Cobalt–bis(imino)pyridine complexes as catalysts for hydroalumination-isomerisation of internal olefins

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Cobalt complex spin states

For the formally Co(I) complexes studied herein a number of spin states can be computed, these being a closed shell singlet (css), a triplet, a quintet and an open shell singlet (oss, a biradical where the Co centre has one unpaired electron with another of opposite spin on the ligand). For simple 4-coordinate LCo-alkyl or hydride complexes, the css solution is unstable and instead the broken symmetry oss is lowest in energy. For all other complexes, a css solution is stable, and we could not compute the biradical solution.

The relative energies of the complexes that are indicated in the text are those resulting from use of the local functional BLYP (0% HF exchange). It is well known that different density functionals lead to differing predictions for relative spin state energies in transition metals, with one of the main factors being the amount of HF exchange included in hybrid functionals. It is found that high amounts of HF exchange lead to an overestabilisation of the high spin states, which in this work correspond to the triplet, quintet and oss.[1] For these reasons, we have also evaluated the different spin state energies of LCoMe (complex **6**) with the B3LYP hybrid functional, being an example of a functional with moderate (20%) HF exchange. The results are shown in Table S1.

Table S1. Relative Gibbs free energies (kJ·mol^{-1}) calculated with different functionals for spins states of complex **6**.

Spin State	Δ*G* (BLYP)	Δ*G* (B3LYP)
oss_{corr}[a]	0	0
oss[b]	9	20
triplet	41	34
quintet	129	32

[a] After spin correction to the energy of the oss, see text. [b] without spin correction.

Two relative energies are included for the oss; a value in which a spin projected correction[2] has been applied, and a value without this correction. In each case, and with each functional, the oss is the most stable spin state. The singlet-triplet gap is reasonably similar with both functionals, while the local functional predicts the quintet to be much higher in energy. This latter effect is probably due to stabilisation of the highest spin state by inclusion of 20% HF exchange in the B3LYP functional. While both functionals predict the experimentally observed ground spin state, we have employed the BLYP functional in this work for the reasons discussed below.

An additional issue to consider is that biradicals such as the oss may exhibit significant multi-reference character and as such DFT may not lead to accurate energies for such species. The applicability of UDFT methods to oss biradicals has been studied.[3] The use of DFT methods for

[1] J. N. Harvey, in *Principles and Applications of Density Functional Theory in Inorganic Chemistry I, Structure and Bonding* (Eds N. Kaltsoyannis, J. E. McGrady) **2004**, Vol. 112, pp. 151–184 (Springer: Berlin).
[2] Q. Knijnenburg; D. Hetterscheid; T. M. Kooistra; P. H. M. Budzelaar *Eur. J. Inorg. Chem.* 2004, 1204.
[3] See for instance: J. Gräfenstein; E. Kraka; M. Filatov; D. Cremer, *Int. J. Mol. Sci.* **2002**, *3*, 360, and references therein.

systems with multi-configurational character has also been extensively discussed, and we refer to the papers of Truhlar and references therein.[4] The general conclusions from previous work are that the correct choice of functional can yield accurate results even with multi-reference character. For such systems, non-hybrid (local) methods appear to be more robust than hybrid functionals. Furthermore, Truhlar[4b] has demonstrated the accuracy of BLYP for transition metal dimers and clusters. These considerations form the basis of our choice of the BLYP functional in this work, although the relative energies, particularly for the open shell singlets, should be considered approximate.

Catalyst Lifetime in 1-Octene Hydroalumination

The results obtained by adding additional 1-octene and [Al(oct)$_2$H] (1:1, 51 μmol) to 4.7 μmol of complex **5** in C_6D_6 are shown in Table S2. There were 4 additions over a day, with the insertion of 1-octene monitored by ^{1}H NMR spectroscopy after each. The reaction times indicated in Table S2 are the time since the respective addition of more substrate.

Table S2. Sequential addition of extra 1-octene and [Al(Oct)$_2$H] (1:1) to catalyst **5**.[a]

Addition	Amount Co (mol%)	Time (min)	% insertion
1	9.2	15	96
2	4.6	15	78
3	3.1	15	60
		40	87
4	2.3	15	53
		40	72
		105	82
		180	88
		255	90

[a] 4.7 μmol of **5** in 0.4 mL of C_6D_6. Each addition was 51 μmol each of 1-octene and [Al(Oct)$_2$H].

[4] (a) N. E. Schultz; Y. Zhao; D. G. Truhlar, *J. Phys. Chem. A* **2005**, *109*, 11127; (b) N. E. Schultz; Y. Zhao; D. G. Truhlar, *J. Phys. Chem. A* **2005**, *109*, 4388; (c) C. J. Cramer; D. G. Truhlar, *Phys. Chem. Chem. Phys.* **2009**, *11*, 10757; (d) Y. Zhao; O. Tishchenko; J. R. Gour; W. Li; J. J. Lutz; P. Piecuch; D. G. Truhlar, *J. Phys. Chem. A* **2009**, *113*, 5786.

D_2O Quench

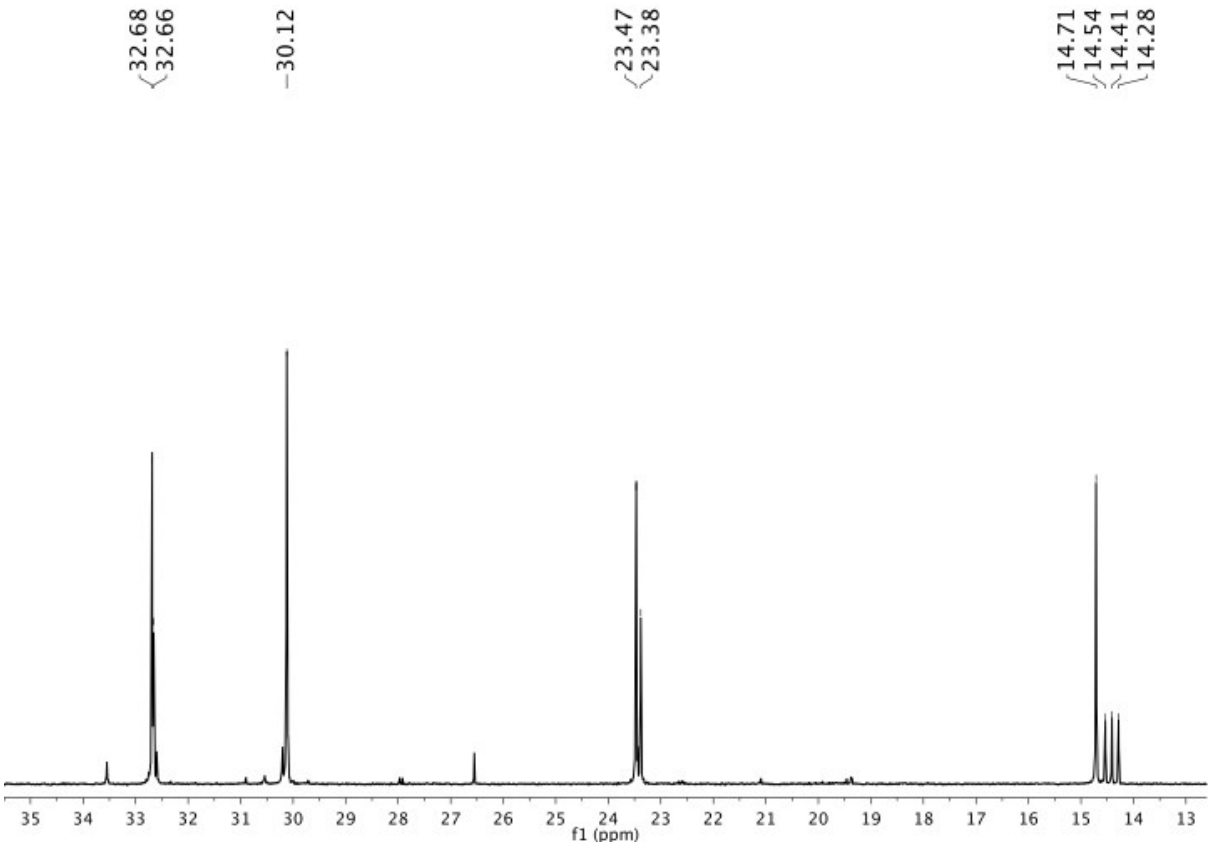


Figure S1. Representative ^{13}C NMR (C_6D_6) of 1-d_1-*n*-octane obtained by quenching the catalyst/[$Al(Oct)_2H$]/octene reaction mixture with D_2O. This example corresponds to hydroalumination of the internal octene mixture with 6 mol% catalyst **5**.

Internal Octene Insertion

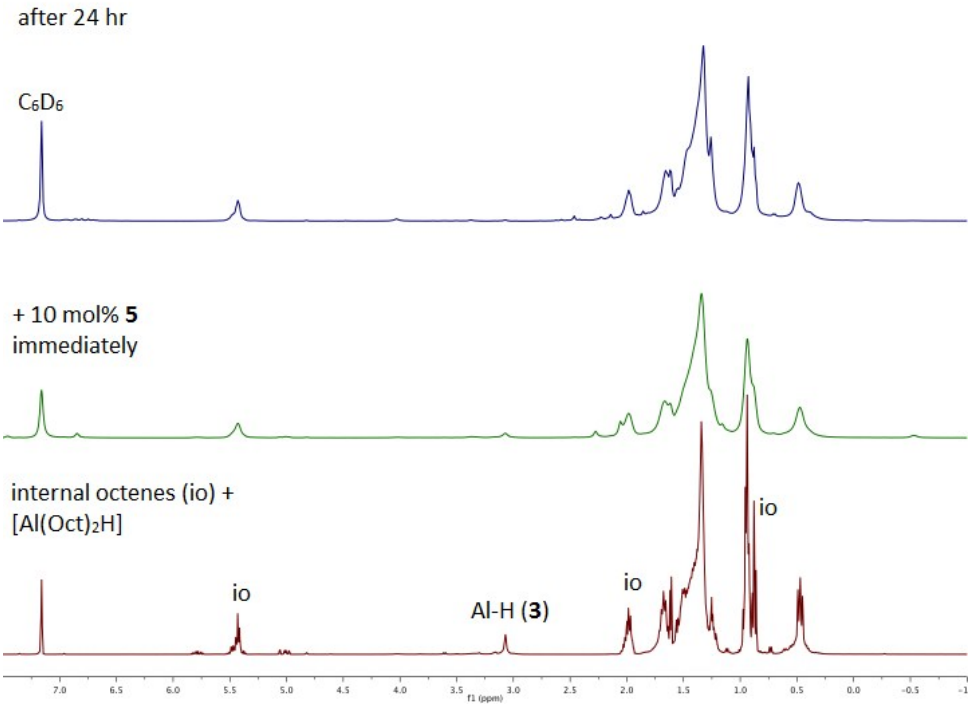


Figure S2. ^{1}H NMR spectra (C_6D_6) of partial insertion of internal octenes into [$Al(Oct)_2H$] catalysed by complex **5**. The Al–hydride and olefinic regions are expanded in Figure S3.

