Electronic Supplementary Material (ESI) for Chemical Communications

ESI

Heterolytic H_2 activation on a carbene-ligated rhodathiaborane promoted by *isonido-nido* cage opening

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General Procedures: Reactions were carried out under an argon atmosphere using standard Schlenk-line techniques. Solvents were obtained dried from a Solvent Purification System of Innovative Technology Inc. Preparative thin-layer chromatography (TLC) was carried out using 1 mm layers of silica gel G (Fluka, type GF254) made from water slurries on glass plates of dimensions 20 × 20 cm and dried in air at 25 °C. Infrared spectra were recorded on a Perkin-Elmer Spectrum 100 spectrometer, using a Universal ATR Sampling Accessory. NMR spectra were recorded on Bruker Avance 300-MHz and AV 400-MHz spectrometers, using ^{31}P-{^{1}H}, ^{11}B, ^{11}B-{^{1}H}, ^{1}H, ^{1}H-{^{11}B} and ^{1}H-{^{11}B(selective)} techniques. Residual solvent protons were used as reference (δ, ppm, $CDCl_3$, 7.26; CD_2Cl_2, 5.33; CD_3CN, 1.96). ^{11}B chemical shifts are quoted relative to [$BF_3(OEt)_2$)] and ^{31}P chemical shifts are quoted relative to 85% aqueous H_3PO_4. Mass spectrometric data were recorded on a MICROFLEX instrument operating in either positive or negative modes, using matrix-assisted laser desorption ionization (MALDI). A nitrogen laser of 337 nm (photon energy of 3.68 eV) was used for the ionization processes, and the molecules under study were protected with a matrix of *trans*-2-[3-(4-*tert*-Butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB).

The main criteria of purity were clean multinuclear NMR spectra allied with mass spectrometric fragmentation patterns. It should be noted that a well-matched isotope pattern may be taken as a good criterion of identity (see W. Henderson, J. S. McIndoe, *Mass Spectrometry of Inorganic and Organometallic Compounds: Tools TechniquesTips*, John Wiley & Sons, 2005).

Reaction of [8,8-$(PPh_3)_2$-*nido*-8,7-$RhSB_9H_{10}$] (1) with IMe:

A Schlenk tube was loaded, in a dry box, with 25.5 mg (0.12 mmol) of 1,3-dimethylimidazolium iodide and 22.7 mg (0.12 mmol) of potassium

bis(trimethylsilyl)amide (commonly abbreviated as KHMDS). The tube was immersed into an isopropyl bath at -20 ^{o}C, and, then, dry THF was added with a syringe upon the reactants via septum to yield a colourless solution. The reaction mixture was stirred until the bath temperature reached 0 ^{o}C, during this time the colour of the solution changed to bright purple. This solution was filtered with a cannula over 38 mg (0.049 mmol) of **1**, dissolved in THF. After 2 h of vigorous stirring, the colour turned from red to orange. Solvent was evaporated to dryness and the residue re-dissolved in the minimum amount of CH_2Cl_2 to be applied to preparative TLC plated. The chromatogram was developed using CH_2Cl_2 as mobile phase to give red and a yellow bands, which were characterized as [8,8-(IMe)(PPh_3)-*nido*-8,7-$RhSB_9H_{10}$] (**2**) y [8,8-$(IMe)_2$-*nido*-8,7-$RhSB_9H_{10}$] (**3**), respectively.

2 (12mg, 0.019 mmol, 39 %): NMR ^{11}B (96 MHz; CD_2Cl_2; 300 K): δ 16.8 (1B, br, BH), 12.8 (1B, br, BH), 6.2 (2B, d, $^{1}J_{BH}$ = 126 Hz, BH), -1.7 (1B, d, $^{1}J_{BH}$ = 132 Hz, BH), -9.1 (1B, d, $^{1}J_{BH}$ = 137 Hz, BH), -19.0 (1B, d, $^{1}J_{BH}$ = 137 Hz, BH), -22.4 (1B, d, $^{1}J_{BH}$ = 132 Hz, BH), -29.4 (1B, br, BH). NMR ^{1}H-{^{11}B} (500 MHz; CD_2Cl_2; 233K): δ 7.53 (3H, t, H_p-PPh_3), 7.41 (6H, t, H_o-PPh_3), 7.11 (6H, t, H_m-PPh_3), 7.06 (1H, d, $^{3}J_{HH}$ = 1,7 Hz, 2*H*-C=C), 6.70 (1H, d, $^{3}J_{HH}$ = 1,8 Hz, 1*H*-C=C), 4.23 (1H, s, BH), 3.69 (3H, s, 1Me), 3.40 (2H, s, BH), 2.75 (1H, s, BH), 2.70 (3H, s, 1Me), 2.68 (1H, s, BH), 1.87 (1H, s, BH), 1.70 (1H, s, BH), 1.23 (1H, s, BH), -0.83 (1H, s, BHB). NMR ^{31}P-{^{1}H} (202 MHz; CD_2Cl_2; 298 K): δ 20.4 (1P, d, $^{1}J_{P,Rh}$ = 127 Hz, PPh_3). NMR ^{13}C-{^{1}H} (126 MHz; CD_2Cl_2; 233 K): δ 172.4 (1C, dd, $^{2}J_{C,P}$ = 17 Hz, $^{1}J_{C,Rh}$ = 56 Hz, C_q), 133.3 (2C, d, $^{2}J_{C,P}$ = 13 Hz, C_o-PPh_3), 131.4 (1C, d, $^{1}J_{C,P}$ = 40 Hz, C_q-PPh_3), 131.0 (2C, s, C_p-PPh_3), 128.9 (C, d, $^{3}J_{C,P}$ = 10 Hz, C_m-PPh_3), 123.7 (1C, s, H-*C*=C), 122.4 (1C, s, H-*C*=C), 37.9 (1C, s, Me), 37.6 (1C, s, Me).

3 (10 mg; 0.024 mmol; 50 %): NMR ^{11}B (128 MHz; CD_2Cl_2; 300 K): δ 15.9 (1B, d, $^1J_{BH}$ = 142 Hz, BH), 10.5 (1B, d, $^1J_{BH}$ = 133 Hz, BH), 3.7 (2B, d, $^1J_{BH}$ = 146 Hz, BH), -4.3 (1B, d, $^1J_{BH}$ = 105 Hz, BH), -7.7 (1B, d, $^1J_{BH}$ = 122 Hz, BH), -23.6 (1B, d, $^1J_{BH}$ = 149 Hz, BH), -25.7 (1B, d, $^1J_{BH}$ = 136 Hz, BH), -28.5 (1B, d, $^1J_{BH}$ = 113 Hz, BH). NMR ^{1}H-{^{11}B} (400 MHz; CD_2Cl_2; 298 K): δ 7.00 (1H, s, *H*-C=C, IMe_A), 6.98 (2H, s br, *H*-C=C, IMe_B), 6.87 (1H, s, *H*-C=C, IMe_A), 4.05 (1B, s, BH), 3.93 (3H, s, Me, IMe_A), 3.46 (6H, s br, Me, IMe_B), 3.32 (1B, s, BH), 3.29 (3H, s, Me, IMe_A), 3.19 (1B, s, BH), 2.93 (1B, s, BH), 2.34 (1H, s, BH), 1.94 (1B, s, BH), 1.39 (1B, s, BH), 1.34 (1B, s, BH), 1.00 (1B, s, BH), -0.48 (1H, s, BHB). ^{1}H-{^{11}B} (400 MHz; CD_2Cl_2; 198 K): δ 7.05 (1H, d, $^3J_{HH}$ = 1.8 Hz, *H*-C=C, IMe_B), 7.03 (1H, d, $^3J_{HH}$ = 1.4 Hz, *H*-C=C, IMe_A), 6.96 (1H, d, $^3J_{HH}$ = 1.8 Hz, *H*-C=C, IMe_B), 6.90 (1H, d, $^3J_{HH}$ = 1.4 Hz, *H*-C=C, IMe_A), 3.88 (3H, s, Me, IMe_A), 3.78 (3H, s, Me, IMe_B), 3.20 (3H, s, Me, IMe_A), 3.02 (3H, s, Me, IMe_B). [^{1}H-^{13}C]-HMBC (126 MHz; CD_2Cl_2; 298 K): δ 179.0 (1C, m, C_q, IMe_B), 174.6 (1C, m, C_q, IMe_A), 123.3 (1C, s, H-*C*=C, IMe_B), 122.9 (1C, s, H-*C*=C, IMe_B), 121.9 (1C, s, H-*C*=C, IMe_A), 120.8 (1C, s, H-*C*=C, IMe_A), 37.8 (3H, s, Me, IMe_B), 37.3 (3H, s, Me, IMe_B), 37.0 (3H, s, Me, IMe_A), 35.6 (3H, s, Me, IMe_A). LRMS (MALDI$^-$/DCTB): *m/z* calcd maximum for [M-(Me + 2H)]$^+$ $C_9H_{21}N_4RhSB_9$, 418; obsd, 418. The mass envelope for the measured masses for **3** matches that calculated from the known isotopic abundances of the constituent elements.

