 0.28217241 | -2.58975679 | 1.94606652 |
| C | -1.08469741 | -0.31083775 | 3.07614733 |
| C | -3.03654152 | -0.39862024 | 0.92814791 |
| C | -1.67015061 | -2.77623734 | -0.16310130 |
| O | -3.25016826 | -3.49616883 | 3.32138792 |
| O | 1.29418628 | -3.10582500 | 2.15127996 |
| O | -0.84935477 | 0.42957024 | 3.92455764 |
| O | -3.86380468 | 0.31596385 | 0.58173520 |
| O | -1.73622403 | -3.41715177 | -1.11590638 |
| C | -0.22458837 | 1.73203941 | 0.64129136 |
| H | -1.27148769 | 2.01515300 | 0.77498588 |
| H | 0.27573961 | 1.77945611 | 1.61421358 |
| H | 0.26187539 | 2.44187817 | -0.03367496 |
| Cl | -1.11314339 | 0.27796923 | -1.86031594 |
| Li | 3.76648678 | -1.38074313 | -1.63889618 |
| O | 3.10541138 | -3.29970222 | -1.64203881 |
| C | 1.71559900 | -2.96882754 | -1.57415472 |
| H | 1.53473192 | -2.30206422 | -0.72405443 |
| H | 1.09778630 | -3.86565492 | -1.46950518 |
| C | 1.39315720 | -2.25727767 | -2.87137851 |
| H | 1.57795847 | -2.92553286 | -3.71665830 |
| H | 0.34824757 | -1.93934576 | -2.87692008 |
| O | 2.25287774 | -1.11449805 | -2.96135959 |
| C | 2.80341504 | -0.79654133 | -4.23923317 |
| H | 2.86542244 | -1.69949017 | -4.85392400 |
| H | 2.17960465 | -0.05865003 | -4.75348279 |
| C | 4.19460846 | -0.23545331 | -4.01947186 |
| H | 4.15391118 | 0.67679634 | -3.41506531 |
| H | 4.66407714 | -0.00333239 | -4.98129125 |
| O | 4.92490678 | -1.24304383 | -3.32291521 |
| C | 6.13044321 | -0.84057524 | -2.67875330 |
| H | 5.93672052 | 0.03539850 | -2.04510666 |
| H | 6.90608272 | -0.58461901 | -3.40817349 |
| C | 6.57060098 | -2.02239289 | -1.83800276 |
| H | 6.74482811 | -2.88569641 | -2.48726288 |
| H | 7.49722889 | -1.78365148 | -1.30696123 |
| O | 5.52449209 | -2.31146913 | -0.90794815 |
| C | 5.20941301 | -3.68605675 | -0.66541738 |
| H | 5.49557956 | -4.29048318 | -1.53116199 |
| H | 5.74356442 | -4.05243565 | 0.21696200 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 3.71285599 | -3.79086749 | -0.44939744 | H | 3.43491110 | -4.83432901 | -0.26759815 |
| H | 3.39536132 | -3.19108047 | 0.40920851 | | | | |

**TS2(8b→9b)**: E = -2784.97211506 au (BP86/def2-TZVP)

ZPE= 0.432960 au

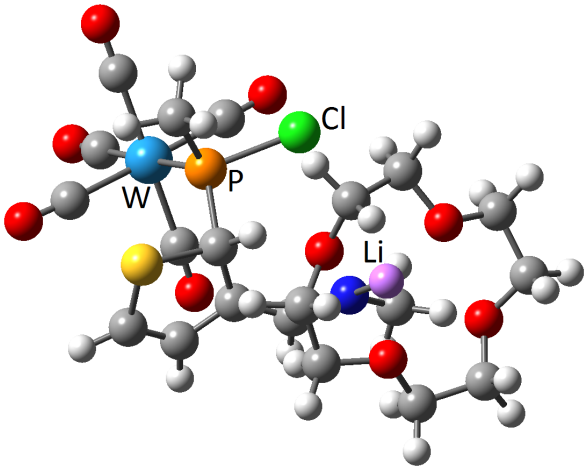
E = -2779.30279830 au ($COSMO_{THF}$/SCS-MP2/def2-TZVPP)