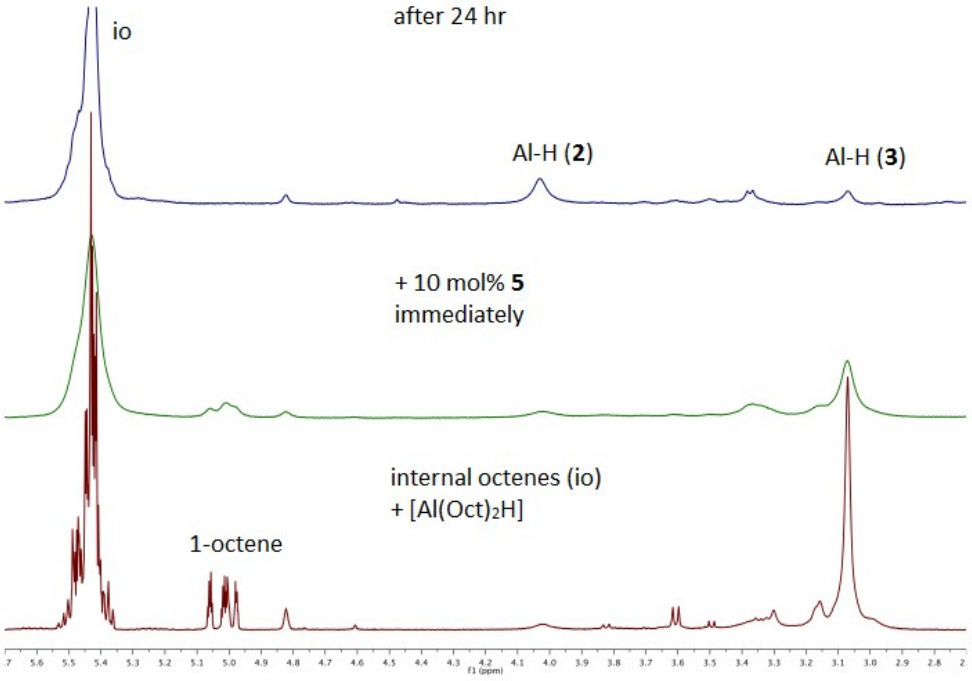


Figure S3. . ^{1}H NMR spectra (C_6D_6) in the olefinic and Al–hydride region of partial insertion of internal octenes into [$Al(Oct)_2H$] catalysed by complex **5**.

Paramagnetism after treatment with [Al(Oct)$_2$H]

To test for the formation of paramagnetic species in solution, complex **5** was treated with 10 equivalents of [Al(Oct)$_2$H] and analysed by the Evans NMR method. Complex **5** (5.5 μmol) and [Al(Oct)$_2$H] (58 μmol) were dissolved in 0.40 mL of C_6D_6 ([Co] = 0.014 M). This solution was added to a capillary tube, which was then inserted into an NMR tube containing C_6D_6. The main solvent residual peak (solution with no metal complex) was measured at 7.1601 ppm and the smaller shoulder peak appears at 7.1792 ppm (Δ = 7.63 Hz, spectrometer frequency = 399.6 MHz).

Reaction of Complex 6 with [Al(Oct)$_2$H]

The ^{1}H NMR spectrum of LCoMe, **6**, is shown in Figure S4 for comparative purposes. In Figures S5-S7 the effect of different Al:Co ratios on the ^{1}H NMR signals is illustrated, which shows the signals associated with proposed complex **7a** diminish as additional [Al(Oct)$_2$H] is added. The presence of minor species **7a** is also evident in the ^{13}C NMR spectrum (Figures S8 and S9).

The ^{1}H and ^{13}C NMR assignments for **7a** and **7b** are listed in the experimental section of the main text, as well as shown in the figures below. These assignments are also supported by ^{1}H–^{13}C HSQC correlations as listed in Table S3. The proposed complexes account for all of the major signals observed in the aromatic region of the ^{1}H and ^{13}C NMR spectra (Figures S5 and S9). In the alkyl region of the ^{1}H NMR spectrum (Figure S6), large and broad peaks appear at ca 1.2–1.5 ppm (internal C*H*$_2$ groups of the octyl chain) and 0.93 ppm (M–C_7H_{14}C*H*$_3$) which are due to the excess of octylaluminium groups present (relative to the observed Co complex). Within these signal groupings, it is not possible to differentiate between octyl CH_2 and CH_3 signals from complexes **7a,b** and those of free alkylaluminium. A further broad signal at 0.35 ppm corresponds to Al–C*H*$_2$ in the free alkylaluminium (cf. -0.60 ppm for Al–C*H*$_2$ in **7a,b**). The corresponding signals for these positions in the ^{13}C NMR spectrum (Figure S8) are multiple signals from 23-33 ppm (internal *C*H$_2$), 11.7 ppm (Al–*C*H$_2$ in free alkylaluminium) and 14.4 ppm (M–C_7H_{14}*C*H$_3$). A remaining signal we cannot assign is a singlet at -1.52 ppm in the ^{1}H NMR spectrum (Figure S7), which is only observed at a Co:Al ratio of 1:1.

Table S3. ^{1}H–^{13}C HSQC correlations in the reaction of complex **6** + 2 [Al(Oct)$_2$H].

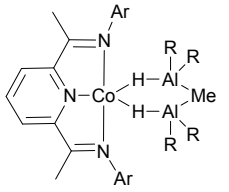
^{1}H NMR shift (ppm)	^{13}C NMR shift (ppm)	Type of carbon	Assignment
7.60	115.1	CH/CH_3	para position, Py
7.46	122.2	CH/CH_3	meta position, Py
6.81	130.0	CH/CH_3	meta position, Ar
2.27	21.2	CH/CH_3	para-Me, Ar
2.02	19.0	CH/CH_3	ortho-Me, Ar
1.15	16.2	CH/CH_3	N=CCH_3
0.93	14.4	CH/CH_3	M–$C_7H_{14}CH_3$
-0.60	9.8	CH_2	Al–CH_2

The formation of complex **7** is also supported by theoretical prediction of the Co–hydride ^{1}H NMR chemical shift. Theoretical NMR shielding values were calculated for a model of complex **7b** with propyl- in place of octyl-substitution. Shielding tensors were computed with the Gauge-Independent Atomic Orbital (GIAO) method,[5] at the BLYP/BS2 level of theory (on BLYP/BS1 geometries). Rather than calculating a predicted chemical shift relative to tetramethylsilane, we have plotted

[5] (a) J. R. Cheeseman; G. W. Trucks; T. A. Keith; M. J. Frisch, *J. Chem. Phys.* **1996**, *104*, 5497; (b) K. Wolinski; J. F. Hinton; P. Pulay, *J. Am. Chem. Soc.* **1990**, *112*, 8251.

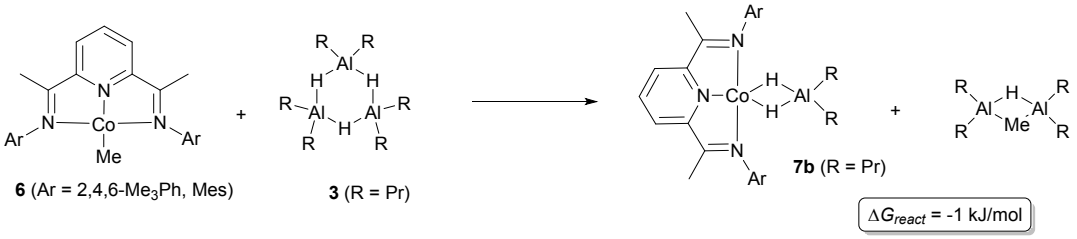
experimental chemical shifts against the absolute calculated isotropic shieldings for several known[6] Co–hydride complexes of phosphine ligands (Figure S10). The relationship derived from this calibration was then employed to calculate predicted chemical shifts for complex **7**. The static nature of the calculation results in slightly different predicted shifts for each Co–hydride (-9.4 and -11.0 ppm), but each is very close to the experimentally observed shift of -10.20 ppm.

Another possibility considered was the 2:1 Al:Co trinuclear complex **9**. While the predicted Co–hydride chemical shifts are almost identical (-9.2 and -11.1 ppm), this structure is not supported by the relative intensity of the Al–CH_2 and Co–*H* signals. Overall, the formation of **7b** along with minor **7a** seems to fit the combined experimental and theoretical data best.



9 (R = Oct, Pr (theory))

The energetics of formation of **7b** (R = propyl) has also been estimated theoretically (BLYP/BS2//BLYP/BS1). The model reaction shown in Scheme S1 has a calculated ΔG_{react} value of -1 kJ·mol^{-1}. While not strongly exergonic, this does show that the formation of complex **7** from these reactants is favourable.