X-ray analysis of compound 2: A single crystal of **2** was analyzed by X-ray diffraction (Figure 1). A static disorder was observed in the thiaborane fragment that was modelled with two sets of positions with equal complementary occupancy factors. The structure illustrated in Figure 1 corresponds to the one of the clusters with 50 % of occupancy, which exhibits a typical 11-vertex *nido*-shape. It is noteworthy that the carbene ligand lies *trans* to the sulphur vertex, which has a

weaker *trans* influence than the cage boron atoms.{McAnaw, 2013 #3437} Thus, the *exo*-polyhedral ligand orientation appears to be controlled by the sulphur atom in the *tetrahapto* face of the $\{SB_9H_{10}\}$ fragment with the ligand that has the stronger *trans* influence (i. e. IMe) lying effectively *trans* to the cage S atom.

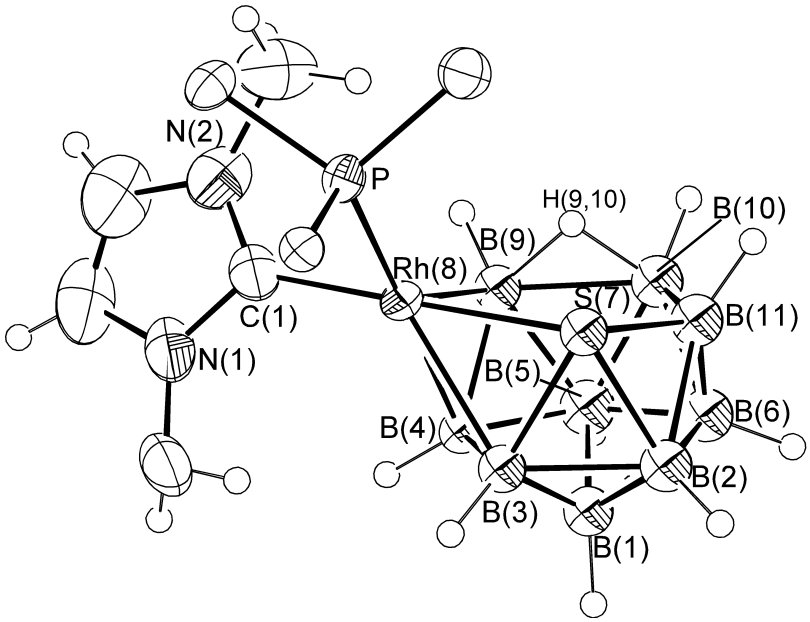

Fig. S1 Molecular structure of **2**. Only the *ipso*-carbon atoms are included to aid clarity. Ellipsoids are shown at 50 % probability levels. Selected interatomic distances (Å) and angles (º): Rh(8)-S(7) 2.523(3), Rh(8)-B(3) 2.294(10), Rh(8)-B(4) 2.133(9), Rh(8)-B(9) 2.122(13), Rh(8)-P(1) 2.3644(13), Rh(8)-C(1) 2.015(4), S(7)-Rh(8)-B(9) 92.0(3), S(7)-Rh(8)-P(1) 82.27(7), P(1)-Rh(8)-B(3) 117.3(3), P(1)-Rh(8)-B(4) 166.2(3), P(1)-Rh(8)-C(1) 93.42(10), C(1)-Rh(8)-B(9) 92.2(4). CCDC934329.

Reaction of 2 with pyridine

A Schlenk flask was charged with **2** (30 mg, 0.048 mmol) and 15 mL of dry CH_2Cl_2. Then, degassed pyridine (19.4 μL, 19 mg; 0.24 mmol) was added to the solution under an atmosphere of argon. The reaction mixture was stirred for 12 h. The solvent was evaporated under reduced pressure and the residue was washed with

hexane. The final product was characterized as [1,1-(IMe)(PPh_3)-3-(NC_5H_5)-*isonido*-1,2-$RhSB_9H_8$] (**4**) (23.42 mg; 0.035 mmol; 72 %): ^{11}B-{^{1}H} NMR (96 MHz; CD_2Cl_2, 298 K): δ 52.5 (1B, s, B-Py), 24.2 (1B, d, $^1J_{B,H}$ = 125 Hz, BH), -2.6 (2B, br, BH), -15,5 (2B, br, BH), -27.7 (1B, d, $^1J_{B,H}$ = 102 Hz, BH), -32.6 (2B, d, $^1J_{B,H}$ = 136 Hz, BH). ^{1}H-{^{11}B} NMR (500 MHz, CD_2Cl_2, 300 K): δ 8.86 (2H, d, $^3J_{H,H}$ = 5.3 Hz, H_o-NC_5H_5), 7.99 (1H, t, $^3J_{H,H}$ = 7.6 Hz, H_p-NC_5H_5), 7.36 (2H, m, H_m-NC_5H_5), 7.32 to 7.18 (15H, m, PPh_3), 6.38 (2H, s, *H*-C=C, IMe), 4.13 (1B, s, BH), 3.41 (6H, s, $2CH_3$, IMe), 2.37 (2H, s, BH), 1.85 (2H, s, BH), -0,01 (1H, s, BH), -0,14 (2H, s, BH). ^{1}H-{^{11}B} NMR (400 MHz, CD_2Cl_2, 198 K): δ 8.58 (2H, s-br, H_o-NC_5H_5), 8.02 (1H, t, $^3J_{H,H}$ = 7,2 Hz, H_p-NC_5H_5), 7.38 (2H, t, $^3J_{H,H}$ = 6.5 Hz, H_m-NC_5H_5), 7.29 a 7.15 (15H, m, PPh_3), 6.36 (1H, s, *H*-C=C, IMe), 6.30 (1H, s, *H*-C=C, IMe), 3.98 (1H, s, BH), 3.65 (3H, s, Me, IMe), 2.91 (3H, s, Me, IMe), 2.33 (1H, s, BH), 2.20 (1H, s, BH), 1.25 (1H, s, BH), 0.30 (1H, s, BH), -0.28 (1H, s, BH), -0.40 (1H, s, BH), -0.59 (1H, s, BH). RMN ^{31}P-{^{1}H} (121 MHz, CD_2Cl_2, 298 K): δ 35.6 (1P, d, $^1J_{P,Rh}$ = 158 Hz, PPh_3). NMR ^{13}C (126 MHz; CD_2Cl_2; 193 K): δ 176.1 (1C, dd, $^2J_{C,P}$ = 15.7 Hz, $^1J_{CRh}$ = 65.7 Hz, C_q), 146.1 (2C, s, C_o-NC_5H_5), 140.6 (1C, s, C_p-NC_5H_5), 137.4 (3C, d, $^1J_{C,P}$ = 37 Hz, C_q-PPh_3), 132.6 (6C, d, $^2J_{C,P}$ = 11 Hz, C_o-PPh_3), 129.1 (3C, s, C_p-PPh_3), 127.9 (6C, d, $^3J_{C,P}$ = 8.8 Hz, C_m-PPh_3), 126.0 (6C, s, C_m-NC_5H_5), 122.1 (1C, s, H-C=C, IMe), 121.6 (1C, s, H-C=C, IMe), 39.9 (3C, s, Me, IMe), 39.2 (3C, Me, IMe). LRMS (MALDI$^-$/DIT): *m/z* calcd maximum for M^+, $B_9C_{28}H_{36}N_3PRhS$, 678; obsd 678. Calcd maximum for $[M - PPh_3]^+$ $B_9C_{10}H_{21}N_3RhS$, 416 ; obsd. The mass envelope for the measured masses for **4** matches that calculated from the known isotopic abundances of the constituent elements.