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 | Cl | -1.12169380 | -1.29341423 | -1.26835844 |
| N | 4.36766949 | 0.00000000 | 0.00000000 | Li | 4.58308199 | -1.45348602 | -1.40572372 |
| C | 3.64482890 | 1.11824996 | 0.00000000 | O | 5.01807898 | -3.48573566 | -1.14987448 |
| H | 4.09720238 | 1.99972370 | 0.49804956 | C | 3.77076414 | -3.89975956 | -0.57145912 |
| C | 2.40205434 | 1.41011826 | -0.58738392 | H | 3.52028085 | -3.26589095 | 0.29901160 |
| C | 1.44584278 | 0.45042745 | -1.21943557 | H | 3.80416485 | -4.95378250 | -0.24215938 |
| C | 2.05662205 | 2.76767070 | -0.95142958 | C | 2.74589282 | -3.73474582 | -1.68707476 |
| C | 1.23970718 | 2.88565319 | -2.03040769 | H | 2.98984403 | -4.42120714 | -2.51577244 |
| S | 0.77667535 | 1.30575486 | -2.70343667 | H | 1.73358752 | -3.96045754 | -1.31514843 |
| H | 1.85560810 | -0.52949731 | -1.48891154 | O | 2.82120668 | -2.37430440 | -2.15575412 |
| H | 2.48951694 | 3.63496376 | -0.44667963 | C | 2.70059396 | -2.16425185 | -3.57534181 |
| H | 0.86214819 | 3.79208893 | -2.49712396 | H | 3.01752408 | -3.07727487 | -4.10802052 |
| C | 5.56145645 | 0.07211044 | 0.84905679 | H | 1.65605537 | -1.93333526 | -3.84632723 |
| H | 6.46687496 | -0.21410535 | 0.28943097 | C | 3.61456521 | -1.00555506 | -3.95644974 |
| H | 5.72506742 | 1.08882914 | 1.25661885 | H | 3.27768091 | -0.05834237 | -3.49407146 |
| H | 5.47627896 | -0.60537652 | 1.71707349 | H | 3.61338681 | -0.87455018 | -5.05414743 |
| W | 0.16636842 | -0.99666269 | 2.36920758 | O | 4.91293199 | -1.38562838 | -3.47697191 |
| C | 0.03579996 | -1.75443587 | 4.23362666 | C | 5.98555935 | -0.44534102 | -3.57569687 |
| C | 2.19759665 | -0.87328557 | 2.67759375 | H | 5.74206510 | 0.48188041 | -3.02306856 |
| C | -0.01168738 | 0.91915685 | 3.11555617 | H | 6.20236928 | -0.18265101 | -4.62788343 |
| C | -1.88066413 | -1.19840409 | 2.24080201 | C | 7.18640039 | -1.15658145 | -2.96158073 |
| C | 0.43740048 | -2.87215128 | 1.58452498 | H | 7.42885500 | -2.04866937 | -3.56477882 |
| O | -0.05696983 | -2.18991896 | 5.30784280 | H | 8.06472895 | -0.48700952 | -2.94968291 |
| O | 3.31885843 | -0.86699185 | 2.97317609 | O | 6.83592693 | -1.55335207 | -1.62710175 |
| O | -0.09463689 | 1.99089050 | 3.54865307 | C | 7.27818574 | -2.84845472 | -1.19269116 |
| O | -3.03223708 | -1.32519832 | 2.21549394 | H | 7.45202175 | -3.49618414 | -2.06964351 |
| O | 0.62245012 | -3.94008003 | 1.16120507 | H | 8.21913526 | -2.76814367 | -0.61923208 |
| C | -1.09484408 | 1.47051839 | -0.03333965 | C | 6.18514582 | -3.46197450 | -0.32377373 |
| H | -2.02008687 | 1.23199125 | 0.50596028 | H | 6.00905175 | -2.85634551 | 0.58438965 |
| H | -0.57728463 | 2.29566530 | 0.47598173 | **H** | **6.48309295** | **-4.48106757** | **-0.01390869** |
| H | -1.31940990 | 1.75371953 | -1.06927732 | | | | |