6 (Ar = 2,4,6-Me$_3$Ph, Mes) **3** (R = Pr) **7b** (R = Pr)

Scheme S1. Estimated free energy of formation of complex **7b**.

[6] (a) C. Bianchini; P. Innocenti; A. Meli; M. Peruzzini; F. Zanobini; P. Zanello, *Organometallics* **1990**, *9*, 2514; (b) R. Ciancanelli; B. C. Noll; D. L. DuBois; M. R. DuBois; *J. Am. Chem. Soc.* **2002**, *124*, 2984.

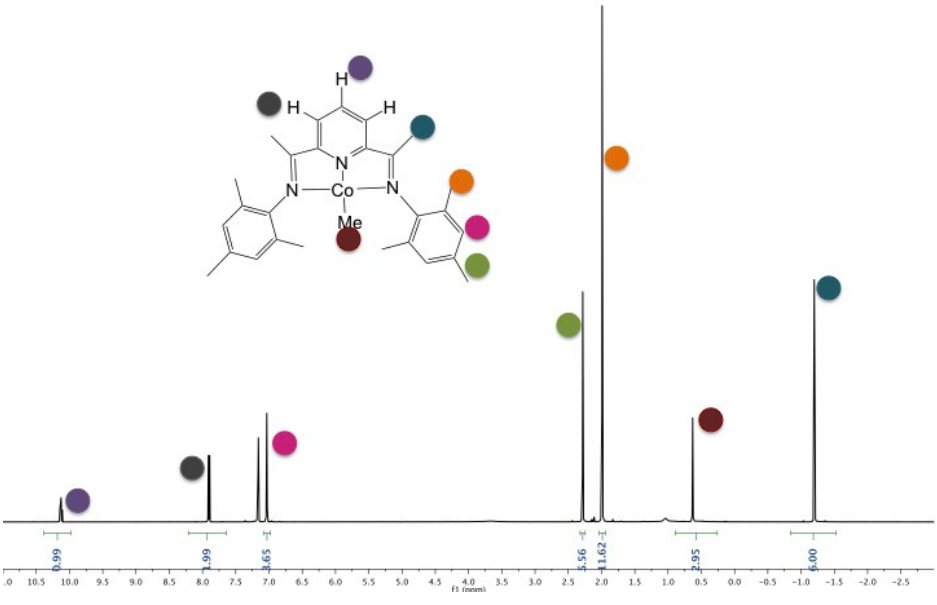


Figure S4. ^{1}H NMR (C_6D_6) of LCoMe (**6**) prior to addition of [Al(Oct)$_2$H].

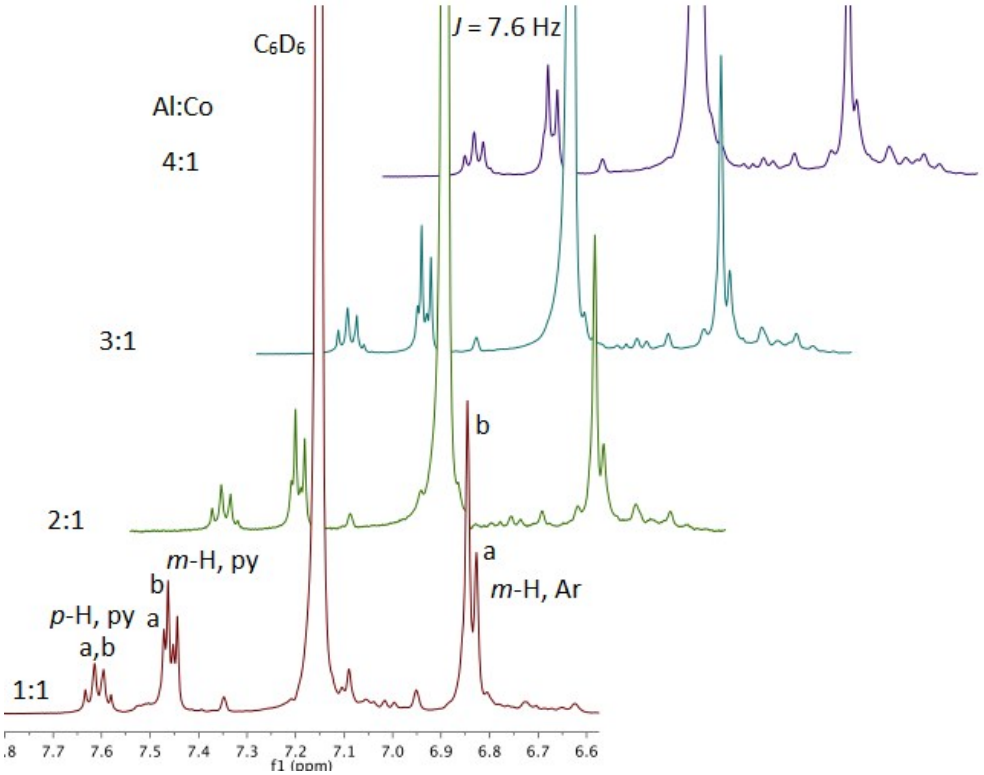


Figure S5. ^{1}H NMR spectra (C_6D_6) in the aromatic region of complex **6** + [Al(Oct)$_2$H] at different Co:Al ratios.

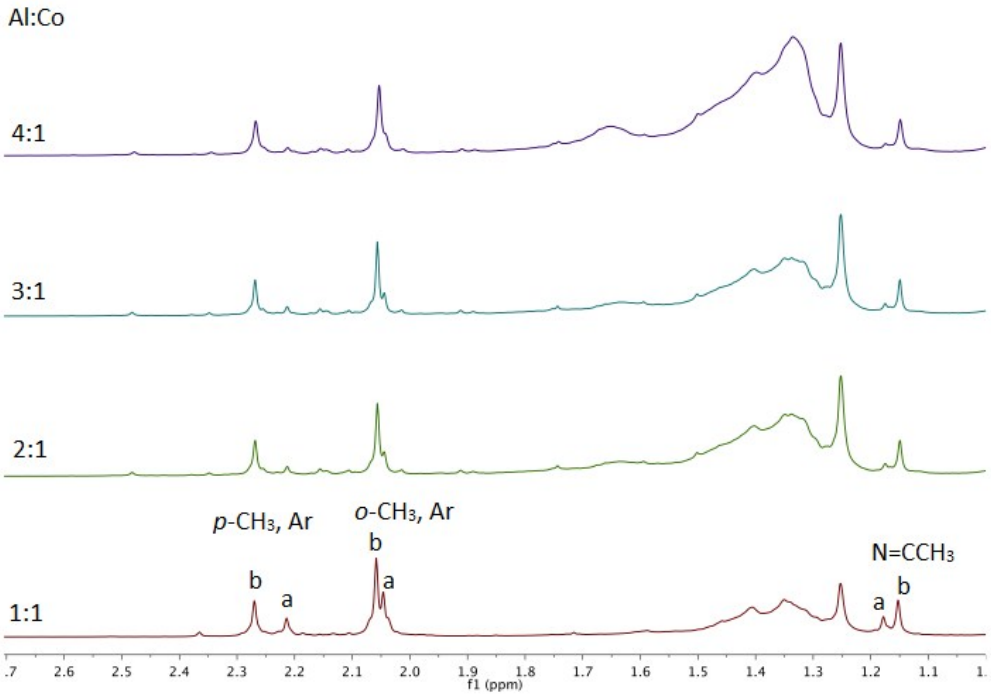


Figure S6. ^{1}H NMR spectra (C_6D_6) in the alkyl region of complex **6** + [Al(Oct)$_2$H] at different Co:Al ratios.

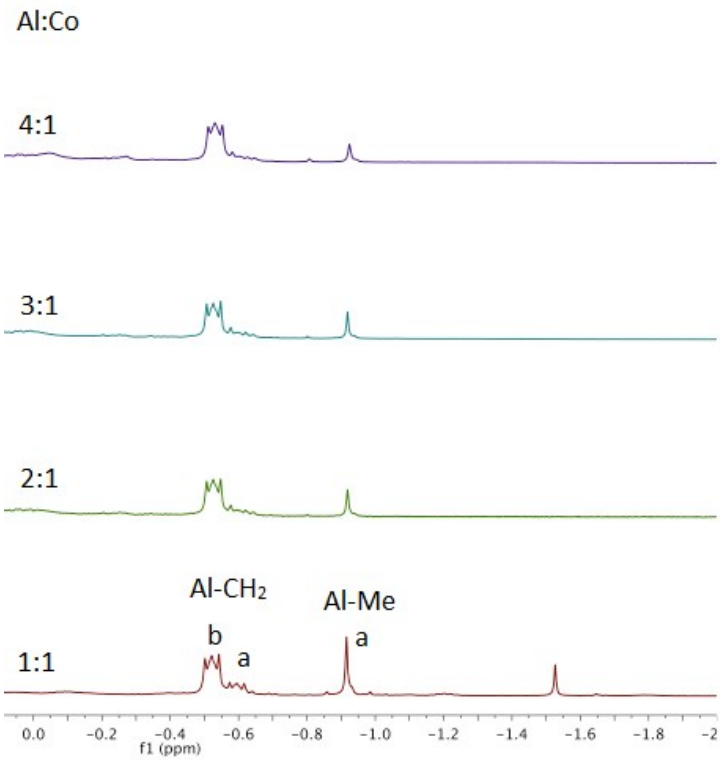


Figure S7. ^{1}H NMR spectra (C_6D_6) in the Al-CH$_x$ region of complex **6** + [Al(Oct)$_2$H] at different Co:Al ratios.