X-ray analysis of compound 4:

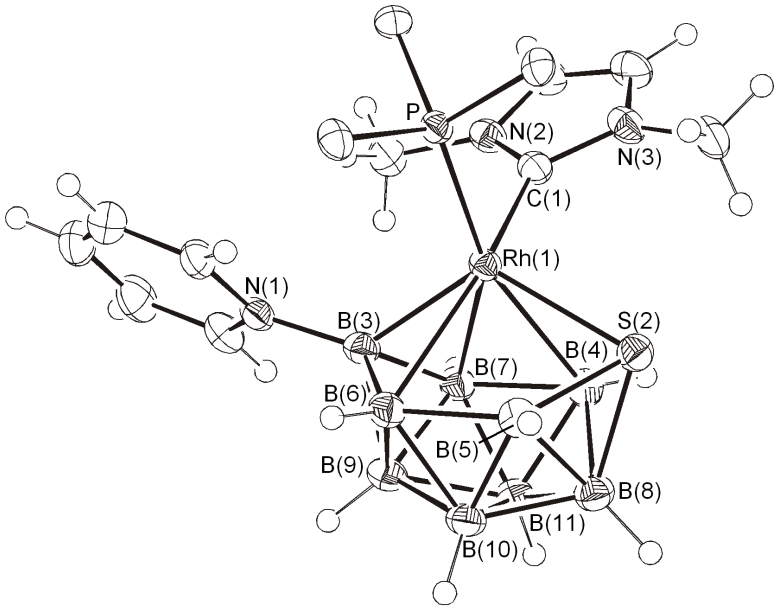

Fig. S2 Molecular structure of **4**. Only the ipso-carbon atoms are included to aid clarity. Ellipsoids are shown at 50 % probability levels. Selected interatomic distances (Å) and angles (º): Rh(1)-S(2) 2.3893(12), Rh(1)-B(3) 2.058(4), Rh(1)-B(5) 2.544(5), Rh(1)-B(4) 2.346(5), Rh(1)-B(7) 2.312(5), Rh(1)-P(1) 2.2798(11), Rh(1)-C(1) 2.018(4), S(2)-Rh(1)-B(3) 119.00(12), C(1)-Rh(1)-P(1) 88.72(11), P(1)-Rh(1)-B(3) 110.93(12), C(1)-Rh(1)-B(3) 114.75(16), P(1)-Rh(1)-S(2) 114.10(4), C(1)-Rh(1)-S(2) 105.30(11). CCDC934330.

The structure of **4** resembles a typical 11-vertex *closo*-cage based on a canonical octadodecahedron, however the cage is quite distorted in the vicinity of the {Rh(1)S(2)B(5)B(6)} face with a Rh(1)–B(5) distance of 2.544(5) Å. A bonding distance would be of the order 2.4 to 2.5 Å, therefore in **4** the Rh(1)–B(5) length lies just on the upper part of the non-bonding limit that leads to the generation a quadrilateral *isonido* open-face.

Reaction of [1,1-(IMe)(PPh$_3$)-3-(NC$_5$H$_5$)-*isonido*-1,3-RhSB$_9$H$_8$] (4) with H$_2$(g):

A quick pressure valve NMR tube was charged with **4** (3 mg, 0.0044 mmol) and 0.3 mL of CD_2Cl_2. The tube was immersed into liquid nitrogen and the system was evacuated under vacuum. Then, the solution was espoused to a H_2 atmosphere of 10 bar. The colour of the solution changed instantaneously from red to yellow. The system was studied by NMR spectroscopy, demonstrating that compound **4** reacts with H_2 to give a new hydridorhodathiaborane, characterized as [8,8,8-(H)(IMe)(PPh_3)-9-(NC_5N_5)-*nido*-8,7-$RhSB_9H_9$] (**5**). The simple opening of the NMR tube and the consequent release of hydrogen lead to the formation of the parent *isonido*-cluster, **4**, showing that the reaction is reversible, which has precluded so far the isolation of **5**. Thus, this labile compound was characterized *in situ* under an atmosphere of H_2.

NMR ^{11}B-{^1H} (96 MHz; CD_2Cl_2, 298 K): δ 9.5 (1B, s, B-Py), 4.1 (1B, br, BH), -9.2 (1B, br, BH), -12.1 (2B, br, BH), -19.0 (1B, br, BH), -27.5 (1B, br, BH), -31.2 (2B, br, BH). RMN ^1H-{^{11}B} (500 MHz, CD_2Cl_2, 273 K): δ 8.32 (2H, d, $^3J_{H,H}$ = 8.7 Hz, H_o-NC_5H_5), 7.89 (1H, t, $^3J_{H,H}$ = 7.4 Hz, H_p-NC_5H_5), 7.30 (2H, t, $^3J_{H,H}$ = 7.2 Hz, H_m-NC_5H_5), 7.5 a 7.0 (15H, m, PPh_3), 7.03 (1H, s, *H*-C=C, IMe), 6.59 (1H, s, *H*-C=C, IMe), 3.96 (1H, s, BH), 3.70 (3H, s, CH_3, IMe), 3.46 (1H, s, BH), 2.40 (1H, s, BH), 2.30 (1H, s, BH), 1.49 (3H, s, CH_3, IMe), 1.45 (1H, s, BH), 1.17 (1H, s, BH), 1.05 (1H, s, BH), -0.07 (1H, s, BHB), -12.26 (1H, t, -12.67, $^1J_{H,Rh}$ = 22.9 Hz, RhH, minor conformer), -12.67 (1H, dd, $^1J_{H,Rh}$ = 23.8 Hz, $^2J_{H,P}$ = 5.4 Hz, RhH, major conformer). ^{31}P-{^1H} (121 MHz, CD_2Cl_2, 183 K): δ 31.3 (1P, d, $^1J_{P,Rh}$ = 99 Hz, PPh_3, minor conformer), 31.3 (1P, d, $^1J_{P,Rh}$ = 99 Hz, PPh_3, major conformer). [^1H-^{13}C]-HMQC (126 MHz; CD_2Cl_2; 183 K): δ 177.7 (1C, C_q), 127 (C, PPh_3), 134 (C, PPh_3), 124.2 (1C, H-*C*=C, IMe), 122 (1C, H-*C*=C, IMe), 40.6 (1C, CH_3, IMe), 36.1 (1C, CH_3, IMe).

With the same amount of rhodathiaborane **4** as above, the quick pressure valve NMR tube was espoused to 6 bar of H_2. And the system was studied by variable temperature NMR (Figures S1 and S2).