**9a**: E = -3602.686700381 au ($COSMO_{THF}$/BP86-D/def2-TZVP)

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 | C | -1.98598177 | 2.77955520 | 3.03001292 |
| N | 4.16303922 | 0.00000000 | 0.00000000 | C | 0.66434915 | 2.29501936 | 2.15644474 |
| C | 3.54818752 | 1.17348263 | 0.00000000 | C | -1.56076745 | 3.04656802 | 0.25874127 |
| H | 4.04492080 | 2.00076727 | 0.54628860 | C | -3.10656421 | 0.92675345 | 1.21438609 |
| C | 2.34279288 | 1.60291120 | -0.57954533 | C | -1.04747263 | 0.11831937 | 3.09932049 |
| C | 1.25639975 | 0.79500790 | -1.23478741 | O | -2.42839010 | 3.48797536 | 3.84262440 |
| C | 2.04947317 | 3.00796068 | -0.64051855 | O | 1.63322250 | 2.76854142 | 2.57863002 |
| C | 1.02719614 | 3.38011104 | -1.45308054 | O | -1.91207778 | 3.92146447 | -0.41610497 |
| S | 0.30321732 | 1.98534489 | -2.26798110 | O | -4.22024465 | 0.66116386 | 1.01624068 |
| H | 1.58204970 | -0.06109566 | -1.83803930 | O | -0.99720925 | -0.65676204 | 3.96292326 |
| H | 2.65105295 | 3.73187289 | -0.08581957 | Cl | 1.46197305 | -1.11163996 | 1.11712283 |
| H | 0.62404029 | 4.37217275 | -1.63470624 | Li | 3.81525651 | -1.80281177 | -0.97202213 |
| C | 5.28992511 | -0.07507404 | 0.92913432 | O | 3.32806175 | -3.91263717 | -1.03522337 |
| H | 6.20686010 | -0.44743171 | 0.44342359 | C | 1.92292496 | -3.92151546 | -1.29109618 |
| H | 5.52423999 | 0.90621919 | 1.38963757 | H | 1.38737318 | -3.35183000 | -0.50942961 |
| H | 5.07271748 | -0.78458347 | 1.74846697 | H | 1.52340812 | -4.95035170 | -1.32029713 |
| W | -1.20712448 | 1.55073430 | 1.64194192 | C | 1.77573755 | -3.26010318 | -2.64702626 |