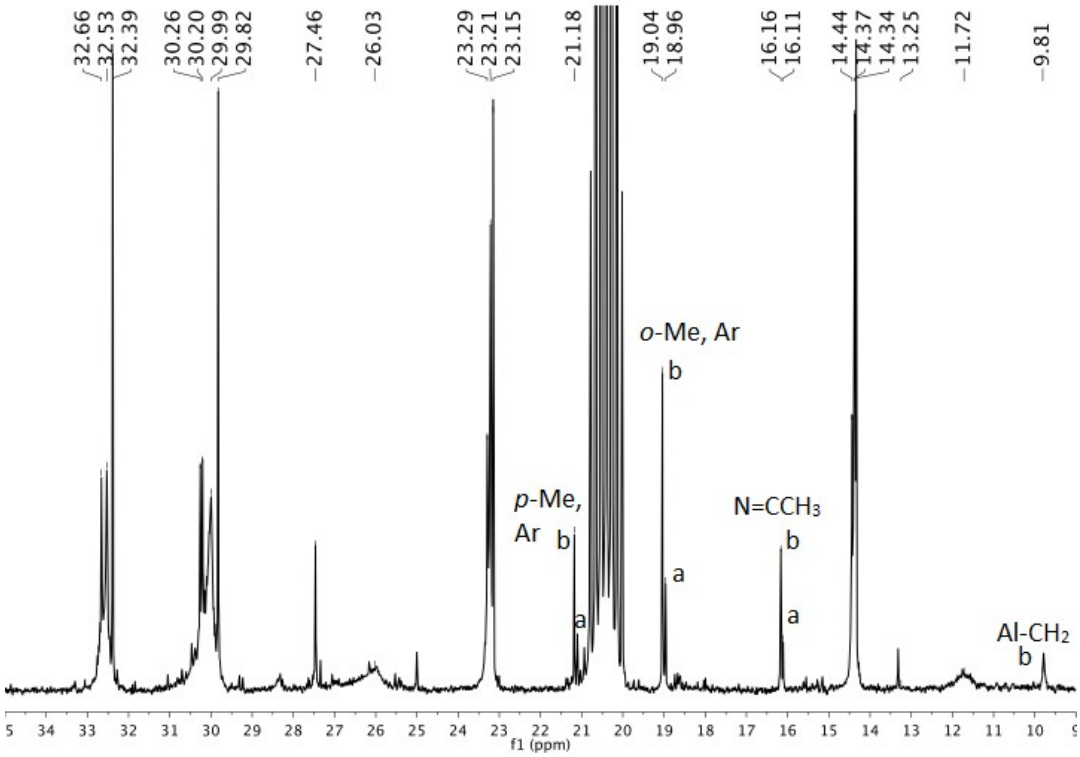


Figure S8. ^{13}C NMR spectrum (toluene-d_8) of complex **6** + 2 [Al(Oct)$_2$H] (alkyl region).

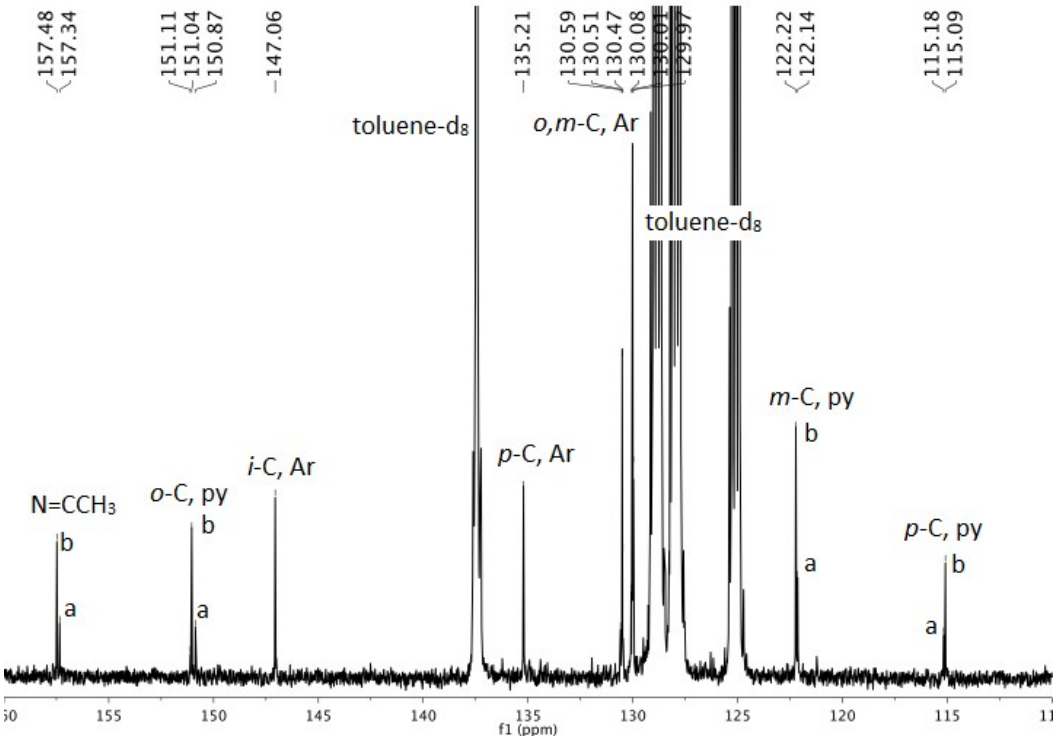


Figure S9. ^{13}C NMR spectrum (toluene-d_8) of complex **6** + 2 [Al(Oct)$_2$H] (aromatic region).

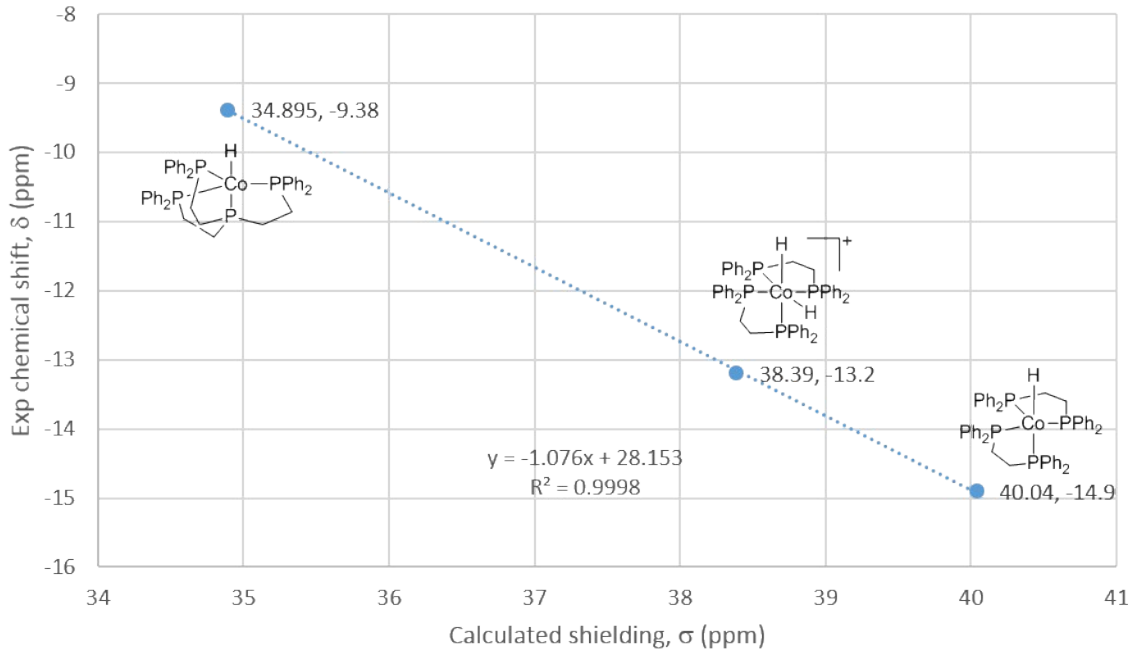


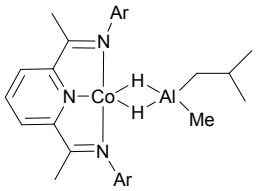
Figure S10. Experimental ^{1}H NMR Co–H chemical shift versus calculated (BLYP/BS2//BLYP/BS1) shielding for known Co–hydrides. Experimental values from references 6a,b.

Reaction of Complex 6 with [Al(^{i}Bu)$_2$H]

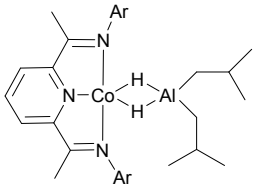
Complex **6** was also reacted with [Al(^{i}Bu)$_2$H] in the hope that *iso*-butyl in place of octyl substitution may lead to a cleaner spectrum in the alkyl region. While this was not the case (in fact it leads to a more complex spectrum in this region), the ^{1}H NMR spectrum observed is again consistent with two very similar diamagnetic Co species forming. Figure S11 shows the Co–hydride region and the ligand aromatic region. Again the pyridyl signals can be interpreted as overlapping triplets (7.6 ppm) and overlapping doublets (7.46 ppm). In this case the Co–hydride signal has a pronounced shoulder which is attributed to the second species. In Figure S12 the minor species is observed in the ligand methyl signals, along with the Al-CH$_2$ signal. The signal at -0.91 ppm is again consistent with an Al–Me group in minor species **7a**. It was not possible to assign the *iso*-butyl CH$_3$ and CH signals as this region (ca. 0.5–2.0 ppm) is very complex, and evidently there are multiple species present apart from the Co complex. Nonetheless, the bis(imino)pyridine ligand resonances and the signals below 0 ppm (Al–C*H*$_2$, Al–C*H*$_3$, Co–*H*) are cleaner and, together with the ^{13}C NMR spectrum, allow us to tentatively proposed structures **7a** and **7b** again. The NMR assignments are listed below with ^{1}H-^{13}C HSQC correlations in Table S4.