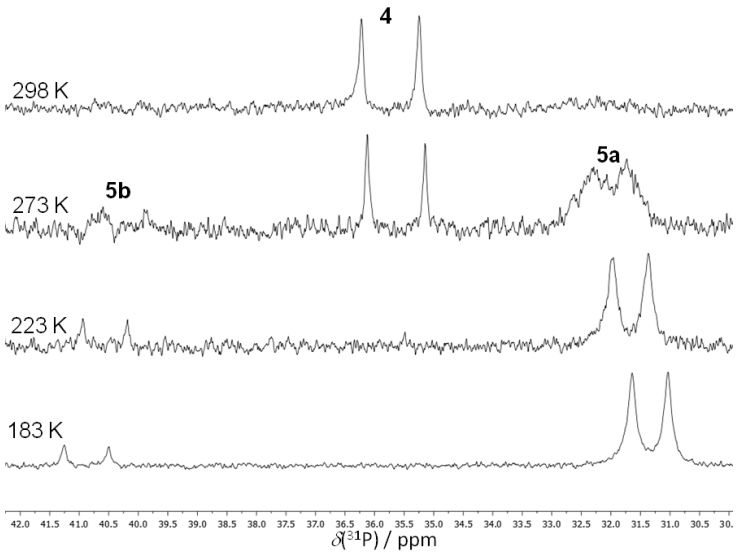

Fig. S3 VT ^{31}P-{^{1}H} NMR spectra of **4** under a 6 bar atmosphere of H_2

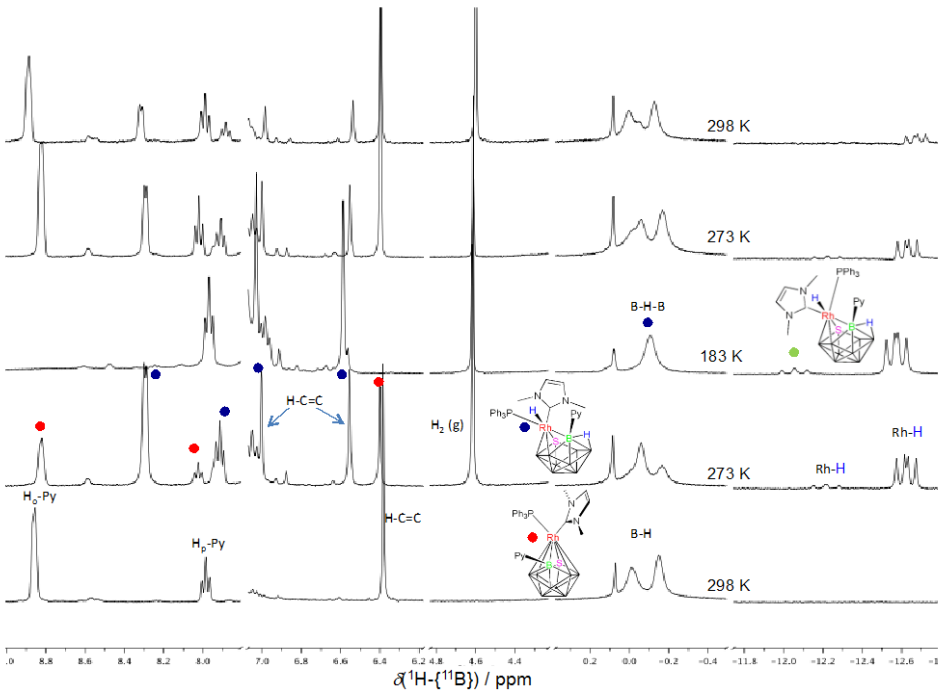

Fig. S4. VT ^{1}H NMR spectra of **4** under a 6 bar atmosphere of H_2, illustrating the H_2-driven equilibrium between **5** and **4**. The bottom trace corresponds to the spectrum of the isonido-cluster in the absence of H_2.

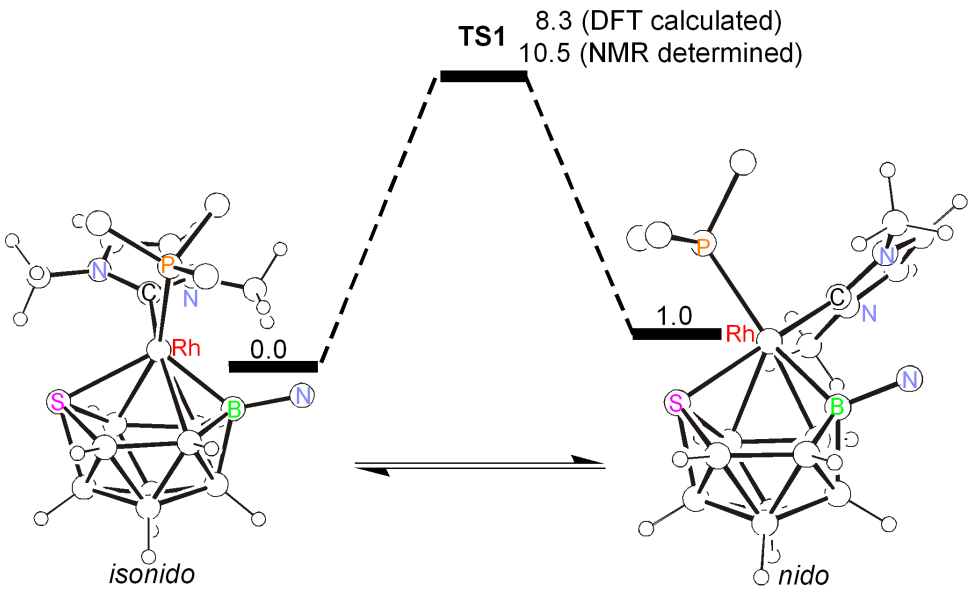

Fig. S5. Proposed *isonido*↔*nido* equilibirum, showing the DFT-calculated relative free energies, ΔG_{253} (kcal/mol). The NMR-determined activation energy, $\Delta G^{\ddagger}_{253}$, was measured at the coalesce temperature.

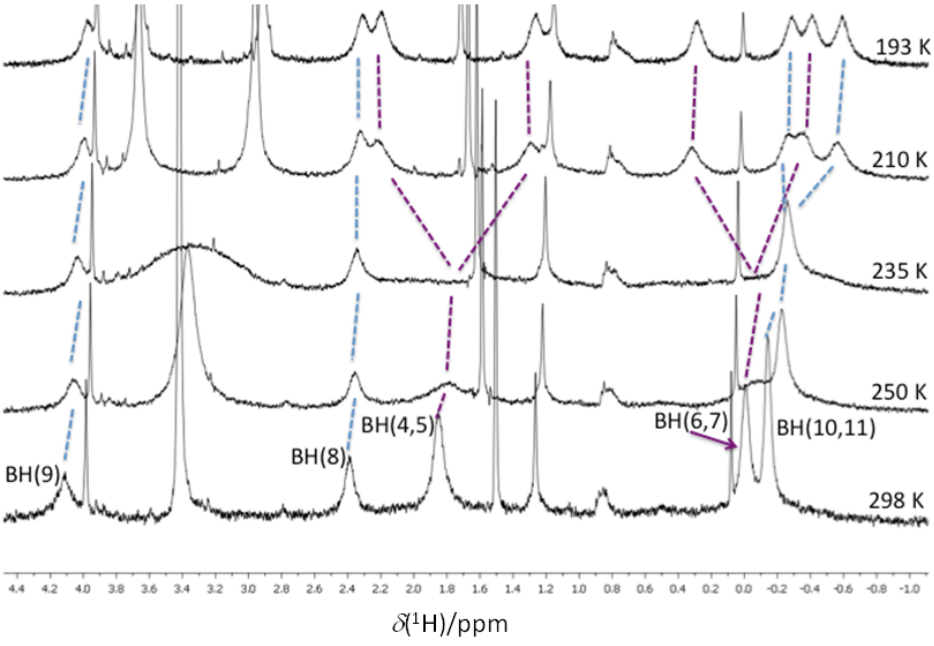

Fig. S6. ^{1}H-{^{11}B} NMR spectra of carbene-ligated rhodathiaborane, **4**, at different temperatures. The measured $\Delta G^{\ddagger}$ at the coalescence temperature of 253 K is 10.5 kcal/mol.

Reaction of [1,1-(IMe)(PPh_3)-3-(NC_5H_5)-*isonido*-1,3-$RhSB_9H_8$] (4) with D_2(g): A quick pressure valve NMR tube was charged with 4.0 mg (0.0058 mmol) of **4** and 0.3 mL of CD_2Cl_2. The tube was espoused to 1.7 bar of D_2 at room temperature. The system was studied by NMR spectroscopy. ^{11}B and ^{31}P-{^1H} NMR spectra correspond to cluster **5**. However, the ^1H-{^{11}B} was devoid of the resonances due to the B-H-B bridging hydrogen atom and the Rh-H hydride ligand, maintaining the B-H terminal hydrogen resonances.