| | | | |
|---|---|---|---|
| H | 2.37171213 | -3.81160208 | -3.39255042 |
| H | 0.72057634 | -3.25480381 | -2.97120378 |
| O | 2.26994249 | -1.91667430 | -2.52177160 |
| C | 2.87025643 | -1.33654293 | -3.70098004 |
| H | 3.00154585 | -2.11175838 | -4.47206601 |
| H | 2.21431840 | -0.54456142 | -4.09738793 |
| C | 4.21398657 | -0.75812970 | -3.30219549 |
| H | 4.09264867 | 0.01564142 | -2.51822631 |
| H | 4.71206200 | -0.31142535 | -4.18090817 |
| O | 4.96883251 | -1.85697075 | -2.76821583 |
| C | 6.20788247 | -1.49698209 | -2.13930476 |
| H | 6.06882629 | -0.55978976 | -1.57504154 |
| H | 7.00449998 | -1.35243382 | -2.89099406 |
| C | 6.58090793 | -2.64530467 | -1.21733373 |
| H | 6.63595174 | -3.58041074 | -1.80147762 |
| H | 7.56812634 | -2.45137092 | -0.76223301 |
| O | 5.57254766 | -2.76429441 | -0.20014787 |
| C | 5.26199424 | -4.08746603 | 0.26221648 |
| H | 5.67408839 | -4.83942249 | -0.43159235 |
| H | 5.68831337 | -4.25343568 | 1.26580115 |
| C | 3.74802802 | -4.21528214 | 0.29861048 |
| H | 3.29862477 | -3.49345457 | 1.00814370 |
| H | 3.45440649 | -5.23747874 | 0.59597103 |
| C | -1.52896721 | -4.34324604 | -1.08359823 |
| Si | -1.62121742 | -2.80609760 | 0.03222420 |
| H | -1.16515036 | -5.19606367 | -0.48795669 |
| H | -2.51458200 | -4.60481307 | -1.49433476 |
| H | -0.84561005 | -4.21231378 | -1.93517483 |
| C | -0.78032711 | -1.37469726 | -0.95161311 |
| C | -3.40826908 | -2.38248139 | 0.45435663 |
| C | -0.79083668 | -3.34147830 | 1.63698609 |
| H | 0.10392460 | -1.84419280 | -1.41986282 |
| Si | -1.85417239 | -0.92507525 | -2.49734959 |
| H | -3.98526478 | -3.31731435 | 0.55170604 |
| H | -3.46427762 | -1.85375650 | 1.41722082 |
| H | -3.90089964 | -1.75383295 | -0.30040911 |
| H | 0.22456728 | -3.72825675 | 1.46488580 |
| H | -0.73242388 | -2.55314985 | 2.39712448 |
| H | -1.40765153 | -4.16662185 | 2.03624504 |
| C | -0.67998938 | -0.73049864 | -3.96573594 |
| C | -2.97693249 | -2.35466992 | -3.02538133 |
| C | -2.98828495 | 0.54413884 | -2.21204585 |
| H | -0.20425238 | -1.70342314 | -4.17215001 |
| H | -1.25553924 | -0.44600159 | -4.86240997 |
| H | 0.11673334 | 0.01371906 | -3.82994189 |
| H | -3.56968007 | -1.97937807 | -3.87773181 |
| H | -2.40421614 | -3.22702450 | -3.37068736 |
| H | -3.67836134 | -2.68733992 | -2.24811116 |
| H | -2.45625296 | 1.42605573 | -1.83184403 |
| H | -3.47076885 | 0.81016505 | -3.16768841 |
| H | -3.78216932 | 0.27623245 | -1.49768960 |




**9b**: E = -2784.97249121 au (BP86/def2-TZVP)

ZPE= 0.432539 au

E = -2779.30404145 au ($COSMO_{THF}$/SCS-MP2/def2-TZVPP)

| | | | |
|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 4.04238851 | 0.00000000 | 0.00000000 |
| C | 3.46493260 | 1.20620410 | 0.00000000 |
| H | 3.96145513 | 1.99866536 | 0.59912791 |
| C | 2.30730399 | 1.64973873 | -0.64923000 |
| C | 1.23123519 | 0.78854910 | -1.25407666 |
| C | 1.98175306 | 3.04816185 | -0.76679096 |
| C | 0.93247904 | 3.35591894 | -1.56907166 |
| S | 0.21197353 | 1.91171123 | -2.30284201 |
| H | 1.57908335 | -0.06255719 | -1.85465708 |
| H | 2.56208798 | 3.81302066 | -0.24583799 |
| H | 0.49495949 | 4.32854218 | -1.77530803 |
| C | 4.97520970 | -0.18245100 | 1.11422742 |
| H | 5.77112651 | -0.89595321 | 0.85481610 |
| H | 5.45239040 | 0.77110613 | 1.42696622 |
| H | 4.45722850 | -0.58202046 | 2.00696749 |
| W | -0.85259312 | 1.19845622 | 2.07015380 |
| C | -1.65412552 | 2.12013617 | 3.68053192 |
| C | 0.83123227 | 2.38051638 | 2.32926650 |
| C | -1.72689572 | 2.63527767 | 0.87251174 |
| C | -2.54238401 | 0.04296177 | 1.94634991 |
| C | 0.01168723 | -0.20231012 | 3.31323462 |
| O | -2.12911396 | 2.64540153 | 4.60195290 |
| O | 1.71606366 | 3.07686841 | 2.60165682 |
| O | -2.25437656 | 3.46127240 | 0.25501713 |
| O | -3.50470177 | -0.60627320 | 1.90586273 |
| O | 0.48704173 | -0.97399073 | 4.03358380 |
| C | -1.30298132 | -0.68634401 | -1.11319585 |
| H | -1.87802977 | -1.42838177 | -0.54458751 |
| H | -1.97227430 | 0.12052970 | -1.43627800 |