^{1}H NMR: δ 7.61 (1H, overlapping triplets, *J* = 7.6 Hz, *p*-*H*, py$_{a+b}$); 7.46 (2H, overlapping doublets, *J* = 7.6 Hz, *m*-*H*, py$_{a+b}$); 6.81 (4H, s, *m*-*H*, Ar$_{a+b}$); 2.23 (6H, s, *o*-C*H*$_3$, Ar$_b$); 2.20 (6H, s, *p*-C*H*$_3$, Ar$_a$); 2.04 (12H, overlapping singlets, *o*-C*H*$_3$, Ar$_{a+b}$); 1.18, 1.16 (6H, overlapping singlets, N=CC*H*$_{3(a+b)}$); -0.62 (4H, d, *J* = 7.2 Hz, Al–C*H*$_{2(b)}$); -0.65 (2H, d, *J* = 7.2 Hz, Al–C*H*$_{2(a)}$); -0.91 (3H, s, Al-C*H*$_{3(a)}$); -10.26 (2H, s with shoulder, Co–*H*$_{(a+b)}$). ^{13}C NMR (toluene-d$_8$): Only the major species is observed by ^{13}C NMR, thought to be **7b**, δ 157.5 (N=*C*CH$_3$); 151.1 (*o*-*C*, py); 146.8 (*i*-*C*, Ar); 135.3 (*p*-*C*, Ar); 130.6, 130.1 (*o,m*-*C*, Ar); 122.3 (*m*-*C*, py); 114.9 (*p*-*C*, py); 21.1 (*p*-*C*H$_3$, Ar); 19.0 (*o*-*C*H$_3$, Ar); 16.2 (N=C*C*H$_3$). Additional signals,

which may be due to either **7a,b** or free alkylaluminium, appear at 28.3 and 24.8 ppm (*iso*-Bu CH_3) and 27.3 ppm (*iso*-Bu $CHMe_2$).



7a



7b

Table S4. ^{1}H–^{13}C HSQC correlations in the reaction of complex **6** + 2 [Al(*i*-Bu)$_2$H].

^{1}H NMR shift (ppm)	^{13}C NMR shift (ppm)	Type of carbon	Assignment
7.61	114.6	CH/CH_3	para position, Py
7.46	122.3	CH/CH_3	meta position, Py
6.78	130.1	CH/CH_3	meta position, Ar
2.23	21.1	CH/CH_3	para-Me, Ar
2.04	19.0	CH/CH_3	ortho-Me, Ar
1.93	27.3	CH/CH_3	*CH*Me_2
1.18	16.2	CH/CH_3	N=CCH_3
1.01	28.3	CH/CH_3	*CH*$_3$ *iso*-Bu
0.87	24.8	CH/CH_3	*CH*$_3$ *iso*-Bu

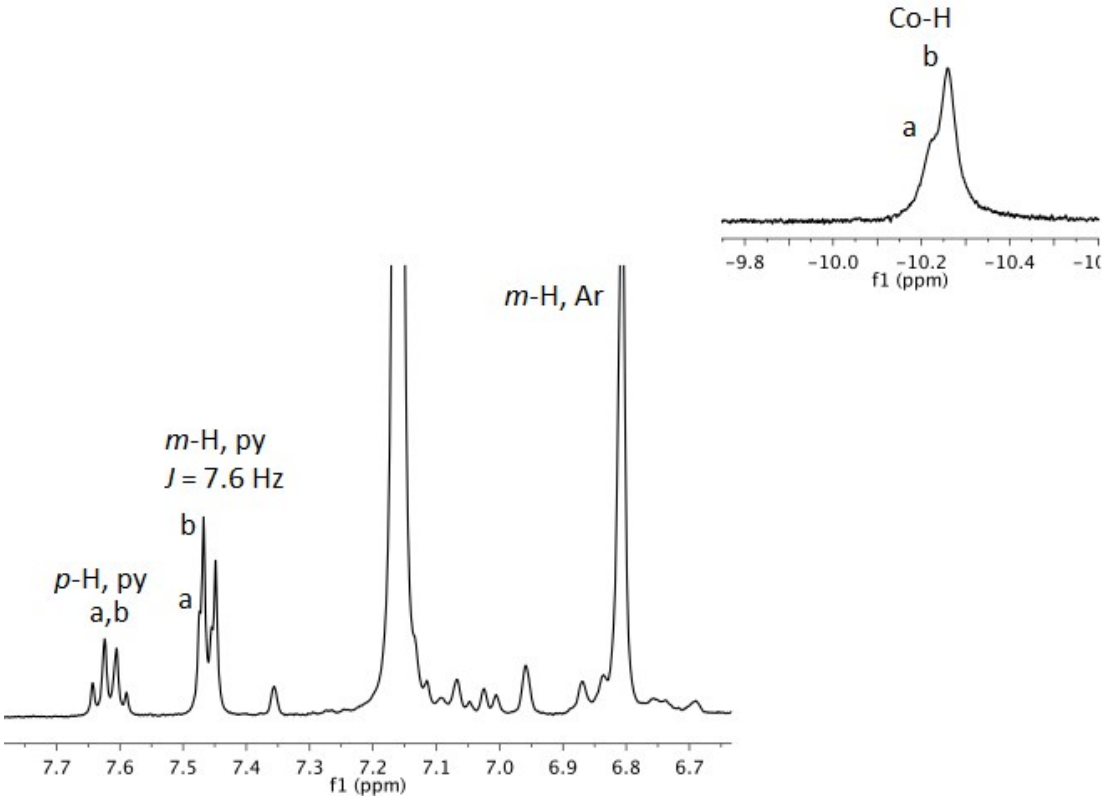


Figure S11. ^{1}H NMR spectra (C_6D_6) of complex **6** + 2 [Al(^{i}Bu)$_2$H] in the aromatic and Co–hydride regions.

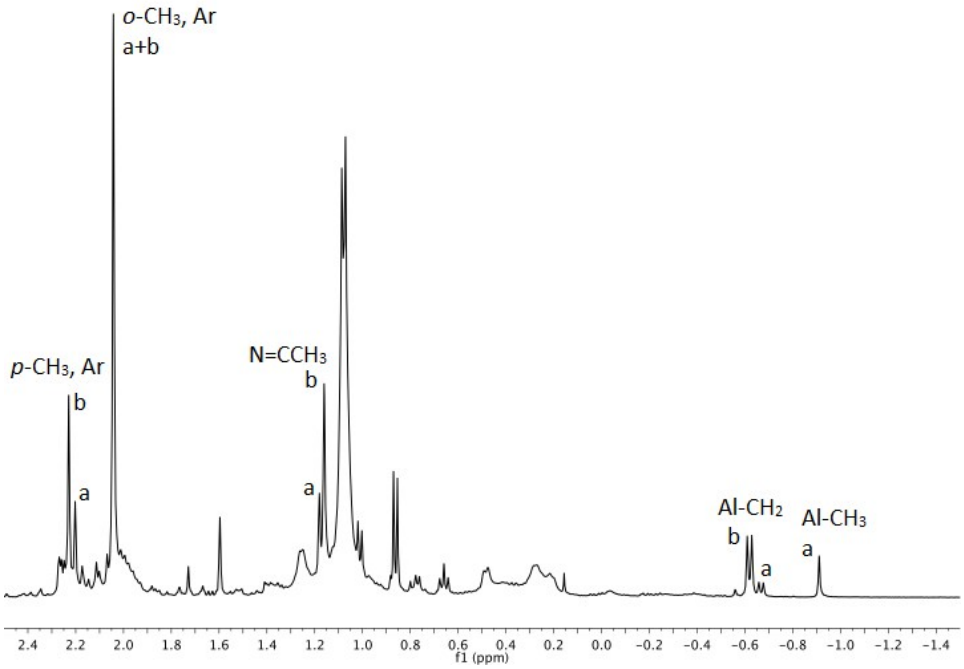


Figure S12. ^{1}H NMR spectra (C_6D_6) of complex **6** + 2 [Al(^{i}Bu)$_2$H] in the alkyl and Al–CH$_x$ regions.

<u>Formation of [LCo(*n*-octyl)], 8, during hydroboration with complex 6</u>

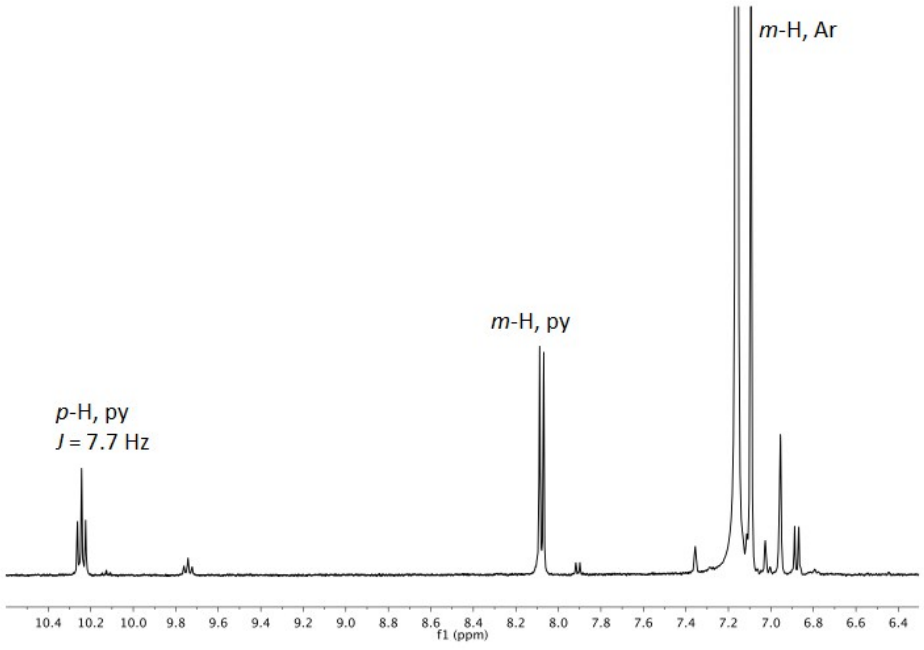


Figure S13. ^{1}H NMR spectrum (C_6D_6) following hydroboration of internal octenes with HBPin catalysed by 10 mol% complex **6**.