Reaction of [1,1-(IMe)(PPh_3)-3-(NC_5H_5)-*isonido*-1,3-$RhSB_9H_8$] (4) with $H_2C{=}CH_2$(g): A quick pressure valve NMR tube was charged with 2.8 mg (0.0041 mmol) of **4** and 0.3 mL of CD_2Cl_2. The tube was immersed in liquid N_2 and evacuated. Then, the system was espoused to 1 bar of ethylene at room temperature. This reaction system was cooled to the temperature of liquid N_2 and subjected to dynamic vacuum; then, the tube was espoused to 5 bar H_2 atmosphere. The reaction was studied by NMR spectroscopy, demonstrating formation of ethane (δ_H = +0.85 ppm) as a function of time, obtaining a conversion of 73 % after 12 h. The experiments are illustrated

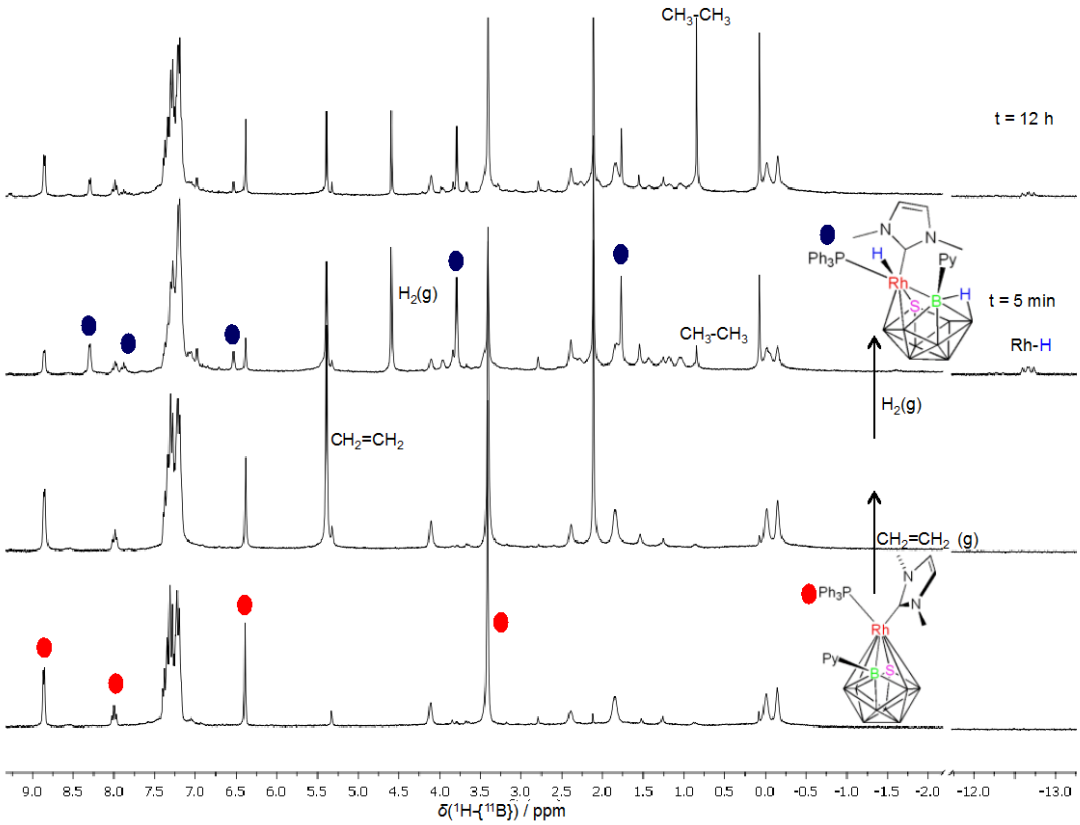

Fig. S7. ^{1}H NMR spectra of **4** (bottom trace), **4** espoused to an atmosphere of C_2H_4 (second trace from the bottom), **4** with C_2H_4 and an atmosphere of H_2 (third trace from the bottom and upper trace)

Reaction of [1,1-(IMe)(PPh$_3$)-3-(NC$_5$H$_5$)-*isonido*-1,3-RhSB$_9$H$_8$] (4) with CH$_3$CH$_2$CH$_2$CH$_2$CH=CH$_2$: The reaction was carried out in a pressure glass reactor (20 mL capacity), under an H_2 atmosphere of 6 bar. The conditions were as follow: 3 mg (0,0044 mmol) of the carbene-ligated rhodathiaborane, **4**, dissolved in 10 mL of CH_2Cl_2, room temperature. To the solution of the catalyst, 0,6 µL of 1-hexene were added. The conversion was determined by GC. The results are gathered in the following Table

Table S1 Hydrogenation results for 1-hexene

time(h)	substrate	% conversion	TOF (h^{-1})	% hydrogenation / isomerization
5	1-hexene	69	14	51/18

Computational details

The geometry of all structures has been optimized with the G09 program package[1] at the DFT level using the B3LYP approximation[2] combined with the def2-SVP basis set for all atoms[3] and pseudo-potentials[4] for Rh. The nature of the stationary points has been confirmed by frequency analysis and intrinsic reaction paths have been traced connecting the transition structures with the respective minima.

References for the computational study

[1] Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski,

G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

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[4] K. A. Peterson, D. Figgen, E. Goll, H. Stoll, M. Dolg, *J. Chem. Phys..* **2003**, *119*, 11113-11123.

Total energies and Cartesian coordinates (in Å) of calculated structures

Compound 4 (E=-2325.64114259 a.u.)

Atomic number	X	Y	Z
45	-0.596939	-1.011016	-0.233900
5	-3.333947	-2.662477	-1.379185
5	-2.405068	-0.022498	-0.586379
5	-1.831859	-3.030394	-0.520755
5	-2.862713	-1.587681	-0.014628
5	-1.040224	-1.743136	-2.879941
5	-1.968036	-0.296415	-2.216665
5	-2.065217	-3.270484	-2.413454
5	-3.557041	-0.914828	-1.527495
5	-2.796769	-1.754135	-2.881804
16	-0.222174	-2.993260	-1.692096
6	-0.103795	-1.714276	1.632408
6	0.658304	-3.001978	3.350715
6	-0.208852	-2.100112	3.874505
7	0.721897	-2.750112	1.988830
7	-0.656891	-1.321624	2.821277
6	-1.604429	-0.237904	3.005904
6	1.525739	-3.564530	1.089930
1	-4.301738	-3.375618	-1.298499
1	-1.744353	-3.958025	0.242458
1	-3.437608	-1.759276	1.039228
1	-0.416438	-1.607293	-3.901286
1	-1.879177	0.660129	-2.954978
1	-2.139239	-4.308911	-3.007957
1	-4.650688	-0.416707	-1.663121
1	-3.370016	-1.708565	-3.940535
1	1.233655	-3.793955	3.821713
1	-0.538762	-1.940216	4.896980
1	-1.642805	0.331741	2.073894
1	-2.604675	-0.636955	3.229403