| | | | |
|---|---|---|---|
| H | -0.85116219 | -1.17013548 | -1.99105804 |
| Cl | 0.95855770 | -1.87523436 | 0.41997174 |
| Li | 4.36061584 | -1.21288598 | -1.56891917 |
| O | 4.37246990 | -3.20131346 | -2.28810690 |
| C | 2.98298216 | -3.45823221 | -2.52415968 |
| H | 2.38837441 | -3.27627100 | -1.60948301 |
| H | 2.81522964 | -4.49792686 | -2.86086009 |
| C | 2.59699911 | -2.48354240 | -3.63005531 |
| H | 3.17097249 | -2.71568062 | -4.54390963 |
| H | 1.51901274 | -2.56551641 | -3.85612642 |
| O | 2.92613713 | -1.16151963 | -3.17735031 |
| C | 3.38188714 | -0.21817380 | -4.17019233 |
| H | 3.74155007 | -0.76709488 | -5.05711167 |
| H | 2.55641727 | 0.45183640 | -4.46512371 |
| C | 4.52192978 | 0.58929485 | -3.56328970 |
| H | 4.17036035 | 1.17396271 | -2.69147998 |
| H | 4.92998826 | 1.28547014 | -4.31916150 |
| O | 5.50151225 | -0.38272333 | -3.16172984 |
| C | 6.62501716 | 0.07203508 | -2.39882644 |
| H | 6.28170426 | 0.66824040 | -1.53322311 |
| H | 7.30895388 | 0.68761740 | -3.01285963 |
| C | 7.34257100 | -1.19120840 | -1.93965777 |
| H | 7.65996820 | -1.77472355 | -2.82153264 |
| H | 8.23709996 | -0.92688049 | -1.34802612 |
| O | 6.42694048 | -1.96827747 | -1.14975676 |
| C | 6.48161264 | -3.39354736 | -1.29537170 |
| H | 6.94011631 | -3.65377777 | -2.26530575 |
| H | 7.08118766 | -3.84779182 | -0.48627871 |
| C | 5.05123055 | -3.92260446 | -1.25757480 |
| H | 4.57879301 | -3.73824670 | -0.27419396 |
| **H** | **5.04649503** | **-5.01145007** | **-1.45075402** |

**TS3(9b→5b)**: E = -2784.96211622 au (BP86/def2-TZVP)

ZPE= 0.432109 au

E = -2779.29747526 au ($COSMO_{THF}$/SCS-MP2/def2-TZVPP)