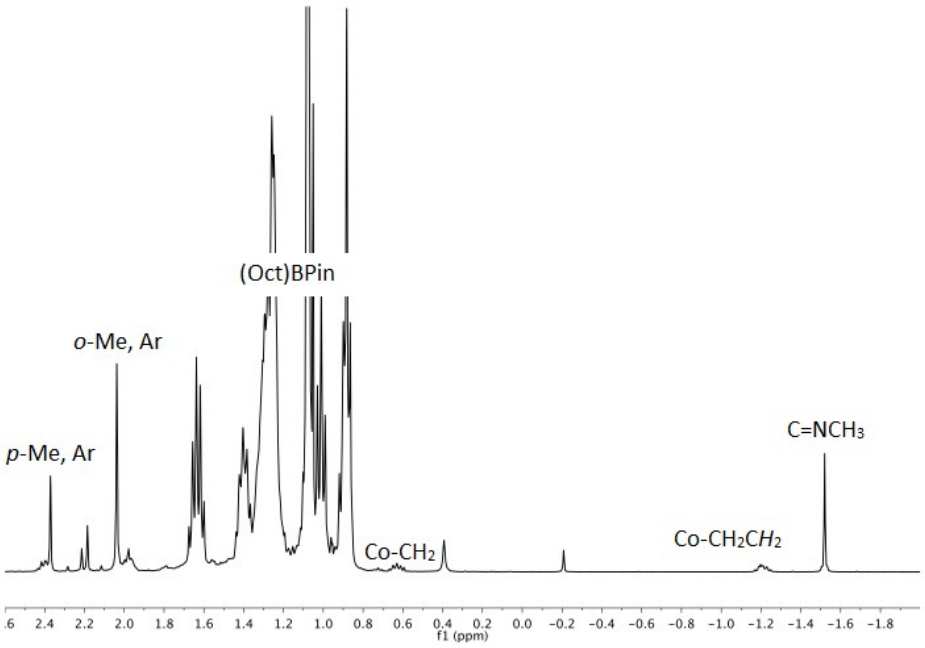


Figure S14. ^{1}H NMR spectrum (C_6D_6) following hydroboration of internal octenes with HBPin catalysed by 10 mol% complex **6**.

Optimised geometries and energies (Hartrees) of all stationary points

[LCoMe] (complex **6**, oss)

```
UBLYP/BS1:
 Zero-point correction=                           0.538255 (Hartree/Particle)
 Thermal correction to Energy=                    0.573009
 Thermal correction to Enthalpy=                  0.573953
 Thermal correction to Gibbs Free Energy=         0.469894
 Sum of electronic and zero-point Energies=          -1396.618416
 Sum of electronic and thermal Energies=             -1396.583662
 Sum of electronic and thermal Enthalpies=           -1396.582718
 Sum of electronic and thermal Free Energies=        -1396.686777
E(UB-LYP/BS2) =  -1396.67408686

0 1
 C                 -1.22798100    2.75796000    0.13357800
 C                 -1.22869100    4.16196300    0.24631200
 C                  0.00618000    4.84176900    0.28566300
 C                  1.22293500    4.13173700    0.22161400
 C                  1.18547700    2.72823700    0.10934400
 N                 -0.03003700    2.07900100    0.06068100
 H                  0.02053600    5.93064300    0.37529300
 H                 -2.16914400    4.71264100    0.31099800
 H                  2.17764600    4.65935200    0.26708400
 C                 -2.33200300    1.82078900    0.08400400
 C                  2.26490800    1.76420300    0.03724300
 N                 -1.94195800    0.53092500    0.03199300
 N                  1.84228700    0.48441500   -0.00608200
 Co                -0.05345400    0.21215400    0.02485600
 C                 -2.94020900   -0.49941700   -0.03484700
 C                 -3.45802100   -1.04340200    1.16366700
 C                 -3.33060500   -0.99621000   -1.29936100
 C                 -4.40033600   -2.08315500    1.06976800
 C                 -4.27904200   -2.03460800   -1.34330700
```

C	-4.82614300	-2.59243300	-0.17230400
H	-4.80585700	-2.51061500	1.99304200
H	-4.59232700	-2.42059000	-2.31915900
C	2.81224600	-0.57111300	-0.09374500
C	3.15880300	-1.08082600	-1.36600400
C	3.34441100	-1.12590200	1.09337400
C	4.07752500	-2.14447500	-1.42990500
C	4.25576300	-2.19106000	0.97962700
C	4.63742400	-2.71447000	-0.27075600
H	4.35689300	-2.54060500	-2.41198500
H	4.67222700	-2.62704600	1.89399500
C	-2.97686000	-0.52852000	2.50564600
H	-1.87540300	-0.57393300	2.56211500
H	-3.25749700	0.52692900	2.67062900
H	-3.39964400	-1.12333300	3.33031000
C	-2.73038100	-0.41578700	-2.56455300
H	-2.98589200	0.65161300	-2.68925500
H	-1.62811100	-0.46839700	-2.53154900
H	-3.08458300	-0.95812500	-3.45504500
C	-5.81944000	-3.73938200	-0.24370400
H	-5.31240900	-4.71708200	-0.14516600
H	-6.56582600	-3.67907500	0.56601700
H	-6.35835900	-3.74677100	-1.20529700
C	2.54553200	-0.48619000	-2.61831100
H	1.44328600	-0.50543700	-2.55882500
H	2.83009200	0.57266600	-2.75290900
H	2.86176800	-1.04139800	-3.51514800
C	2.91195700	-0.59403900	2.44531900
H	3.23225400	0.45140500	2.60189500
H	1.81129500	-0.60220300	2.52805400
H	3.33391000	-1.20193600	3.26080800
C	5.59740200	-3.88802900	-0.36303100
H	6.34784300	-3.86056900	0.44455100
H	5.06307700	-4.85231300	-0.27714300
H	6.13248800	-3.89670400	-1.32683200
C	-3.77569600	2.25661200	0.11107000
H	-4.16504700	2.29946100	1.14560100
H	-3.88985200	3.26013400	-0.32750900
H	-4.41104700	1.55186400	-0.44494500
C	3.71890300	2.16499500	0.03319000
H	4.12760400	2.21129800	1.06007800
H	4.32671300	1.43832800	-0.52526400
H	3.84915200	3.16016300	-0.41991000
C	-0.07262400	-1.73534700	0.21112600
H	0.82323300	-2.14368900	0.70629400
H	-0.98324000	-2.13108900	0.68893300
H	-0.06375200	-2.09103000	-0.84280200

[LCoMe] (triplet)

```
UBLYP/BS1:
 Zero-point correction=                           0.537404 (Hartree/Particle)
 Thermal correction to Energy=                    0.571462
 Thermal correction to Enthalpy=                  0.572406
 Thermal correction to Gibbs Free Energy=         0.470012
 Sum of electronic and zero-point Energies=          -1396.606985
 Sum of electronic and thermal Energies=             -1396.572927
 Sum of electronic and thermal Enthalpies=           -1396.571983
 Sum of electronic and thermal Free Energies=        -1396.674377
E(UB-LYP/BS2) =  -1396.66178134

0 3
 C                 -1.23481800    2.74743600    0.10454600
 C                 -1.22977600    4.15282200    0.13329700
 C                  0.00696200    4.83370900    0.13520900
 C                  1.22530900    4.12085100    0.11040800
 C                  1.19350700    2.71582000    0.08168400
```

N	-0.02938200	2.07249500	0.07847600
H	0.02143400	5.92582700	0.15725100
H	-2.16618500	4.71427100	0.15485200
H	2.17614100	4.65793300	0.11428200
C	-2.34154600	1.81695600	0.08816600
C	2.27505900	1.75674600	0.04369400
N	-1.96368500	0.51564800	0.06970800
N	1.86308000	0.46570800	0.03259200
Co	-0.05396000	0.17984400	0.08665200
C	-2.97499900	-0.49858200	0.00702200
C	-3.46329900	-1.06657400	1.20717800
C	-3.41777300	-0.95746200	-1.25495200
C	-4.43324200	-2.08111300	1.12097500
C	-4.38917500	-1.97453100	-1.29295800
C	-4.91156200	-2.54854900	-0.11858600
H	-4.81888400	-2.52197700	2.04651400
H	-4.74086200	-2.33159800	-2.26678700
C	2.84613200	-0.57423100	-0.05266300
C	3.25073800	-1.04067300	-1.32461400
C	3.34497600	-1.15719600	1.13580900
C	4.19640800	-2.08057300	-1.38527400
C	4.28801100	-2.19469300	1.02704400
C	4.72941600	-2.66983500	-0.22322900
H	4.51899800	-2.44340900	-2.36702100
H	4.68223100	-2.64717000	1.94331600
C	-2.92178500	-0.59770500	2.54297000
H	-1.82812100	-0.74634700	2.58808300
H	-3.09794700	0.47975000	2.70746700
H	-3.38456100	-1.15171400	3.37455600
C	-2.83383700	-0.37415400	-2.52691500
H	-3.01327100	0.71226100	-2.60710000
H	-1.73841000	-0.51124100	-2.55001700
H	-3.26416900	-0.85841700	-3.41734400
C	-5.93427800	-3.66965400	-0.18508200
H	-5.45092400	-4.66062100	-0.10127800
H	-6.66781500	-3.59763300	0.63550700
H	-6.48655900	-3.65521100	-1.13891000
C	2.65379200	-0.44006400	-2.58234400
H	1.55483000	-0.54756800	-2.57973200
H	2.86048700	0.64126600	-2.66581800
H	3.05013800	-0.93452900	-3.48287300
C	2.84322200	-0.67853800	2.48357900
H	3.04835100	0.39407900	2.64595100
H	1.74753200	-0.80128400	2.55181700
H	3.31029000	-1.24513500	3.30421200
C	5.72412300	-3.81431100	-0.31331100
H	6.47142100	-3.76535100	0.49641800
H	5.21883000	-4.79423500	-0.22900900
H	6.26202600	-3.80594700	-1.27541200
C	-3.79086800	2.23631000	0.07978100
H	-4.33637500	1.80570700	0.93721300
H	-3.88911300	3.33036700	0.12267000
H	-4.30652100	1.87906800	-0.82868600
C	3.73432100	2.13838300	0.00575100
H	4.28654000	1.69126900	0.85032300
H	4.22142400	1.77101900	-0.91447200
H	3.86155800	3.22940900	0.04940400
C	-0.07953800	-1.79116000	0.06200000
H	0.81767600	-2.23159300	0.53013700
H	-0.98314200	-2.20861300	0.53851700
H	-0.08828000	-2.11081200	-1.00152800