1	-1.267822	0.411559	3.826793
1	1.968599	-2.937328	0.310257
1	2.332394	-4.035690	1.668205
1	0.915582	-4.346748	0.615745
15	1.188539	0.525788	-0.185402
7	-2.925014	1.348890	-0.082109
6	-3.952058	1.405749	0.799786
6	-2.397235	2.504169	-0.553532
6	-4.459161	2.616219	1.256252
1	-4.349592	0.440978	1.114880
6	-2.865598	3.743847	-0.141786
1	-1.590602	2.390885	-1.276978
6	-3.913418	3.811644	0.783295
1	-5.287468	2.610562	1.966847
1	-2.411228	4.645073	-0.556603
1	-4.300693	4.775578	1.120701
6	1.373748	1.291064	1.497836
6	0.565678	2.379169	1.875948
6	2.197785	0.708928	2.477002
6	0.604809	2.888923	3.176250
1	-0.103519	2.838815	1.146229
6	2.229733	1.211083	3.781907
1	2.824255	-0.148497	2.224248
6	1.439275	2.307710	4.136485
1	-0.023466	3.743899	3.440299
1	2.881143	0.741403	4.523552
1	1.472274	2.706550	5.153585
6	1.213574	1.989515	-1.344948
6	0.814069	1.765105	-2.673739
6	1.706149	3.259900	-0.995572
6	0.886822	2.789541	-3.622703
1	0.435175	0.786471	-2.970263
6	1.769253	4.285191	-1.944368
1	2.052375	3.458821	0.019745
6	1.357097	4.054625	-3.260352
1	0.567166	2.593029	-4.649054
1	2.151509	5.267247	-1.652655
1	1.408473	4.856609	-4.001413
6	2.919763	-0.078887	-0.564719
6	4.071525	0.624900	-0.168124
6	3.073390	-1.211692	-1.377682
6	5.340899	0.189531	-0.554644
1	3.982740	1.524660	0.444130
6	4.344749	-1.641775	-1.775451
1	2.187718	-1.753818	-1.714553
6	5.481912	-0.946571	-1.359381
1	6.225041	0.746057	-0.232262
1	4.440908	-2.523165	-2.414669
1	6.475893	-1.282623	-1.665792

TS1 (E=-2325.62941558 a.u.)

Atomic number	**X**	**Y**	**Z**
45	-0.507525	-0.599080	-0.672295
5	-2.211086	-3.917686	0.117366
5	-2.385469	-1.089484	0.282280

5	-0.561521	-3.387567	0.464017
5	-2.002842	-2.487507	1.140997
5	-1.174199	-2.469882	-2.183096
5	-2.536440	-1.504538	-1.412646
5	-1.067048	-4.097991	-1.211483
5	-3.275921	-2.542842	-0.137392
5	-2.586836	-3.304675	-1.577271
16	0.430784	-2.796730	-1.126009
6	-1.091485	1.205434	-1.271689
6	-1.756279	3.385417	-1.426896
6	-1.728442	2.878068	-2.685462
7	-1.370932	2.360459	-0.575409
7	-1.318090	1.559390	-2.580493
6	-1.133473	0.687908	-3.732304
6	-1.231519	2.552425	0.856093
1	-2.609925	-4.956307	0.581589
1	0.201073	-3.949388	1.207495
1	-2.223960	-2.659286	2.324152
1	-0.920990	-2.414385	-3.357987
1	-3.224110	-0.876750	-2.191439
1	-0.690937	-5.139199	-1.672497
1	-4.466602	-2.566257	0.069915
1	-3.320563	-3.834214	-2.372868
1	-2.000800	4.380441	-1.065944
1	-1.955700	3.340580	-3.642072
1	-0.331860	-0.026960	-3.513511
1	-2.045863	0.114293	-3.945644
1	-0.864198	1.301168	-4.603985
1	-0.437976	3.283140	1.069790
1	-2.177551	2.913169	1.287848
1	-0.963639	1.593499	1.310475
15	1.577739	0.205935	0.227824
7	-3.333728	-0.001761	0.922188
6	-3.450415	0.081018	2.266224
6	-4.096592	0.800002	0.146842
6	-4.316080	0.980287	2.875974
1	-2.837574	-0.626034	2.825183
6	-4.982353	1.722573	0.691776
1	-3.981218	0.653304	-0.926740
6	-5.098024	1.822595	2.080329
1	-4.379226	1.004773	3.965112
1	-5.581740	2.343345	0.023800
1	-5.791930	2.534194	2.533922
6	3.116710	-0.713203	-0.286538
6	4.041649	-0.218790	-1.219441
6	3.324504	-1.997836	0.251246
6	5.145397	-0.987749	-1.604712
1	3.918430	0.776717	-1.647351
6	4.427755	-2.761638	-0.133742
1	2.623660	-2.407595	0.981964
6	5.342423	-2.260397	-1.064974
1	5.856629	-0.582059	-2.329124
1	4.568551	-3.756827	0.295336
1	6.204786	-2.859864	-1.367481
6	2.024653	1.972550	-0.154044
6	1.953156	2.388083	-1.497483
6	2.395209	2.920017	0.814667

6	2.266691	3.699053	-1.863699
1	1.642354	1.677094	-2.266223
6	2.697531	4.237063	0.449354
1	2.445504	2.638332	1.866973
6	2.640362	4.630464	-0.889569
1	2.212155	3.995174	-2.914418
1	2.983530	4.957027	1.220837
1	2.882152	5.657940	-1.173265
6	1.735752	0.070892	2.073822
6	0.629114	-0.335197	2.832980
6	2.958791	0.311320	2.729658
6	0.731885	-0.472300	4.222590
1	-0.301345	-0.592057	2.320841
6	3.057069	0.182715	4.116138
1	3.845199	0.585473	2.152868
6	1.940913	-0.205582	4.867134
1	-0.134663	-0.809003	4.797361
1	4.012430	0.373550	4.612038
1	2.022564	-0.316673	5.951581

4' (E = -2325.63821100 a.u.)

Atomic number	**X**	**Y**	**Z**
45	0.543950	-0.517925	-0.558240
5	2.651577	-3.047941	-1.780429
5	2.636771	-0.980649	0.184722
5	1.041846	-2.386407	-1.832610
5	2.469064	-1.274119	-1.532912
5	1.505111	-3.519147	0.851013
5	2.896416	-2.421544	1.034300
5	1.417864	-4.006110	-0.963389
5	3.654489	-2.212849	-0.579796
5	2.962711	-3.760679	-0.116950
16	-0.010159	-2.865080	-0.171341
6	0.942179	1.356257	-1.180042
6	1.252137	3.102631	-2.607960
6	1.409422	3.581376	-1.347073
7	0.962570	1.752354	-2.492640
7	1.214883	2.509047	-0.488045
6	1.223943	2.648292	0.957338
6	0.698441	0.895812	-3.641313
1	3.111731	-3.485667	-2.804786
1	0.342437	-2.398062	-2.815688
1	2.868191	-0.562638	-2.429577
1	1.124906	-4.279879	1.704172
1	3.586323	-2.499488	2.032043
1	0.968180	-5.045695	-1.358645
1	4.837544	-2.018824	-0.743122
1	3.637453	-4.743901	0.063215
1	1.318617	3.601239	-3.571256
1	1.630085	4.582505	-0.987402
1	1.013397	1.668718	1.400413
1	2.205321	3.005386	1.303569
1	0.448666	3.360077	1.275832
1	-0.078319	1.353732	-4.272496
1	1.613400	0.746306	-4.232168

1	0.355170	-0.078923	-3.279679
15	-1.683020	0.056378	0.228422
7	3.470782	0.251319	0.721072
6	4.152981	1.047306	-0.129685
6	3.619453	0.425794	2.052163
6	5.004180	2.048124	0.326078
1	4.000014	0.833836	-1.187784
6	4.448650	1.411044	2.575337
1	3.069715	-0.280391	2.673890
6	5.159902	2.237485	1.701373
1	5.545454	2.658953	-0.398217
1	4.544015	1.509650	3.657879
1	5.830667	3.009661	2.085712
6	-3.037805	-0.312396	-0.987396
6	-4.278126	0.352169	-0.960732
6	-2.822253	-1.300849	-1.963138
6	-5.278269	0.028615	-1.881770
1	-4.466910	1.134357	-0.222629
6	-3.826081	-1.624724	-2.880942
1	-1.864536	-1.821082	-2.009527
6	-5.055578	-0.961982	-2.843248
1	-6.235821	0.554979	-1.847231
1	-3.639304	-2.398090	-3.630102
1	-5.838274	-1.213557	-3.563622
6	-2.067255	1.817697	0.677639
6	-2.061465	2.793089	-0.337069
6	-2.302668	2.227350	2.000114
6	-2.288395	4.137568	-0.037992
1	-1.884240	2.499006	-1.374768
6	-2.523877	3.576720	2.300495
1	-2.318351	1.489925	2.804679
6	-2.517061	4.535953	1.284833
1	-2.287069	4.878278	-0.841896
1	-2.709838	3.875120	3.335648
1	-2.696142	5.588379	1.519532
6	-2.164395	-0.866540	1.760343
6	-3.495435	-1.190933	2.071773
6	-1.145184	-1.243461	2.651470
6	-3.799547	-1.866460	3.256734
1	-4.301718	-0.928339	1.384532
6	-1.452733	-1.913938	3.838825
1	-0.101708	-1.039793	2.397111
6	-2.780201	-2.225683	4.144226
1	-4.838460	-2.120427	3.482655
1	-0.647206	-2.211912	4.514277
1	-3.019931	-2.760955	5.066623

TS2 (E= -2326.79704537 a.u.)