| | | | |
|---|---|---|---|
| P | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.72221500 | 0.00000000 | 0.00000000 |
| C | 2.74315436 | 1.32091240 | 0.00000000 |
| H | 3.38965487 | 1.89160044 | 0.68792242 |
| C | 1.78721566 | 2.00051538 | -0.77720311 |
| C | 0.73152160 | 1.14485213 | -1.38309076 |
| C | 1.50598311 | 3.38291836 | -0.84003168 |
| C | 0.31127936 | 3.68594775 | -1.45205764 |
| S | -0.53113284 | 2.29128870 | -2.03800322 |
| H | 1.06760653 | 0.46314284 | -2.17843424 |
| H | 2.13546113 | 4.14004552 | -0.37116226 |
| H | -0.17109185 | 4.66006699 | -1.49461586 |
| C | 3.47547653 | -0.66243959 | 1.05076645 |
| H | 2.85900116 | -1.47945434 | 1.45866745 |
| H | 4.39041532 | -1.11712679 | 0.62593814 |
| H | 3.77926515 | 0.00746504 | 1.87736260 |
| W | -0.91059581 | 0.98642535 | 2.18886673 |
| C | -1.77142150 | 1.68753181 | 3.87363734 |
| C | 0.34545031 | -0.18187884 | 3.34808714 |
| C | 0.46179068 | 2.51657576 | 2.32622238 |
| C | -2.21241366 | 2.18678170 | 1.13684304 |
| C | -2.28471671 | -0.54465289 | 2.16776861 |
| O | -2.28826986 | 2.09534103 | 4.83312834 |
| O | 1.02191413 | -0.79621882 | 4.05812947 |
| O | 1.19725196 | 3.39773692 | 2.50623756 |
| O | -2.98330890 | 2.87101391 | 0.60553597 |
| O | -3.07523472 | -1.39283740 | 2.18841077 |
| C | -1.27605599 | -0.86666010 | -1.03742510 |
| H | -1.81151036 | -1.58982029 | -0.41398288 |
| H | -1.99373198 | -0.14366005 | -1.45194113 |
| H | -0.77418550 | -1.40387660 | -1.85633643 |
| Cl | 0.52297149 | -2.78232062 | 0.77414816 |
| Li | 1.60726925 | -3.98283672 | -0.80142427 |
| O | 0.65294514 | -5.69695504 | -1.44813429 |
| C | -0.52134554 | -5.07990609 | -1.99939936 |
| H | -1.00766182 | -4.44321691 | -1.23787176 |
| H | -1.24197586 | -5.83829742 | -2.35725160 |
| C | -0.02805757 | -4.23957578 | -3.17130370 |
| H | 0.48298064 | -4.88853126 | -3.90427150 |
| H | -0.88091025 | -3.74456135 | -3.66867426 |
| O | 0.89573823 | -3.26341414 | -2.65946721 |
| C | 2.02318746 | -2.92182462 | -3.48318025 |
| H | 2.22661770 | -3.74005884 | -4.19615280 |
| H | 1.82390352 | -1.99647993 | -4.05190602 |
| C | 3.22514559 | -2.72986388 | -2.56565881 |
| H | 3.05087922 | -1.90463452 | -1.84630737 |
| H | 4.12495181 | -2.50064051 | -3.16556367 |
| O | 3.36226416 | -3.98701460 | -1.87938372 |
| C | 4.33626250 | -4.09950075 | -0.83389026 |
| H | 4.22635891 | -3.27028435 | -0.11207165 |
| H | 5.36510450 | -4.08488909 | -1.23862714 |
| C | 4.05588097 | -5.44031468 | -0.16522862 |
| H | 4.18527642 | -6.25383558 | -0.90129216 |
| H | 4.75935206 | -5.60264809 | 0.67110180 |
| O | 2.70128760 | -5.41558533 | 0.30431422 |
| C | 1.96685440 | -6.65057226 | 0.25946811 |
| H | 2.42997314 | -7.33330484 | -0.47473366 |
| H | 1.96990865 | -7.13776414 | 1.25019723 |
| C | 0.53700184 | -6.33557870 | -0.16459002 |
| H | 0.05592263 | -5.64962065 | 0.55704686 |
| **H** | **-0.05048738** | **-7.26961568** | **-0.23309860** |