[LCoMe] (quintet)

```
UBLYP/BS1:
 Zero-point correction=                           0.535336 (Hartree/Particle)
 Thermal correction to Energy=                    0.570469
 Thermal correction to Enthalpy=                  0.571413
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```
 Thermal correction to Gibbs Free Energy=          0.465364
 Sum of electronic and zero-point Energies=          -1396.573041
 Sum of electronic and thermal Energies=             -1396.537909
 Sum of electronic and thermal Enthalpies=           -1396.536965
 Sum of electronic and thermal Free Energies=        -1396.643014
E(UB-LYP/BS2) =  -1396.62681287

0 5
 C                 -1.22131400    2.75235300    0.42158500
 C                 -1.23106300    4.18401600    0.48397600
 C                  0.00905700    4.84839600    0.51996300
 C                  1.23168100    4.15418000    0.45376500
 C                  1.18576000    2.72334200    0.39239100
 N                 -0.02446600    2.10175900    0.48327500
 H                  0.02294500    5.94141400    0.57122600
 H                 -2.16984300    4.73859900    0.48679700
 H                  2.18325800    4.68611500    0.43289800
 C                 -2.33106200    1.84464900    0.22652400
 C                  2.26809500    1.78862600    0.17144400
 N                 -1.99498100    0.56378100   -0.10616500
 N                  1.89286400    0.51691500   -0.15363200
 Co                -0.05144200    0.15730700    0.24295900
 C                 -2.96222100   -0.47796000   -0.18265000
 C                 -3.68017400   -0.91985700    0.96161200
 C                 -3.11420600   -1.14472100   -1.42895300
 C                 -4.56273500   -2.00827800    0.82066400
 C                 -4.01039000   -2.22095400   -1.51948400
 C                 -4.74724700   -2.67127300   -0.40537500
 H                 -5.11269400   -2.35406800    1.70258900
 H                 -4.13699700   -2.72256300   -2.48497300
 C                  2.83208200   -0.54884600   -0.24930700
 C                  2.94028900   -1.22053800   -1.49761500
 C                  3.56199100   -1.00794300    0.88034400
 C                  3.80624700   -2.31949100   -1.60540100
 C                  4.41279800   -2.11926300    0.72254000
 C                  4.55452600   -2.78762000   -0.50616600
 H                  3.89915100   -2.82549600   -2.57244400
 H                  4.97167300   -2.47874600    1.59328300
 C                 -3.49231000   -0.26751100    2.31893800
 H                 -2.43929400    0.00593100    2.49084500
 H                 -4.08821200    0.65646000    2.42197200
 H                 -3.80960500   -0.95149300    3.12193100
 C                 -2.32054800   -0.68379500   -2.63502200
 H                 -2.48944600    0.38518700   -2.84959300
 H                 -1.23501500   -0.79337100   -2.46191300
 H                 -2.58669500   -1.26756100   -3.53035600
 C                 -5.68318300   -3.86150000   -0.52072400
 H                 -5.12855500   -4.81683600   -0.47010400
 H                 -6.42582600   -3.87032600    0.29353300
 H                 -6.22779000   -3.85564300   -1.48006900
 C                  2.13212600   -0.74068200   -2.68645200
 H                  1.04840100   -0.81989300   -2.48749200
 H                  2.32522700    0.32281000   -2.90778700
 H                  2.36128100   -1.33349300   -3.58604500
 C                  3.41825500   -0.35017600    2.24042700
 H                  4.03412700    0.56213000    2.32832800
 H                  2.37492600   -0.05581800    2.43588000
 H                  3.74020400   -1.03923400    3.03719400
 C                  5.45753100   -4.00108200   -0.64049200
 H                  6.19425900   -4.04733800    0.17775400
 H                  4.87606200   -4.94123400   -0.61377000
 H                  6.00867200   -3.99076700   -1.59622800
 C                 -3.75255200    2.35044100    0.26069300
 H                 -4.04120300    2.69788700    1.26941900
 H                 -3.86324200    3.21675500   -0.41684500
 H                 -4.46076400    1.57185900   -0.05393700
 C                  3.70212100    2.25916400    0.17313500
 H                  4.02051800    2.60357800    1.17389400
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 H                  4.38409500    1.46211900   -0.15288000
 H                  3.81970400    3.11974300   -0.51059500
 C                 -0.06139700   -1.61477100    1.09823600
 H                  0.85257600   -1.81125900    1.67938100
 H                 -0.96091200   -1.78646100    1.70907600
 H                 -0.08481700   -2.28270600    0.21311300
```

[LCo(*sec*-Bu)] (oss)

```
UBLYP/BS1:
 Zero-point correction=                           0.622891 (Hartree/Particle)
 Thermal correction to Energy=                    0.661529
 Thermal correction to Enthalpy=                  0.662473
 Thermal correction to Gibbs Free Energy=         0.551472
 Sum of electronic and zero-point Energies=          -1514.403908
 Sum of electronic and thermal Energies=             -1514.365270
 Sum of electronic and thermal Enthalpies=           -1514.364326
 Sum of electronic and thermal Free Energies=        -1514.475327
E(UB-LYP/BS2) =  -1514.58542757

0 1
 C                 -1.24965200    2.74894800    0.14906400
 C                 -1.25376900    4.15376300    0.25489300
 C                 -0.02212300    4.83889800    0.28900700
 C                  1.19465500    4.12916800    0.22613800
 C                  1.15899500    2.72514600    0.12229100
 N                 -0.05310900    2.06710000    0.07117500
 H                 -0.01021800    5.92819100    0.37392600
 H                 -2.19769800    4.69913900    0.31648800
 H                  2.15069200    4.65536400    0.26317400
 C                 -2.35880900    1.82569500    0.08289100
 C                  2.24637900    1.77618400    0.04520400
 N                 -1.98586300    0.52554500    0.09378800
 N                  1.83761400    0.49109200    0.04727600
 Co                -0.07546800    0.19806800    0.17480400
 C                 -2.99140500   -0.48627500   -0.06965300
 C                 -3.84232300   -0.84239700    1.00430800
 C                 -3.07981200   -1.14747200   -1.32091100
 C                 -4.76013100   -1.89323400    0.81005300
 C                 -4.01291800   -2.18763400   -1.46630400
 C                 -4.85589800   -2.58571800   -0.40964000
 H                 -5.41109100   -2.18108300    1.64242700
 H                 -4.08351300   -2.69957100   -2.43190000
 C                  2.79989700   -0.56319300   -0.09809600
 C                  2.99085100   -1.13798000   -1.37811900
 C                  3.46505800   -1.07373400    1.04190800
 C                  3.84293000   -2.25014000   -1.49112400
 C                  4.30788100   -2.18934400    0.87911800
 C                  4.50103600   -2.80036400   -0.37353200
 H                  3.99232700   -2.70110100   -2.47784200
 H                  4.81711900   -2.59647100    1.75890700
 C                 -3.77498100   -0.11659500    2.33533700
 H                 -2.74603000    0.19361800    2.56882700
 H                 -4.40263700    0.79290900    2.33299900
 H                 -4.13827700   -0.76270300    3.14996800
 C                 -2.20234500   -0.71517400   -2.47866100
 H                 -2.38961700    0.33698800   -2.75620800
 H                 -1.13375100   -0.77759700   -2.21229800
 H                 -2.38023600   -1.34454000   -3.36467000
 C                 -5.82132200   -3.74550400   -0.57936600
 H                 -5.31348600   -4.71586200   -0.42754200
 H                 -6.64810500   -3.69157900    0.14751100
 H                 -6.25696900   -3.76408200   -1.59257200
 C                  2.30725700   -0.54211600   -2.59368900
 H                  1.22025400   -0.44375700   -2.43379300
 H                  2.68009800    0.47575200   -2.80735400
 H                  2.47825100   -1.16288900   -3.48690500
 C                  3.26785500   -0.42901100    2.40045400
```

H	3.76562800	0.55562400	2.46019200
H	2.19795700	-0.25913900	2.60510500
H	3.68372200	-1.06225200	3.19954200
C	5.36899500	-4.03845300	-0.51440000
H	6.11327100	-4.10413900	0.29592500
H	4.75891200	-4.95968300	-0.47515500
H	5.90817000	-4.04768000	-1.47645000
C	-3.78173900	2.31389500	-0.03702500
H	-4.15309300	2.71346700	0.92479900
H	-3.84678000	3.13305200	-0.77314600
H	-4.45653800	1.50560300	-0.34891100
C	3.68888400	2.21036300	-0.03352900
H	4.06082700	2.54658000	0.95246400
H	4.33174100	1.38557300	-0.37049700
H	3.80445500	3.05835600	-0.72930300
C	0.06046500	-1.65696100	0.91154300
H	1.09735300	-1.69710500	1.28108100
C	-0.03733100	-2.65441800	-0.27206200
H	-1.09747800	-2.80454600	-0.54353100
H	0.46135300	-2.24565400	-1.16906700
C	0.62138100	-4.02578900	0.02529500
H	1.69489500	-3.89366500	0.24226100
H	0.15558600	-4.51744400	0.89566500
H	0.52962200	-4.71027700	-0.83737000
C	-0.85313200	-2.04452000	2.08499800
H	-0.79882400	-1.30112700	2.89935100
H	-1.90585400	-2.13680900	1.77996200
H	-0.56210300	-3.02094400	2.52443000