Atomic number	**X**	**Y**	**Z**
5	-2.286106	-2.992436	1.942830
5	-2.833097	-1.115700	-0.124558
5	-0.742649	-2.270914	1.568571
5	-2.263971	-1.248373	1.524403
5	-1.792187	-3.688193	-0.838350
5	-3.221987	-2.643930	-0.779729

5	-1.248250	-3.981029	0.917259
5	-3.585770	-2.301103	0.942873
5	-2.958584	-3.867882	0.473488
16	-0.126839	-2.843865	-0.290455
6	-0.967019	1.367490	0.865050
6	-1.522672	3.557126	1.193177
6	-1.102832	3.060185	2.384403
7	-1.434663	2.518612	0.277894
7	-0.762417	1.735180	2.170101
6	-0.232267	0.891819	3.234875
6	-1.694648	2.723708	-1.136695
1	-2.464205	-3.350658	3.080112
1	-2.496821	-0.472386	2.422848
1	-1.566432	-4.538933	-1.662073
1	-4.139764	-2.809409	-1.560759
1	-0.639610	-4.948865	1.281805
1	-4.701925	-2.103736	1.367756
1	-3.603766	-4.882848	0.569604
1	-1.871119	4.548319	0.916468
1	-1.021215	3.528305	3.361629
1	0.696203	1.332760	3.628264
1	-0.969165	0.797863	4.044841
1	-0.024638	-0.101523	2.829380
1	-0.884971	3.313818	-1.593946
1	-1.749793	1.755555	-1.638703
1	-2.648422	3.255507	-1.268412
7	-3.823389	0.052128	-0.538143
6	-4.333493	0.893984	0.386209
6	-4.259722	0.132623	-1.814195
6	-5.285373	1.853614	0.059170
1	-3.957942	0.753157	1.399763
6	-5.202539	1.073889	-2.211203
1	-3.839956	-0.609446	-2.493426
6	-5.730188	1.952118	-1.261420
1	-5.677038	2.504663	0.842497
1	-5.526789	1.098013	-3.252857
1	-6.482961	2.692239	-1.543283
45	-0.628264	-0.505626	0.082719
15	1.804434	0.085189	-0.205805
6	2.916519	0.035264	1.278818
6	3.869009	1.022357	1.586070
6	2.819110	-1.092582	2.114141
6	4.691256	0.890986	2.710633
1	3.983628	1.897698	0.945391
6	3.649099	-1.225715	3.229794
1	2.086961	-1.871477	1.895849
6	4.583827	-0.231531	3.535827
1	5.425195	1.669528	2.935378
1	3.557823	-2.110801	3.864287
1	5.228428	-0.333340	4.412680
6	2.058430	1.796515	-0.889681
6	2.414577	2.007902	-2.232914
6	1.803850	2.922691	-0.083542
6	2.512429	3.302978	-2.753598
1	2.623830	1.156806	-2.882823
6	1.915167	4.215601	-0.600525
1	1.525017	2.795429	0.964105

6	2.266143	4.411935	-1.940944
1	2.793198	3.441370	-3.800967
1	1.725765	5.073833	0.049680
1	2.352796	5.423393	-2.346042
6	2.753958	-0.954797	-1.419384
6	4.142650	-1.141234	-1.304823
6	2.080704	-1.555792	-2.496277
6	4.837844	-1.904158	-2.246581
1	4.689227	-0.693267	-0.473330
6	2.778343	-2.314342	-3.440927
1	1.000356	-1.445885	-2.596262
6	4.158450	-2.492043	-3.317669
1	5.916706	-2.042774	-2.138331
1	2.234077	-2.779911	-4.266218
1	4.702632	-3.094474	-4.049530
1	0.134056	-2.254361	2.390534
1	-1.253563	-0.435466	-1.733067
1	-0.638398	0.021302	-1.960473

INT1 (E = -2326.79707167 a.u.)

Atomic number	**X**	**Y**	**Z**
5	-2.261342	-2.982892	1.958604
5	-2.835538	-1.119470	-0.116958
5	-0.724834	-2.259147	1.560942
5	-2.246684	-1.241795	1.529844
5	-1.803634	-3.696626	-0.825194
5	-3.232141	-2.654861	-0.755479
5	-1.235397	-3.974895	0.925142
5	-3.573259	-2.298713	0.968733
5	-2.951228	-3.868667	0.504469
16	-0.135477	-2.840113	-0.307434
6	-0.969757	1.372563	0.845148
6	-1.529592	3.560790	1.174373
6	-1.100106	3.066587	2.363270
7	-1.444862	2.521442	0.259889
7	-0.757289	1.742363	2.148309
6	-0.215982	0.903966	3.211690
6	-1.713904	2.725400	-1.153329
1	-2.424350	-3.334693	3.100160
1	-2.473126	-0.461146	2.425537
1	-1.585077	-4.555641	-1.642371
1	-4.162016	-2.826112	-1.521058
1	-0.616865	-4.937264	1.287671
1	-4.684114	-2.096510	1.405242
1	-3.593463	-4.883787	0.617689
1	-1.883142	4.550513	0.898926
1	-1.013218	3.536109	3.339363
1	0.717224	1.346254	3.592164
1	-0.944058	0.816080	4.030191
1	-0.013884	-0.092180	2.810494
1	-0.899632	3.302022	-1.619694
1	-1.788228	1.756786	-1.651804
1	-2.660709	3.271018	-1.277851

7	-3.837354	0.042278	-0.522665
6	-4.339350	0.886760	0.403563
6	-4.290496	0.113918	-1.793347
6	-5.299169	1.840945	0.083531
1	-3.950803	0.752834	1.413143
6	-5.242261	1.049059	-2.183347
1	-3.876180	-0.630217	-2.473770
6	-5.761239	1.930484	-1.231694
1	-5.683499	2.494581	0.868345
1	-5.580099	1.065996	-3.220818
1	-6.520626	2.665969	-1.507882
45	-0.633877	-0.501920	0.056684
15	1.811742	0.083920	-0.199385
6	2.925160	0.037580	1.284382
6	3.865599	1.033662	1.599473
6	2.839650	-1.096682	2.112503
6	4.687615	0.904624	2.724525
1	3.971405	1.914092	0.964335
6	3.669306	-1.227260	3.228627
1	2.117054	-1.882605	1.887825
6	4.591936	-0.224215	3.542488
1	5.412354	1.690036	2.955151
1	3.587325	-2.117323	3.857395
1	5.236369	-0.324133	4.419677
6	2.063182	1.794500	-0.886833
6	2.425371	2.003664	-2.228830
6	1.801065	2.922159	-0.085255
6	2.521095	3.297634	-2.752660
1	2.640893	1.151710	-2.875488
6	1.910142	4.214081	-0.605265
1	1.518005	2.797205	0.961416
6	2.266740	4.408016	-1.944478
1	2.806481	3.434027	-3.799043
1	1.714615	5.073335	0.041771
1	2.351567	5.418646	-2.352029
6	2.762353	-0.956879	-1.411352
6	4.149800	-1.149140	-1.291369
6	2.091735	-1.551205	-2.493667
6	4.846324	-1.910895	-2.233138
1	4.694454	-0.706367	-0.455860
6	2.790720	-2.308401	-3.438326
1	1.012205	-1.436757	-2.598076
6	4.169626	-2.491747	-3.309702
1	5.924191	-2.053844	-2.120717
1	2.248439	-2.768496	-4.267983
1	4.714847	-3.093046	-4.041718
1	0.162737	-2.238472	2.370357
1	-1.256750	-0.413659	-1.712572
1	-0.600932	0.027378	-1.884300

TS3 (E= -2326.79392773 a.u.)

Atomic number	**X**	**Y**	**Z**
5	-2.322771	-2.952749	1.982677
5	-2.784933	-1.093935	-0.173101
5	-0.747732	-2.261627	1.676722

5	-2.231912	-1.218545	1.520393
5	-1.727222	-3.704641	-0.759492
5	-3.150083	-2.676887	-0.789826
5	-1.253223	-3.972031	1.023450
5	-3.556867	-2.271336	0.900091
5	-2.937052	-3.860575	0.522937
16	-0.087230	-2.831026	-0.160383
6	-0.897690	1.404067	0.910025
6	-1.488424	3.587770	1.193712
6	-1.110627	3.106731	2.405980
7	-1.351075	2.542899	0.292744
7	-0.748065	1.783514	2.217787
6	-0.262168	0.948014	3.309020
6	-1.575992	2.719261	-1.132205
1	-2.569366	-3.266997	3.119790
1	-2.524341	-0.422338	2.383357
1	-1.455082	-4.580385	-1.542198
1	-4.047092	-2.847333	-1.592875
1	-0.659122	-4.933644	1.426110
1	-4.681234	-2.023119	1.272098
1	-3.598385	-4.864227	0.623156
1	-1.831854	4.573894	0.893550
1	-1.067936	3.586949	3.379856
1	0.605499	1.429943	3.784379
1	-1.055195	0.796805	4.054939
1	0.028624	-0.024634	2.903038
1	-0.892522	3.485347	-1.528409
1	-1.375098	1.770526	-1.639608
1	-2.615782	3.027037	-1.321419
7	-3.814143	0.057225	-0.565472
6	-4.327371	0.886078	0.367293
6	-4.261824	0.134888	-1.836952
6	-5.294259	1.834887	0.051818
1	-3.939308	0.746784	1.376365
6	-5.222982	1.062296	-2.221871
1	-3.834344	-0.593752	-2.525935
6	-5.752663	1.930558	-1.263934
1	-5.685462	2.479965	0.840201
1	-5.557228	1.085628	-3.260308
1	-6.517225	2.661977	-1.536649
45	-0.561972	-0.475959	0.113253
15	1.760098	0.075835	-0.205076
6	2.946609	-0.037600	1.218567
6	3.992099	0.877034	1.437120
6	2.816899	-1.136020	2.086642
6	4.876841	0.702656	2.506541
1	4.128080	1.729319	0.769704
6	3.708803	-1.312903	3.147663
1	2.011026	-1.855851	1.937052
6	4.737969	-0.391648	3.364615
1	5.682658	1.424740	2.663230
1	3.592188	-2.175026	3.809052
1	5.431282	-0.527492	4.198710
6	2.026801	1.804997	-0.839882
6	2.309974	2.054447	-2.193163
6	1.870868	2.906246	0.022545
6	2.430819	3.364219	-2.670435

1	2.442848	1.221729	-2.885614
6	2.001413	4.213668	-0.452113
1	1.655307	2.747106	1.080933
6	2.278759	4.448782	-1.803321
1	2.654550	3.533125	-3.727020
1	1.886561	5.052230	0.239793
1	2.382527	5.471429	-2.175096
6	2.615360	-0.947937	-1.501609
6	3.998371	-1.194677	-1.455396
6	1.873262	-1.471948	-2.573248
6	4.621580	-1.939415	-2.460435
1	4.598263	-0.811631	-0.628486
6	2.498805	-2.212271	-3.580302
1	0.794450	-1.313370	-2.613348
6	3.874734	-2.448817	-3.526456
1	5.697116	-2.126324	-2.404619
1	1.901707	-2.617929	-4.400718
1	4.362565	-3.037123	-4.307908
1	0.088669	-2.265965	2.539443
1	-1.653019	-0.730997	-1.279958
1	-0.865174	-0.213349	-1.574682

Compound 5 (E)= -2326.82470781 a.u.)

Atomic number	**X**	**Y**	**Z**
5	2.268665	-2.951021	-2.045879
5	2.735517	-1.027339	0.091774
5	0.690610	-2.237033	-1.703353
5	2.144828	-1.220238	-1.606849
5	1.725615	-3.823185	0.680352
5	3.146847	-2.745260	0.729473
5	1.192344	-3.959886	-1.084175
5	3.496614	-2.228020	-0.965063
5	2.878789	-3.857411	-0.636866
16	0.126810	-2.818315	0.215705
6	0.906633	1.404102	-0.918452
6	1.480168	3.590968	-1.197685
6	1.081479	3.118676	-2.406366
7	1.366486	2.540621	-0.300956
7	0.728464	1.792649	-2.221925
6	0.210318	0.971228	-3.308778
6	1.614270	2.716292	1.121796
1	2.523078	-3.276381	-3.176773
1	2.477248	-0.424373	-2.454760
1	1.496310	-4.746685	1.415904
1	4.073287	-2.853625	1.497580
1	0.587327	-4.912997	-1.488741
1	4.627567	-2.021303	-1.333412
1	3.609241	-4.810815	-0.719469
1	1.822621	4.576727	-0.895581
1	1.015895	3.606619	-3.375048
1	-0.639215	1.484943	-3.783440
1	0.993999	0.785921	-4.056922
1	-0.117779	0.012364	-2.898911
1	0.920528	3.466267	1.530931
1	1.434650	1.754425	1.616751

1	2.650024	3.048374	1.289933
7	3.765054	0.052363	0.537298
6	4.301591	0.894965	-0.377683
6	4.178906	0.133767	1.824713
6	5.245214	1.851142	-0.027987
1	3.950213	0.759210	-1.400100
6	5.127749	1.059553	2.234163
1	3.721772	-0.570932	2.517866
6	5.674861	1.943357	1.298950
1	5.647472	2.505132	-0.803420
1	5.431076	1.078929	3.282196
1	6.423713	2.680641	1.596291
45	0.598084	-0.464654	-0.147464
15	-1.746810	0.073995	0.204711
6	-2.997183	-0.032476	-1.170151
6	-4.058453	0.874828	-1.339385
6	-2.888171	-1.114832	-2.060804
6	-4.977350	0.708812	-2.380894
1	-4.179774	1.714715	-0.653613
6	-3.813824	-1.284862	-3.093904
1	-2.069776	-1.827526	-1.949232
6	-4.858041	-0.370315	-3.261220
1	-5.794922	1.425220	-2.498407
1	-3.712053	-2.135370	-3.772709
1	-5.577981	-0.499260	-4.073637
6	-1.996484	1.803936	0.842312
6	-2.245678	2.062742	2.200059
6	-1.868999	2.899148	-0.031871
6	-2.361594	3.375653	2.669969
1	-2.355378	1.234826	2.901934
6	-1.992109	4.209959	0.435514
1	-1.682172	2.732471	-1.094581
6	-2.236322	4.454380	1.791326
1	-2.559277	3.551685	3.730631
1	-1.897999	5.043473	-0.265611
1	-2.335172	5.479446	2.157902
6	-2.550187	-0.955935	1.528945
6	-3.911331	-1.301629	1.479273
6	-1.783111	-1.392848	2.623270
6	-4.490349	-2.060145	2.500849
1	-4.529153	-0.984798	0.637974
6	-2.365765	-2.145916	3.646034
1	-0.720169	-1.148577	2.661236
6	-3.720746	-2.483372	3.587607
1	-5.549401	-2.324421	2.441559
1	-1.751532	-2.481416	4.485522
1	-4.173812	-3.081244	4.382704
1	-0.179504	-2.288756	-2.529948
1	2.358331	-1.753059	1.145704
1	0.667962	0.053164	1.390035