[LCo(*sec*-Bu)] (with β-agostic interaction, css)

```
BLYP/BS1:
 Zero-point correction=                           0.623309 (Hartree/Particle)
 Thermal correction to Energy=                    0.661361
 Thermal correction to Enthalpy=                  0.662305
 Thermal correction to Gibbs Free Energy=         0.552161
 Sum of electronic and zero-point Energies=          -1514.399963
 Sum of electronic and thermal Energies=             -1514.361911
 Sum of electronic and thermal Enthalpies=           -1514.360966
 Sum of electronic and thermal Free Energies=        -1514.471111
E(RB-LYP/BS2) =  -1514.58443630

0 1
 C                 -1.21043900    2.38450500    0.09961300
 C                 -1.17216000    3.77707400    0.27673600
 C                  0.06710000    4.44570100    0.32216300
 C                  1.26609700    3.71431500    0.20402600
 C                  1.22131800    2.32201800    0.03165300
 N                 -0.01565400    1.66751900   -0.05308500
 H                  0.09924300    5.52817700    0.46394900
 H                 -2.10600300    4.33287000    0.38737200
 H                  2.23184800    4.22184300    0.25771700
 C                 -2.33430600    1.51034000    0.01906200
 C                  2.28986300    1.38217300   -0.08005600
 N                 -1.97549300    0.19913200   -0.02358500
 N                  1.84927800    0.10142200   -0.10926600
 Co                -0.06338900   -0.13551000    0.00379400
 C                 -2.99832700   -0.78822400   -0.22950100
 C                 -3.86592300   -1.16659800    0.82993900
 C                 -3.12378600   -1.39498900   -1.50855600
 C                 -4.78633100   -2.20871700    0.61025100
 C                 -4.06686600   -2.42498800   -1.67860400
 C                 -4.89302800   -2.86538800   -0.62819000
 H                 -5.44334700   -2.50887100    1.43385400
 H                 -4.16512400   -2.88819100   -2.66658900
 C                  2.79755500   -0.96456600   -0.24153600
 C                  2.98212100   -1.56542200   -1.51466000
 C                  3.49622400   -1.44166500    0.89526500
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C	3.84899000	-2.66617400	-1.61869800
C	4.34691600	-2.55451400	0.74104500
C	4.53046300	-3.18758600	-0.49998200
H	4.00071400	-3.12632200	-2.60102300
H	4.88036500	-2.93326200	1.61948600
C	-3.85753400	-0.45612500	2.17280100
H	-2.92769900	0.10279000	2.33464600
H	-4.69735500	0.25898000	2.23943200
H	-3.97852000	-1.17378400	3.00029800
C	-2.29623700	-0.93898200	-2.69928000
H	-1.90885000	0.08006200	-2.56108300
H	-1.42368500	-1.59539400	-2.86590500
H	-2.90282800	-0.96978100	-3.61994600
C	-5.86518300	-4.01492900	-0.82568200
H	-6.23287100	-4.05864800	-1.86432100
H	-5.38621900	-4.98781400	-0.60911100
H	-6.73710100	-3.92591800	-0.15693300
C	2.29127100	-1.00198600	-2.74259900
H	1.19371800	-1.06188200	-2.65894000
H	2.52584800	0.06768600	-2.87876500
H	2.60290900	-1.54347600	-3.64955300
C	3.36622200	-0.76049800	2.24664000
H	4.13535000	0.02358800	2.37277800
H	2.38434600	-0.28007400	2.36368200
H	3.50518600	-1.48462400	3.06559600
C	5.42460900	-4.40772600	-0.63473200
H	4.83272800	-5.34165300	-0.63991500
H	5.99951300	-4.38542500	-1.57598000
H	6.13971800	-4.47749400	0.20087300
C	-3.75794700	2.00640200	-0.06610000
H	-3.79587500	2.98685500	-0.56591300
H	-4.38650900	1.30389700	-0.63322600
H	-4.21870000	2.12517100	0.93176000
C	3.74699100	1.76491800	-0.16617300
H	3.85773300	2.79647300	-0.53331000
H	4.25267400	1.70264800	0.81488400
H	4.28911600	1.09335400	-0.85021300
C	-0.14348600	-2.41702200	-0.19252200
H	-1.11730800	-2.92284600	-0.26305300
H	0.67704700	-3.08296500	-0.50504800
C	0.08953300	-1.75084700	1.15602100
H	1.13028700	-1.85798000	1.47756100
H	-0.17645500	-1.65099500	-1.04915200
C	-0.84249900	-2.08424100	2.30897200
H	-1.89015000	-2.06725500	1.97860100
H	-0.65076400	-3.12670700	2.64991000
C	-0.63848200	-1.13456200	3.50729200
H	0.39841400	-1.19676000	3.88226300
H	-0.81460700	-0.08948600	3.20297300
H	-1.31603700	-1.37777700	4.34382000

TS Co(*sec*-Bu) to CoH(butene)

```
BLYP/BS1:
 Zero-point correction=                           0.620627 (Hartree/Particle)
 Thermal correction to Energy=                    0.657904
 Thermal correction to Enthalpy=                  0.658848
 Thermal correction to Gibbs Free Energy=         0.551251
 Sum of electronic and zero-point Energies=          -1514.388879
 Sum of electronic and thermal Energies=             -1514.351601
 Sum of electronic and thermal Enthalpies=           -1514.350657
 Sum of electronic and thermal Free Energies=        -1514.458255
E(RB-LYP/BS2) =  -1514.56891564

0 1
 C                 -1.20829300    2.30261000    0.25473900
 C                 -1.17131900    3.70004700    0.38320200
 C                  0.06767200    4.36835100    0.44264900
```

C	1.26543800	3.63527800	0.32614900
C	1.22077600	2.23816900	0.20000600
N	-0.01224000	1.57264900	0.24104600
H	0.09888600	5.45538900	0.54336300
H	-2.10593600	4.26406200	0.42164800
H	2.22941400	4.14891200	0.31989700
C	-2.33279500	1.44556500	0.07125400
C	2.28682500	1.31393100	-0.00894700
N	-1.98241300	0.13850800	-0.06097900
N	1.84888300	0.03803700	-0.14576700
Co	-0.06570700	-0.22241600	0.01313300
C	-3.01321500	-0.83852800	-0.27910400
C	-3.89165700	-1.21906700	0.77222300
C	-3.13961000	-1.43740900	-1.56356400
C	-4.80950100	-2.26286100	0.54362000
C	-4.08338300	-2.46450200	-1.74218500
C	-4.91107700	-2.91425300	-0.69655900
H	-5.47232200	-2.56388100	1.36229900
H	-4.18105700	-2.91859300	-2.73432400
C	2.80398000	-1.01968300	-0.29505600
C	2.98084400	-1.61378100	-1.57418300
C	3.53234800	-1.49133300	0.82739900
C	3.85993900	-2.70294200	-1.69445300
C	4.39197700	-2.59512900	0.65591500
C	4.56307400	-3.22264200	-0.58874200
H	4.00492600	-3.15482000	-2.68155600
H	4.94627300	-2.96789400	1.52409400
C	-3.92115700	-0.50959100	2.11624000
H	-3.02329200	0.09457300	2.28967300
H	-4.79589500	0.16314200	2.17474700
H	-4.01647700	-1.23186800	2.94334200
C	-2.32032900	-0.97035700	-2.75427800
H	-2.01150500	0.07931900	-2.64975900
H	-1.39446400	-1.55991300	-2.86895300
H	-2.90351800	-1.08401800	-3.68352100
C	-5.88085400	-4.06362500	-0.90491400
H	-6.28686600	-4.06853800	-1.93028300
H	-5.38589800	-5.03984100	-0.74755800
H	-6.72762100	-4.01008000	-0.20120600
C	2.27075200	-1.05992300	-2.79446100
H	1.18264000	-1.22820700	-2.73933500
H	2.40279900	0.03209800	-2.87407800
H	2.65440400	-1.52842600	-3.71453700
C	3.44200300	-0.81962300	2.18831500
H	4.29198100	-0.13001300	2.34327100
H	2.51753300	-0.23661700	2.29927300
H	3.48357200	-1.56689200	2.99772700
C	5.46910300	-4.43151000	-0.74228400
H	4.88688000	-5.37142100	-0.75054200
H	6.03491200	-4.39475600	-1.68859000
H	6.19252500	-4.50091900	0.08617000
C	-3.74928600	1.95979900	-0.03575000
H	-3.76412400	2.94957200	-0.51875600
H	-4.37166900	1.27621400	-0.63160600
H	-4.23211600	2.06802400	0.95238800
C	3.74124300	1.71091700	-0.08759800
H	3.84165400	2.74292500	-0.45783700
H	4.24165100	1.66233800	0.89677100
H	4.29441400	1.04466100	-0.76695600
C	-0.12643200	-2.32177900	0.02159000
H	-1.12242900	-2.72077400	-0.19644700
H	0.68593100	-2.83057600	-0.50830100
C	0.13653300	-1.81756000	1.33747700
H	1.18211500	-1.84203700	1.64925200
H	-0.15599300	-1.16804900	-1.15266300
C	-0.83448700	-1.89356000	2.49715600
H	-1.86480100	-1.95418500	2.12194700
H	-0.65298500	-2.84204000	3.04791700

```
 C                 -0.67802700   -0.72070300    3.48894600
 H                  0.34973400   -0.68858900    3.89173100
 H                 -0.86021000    0.24012800    2.98112900
 H                 -1.37295100   -0.81272500    4.34137900
```

[LCoH(butene)] isomer 1

```
BLYP/BS1:
 Zero-point correction=                           0.621134 (Hartree/Particle)
 Thermal correction to Energy=                    0.659770
 Thermal correction to Enthalpy=                  0.660715
 Thermal correction to Gibbs Free Energy=         0.548909
 Sum of electronic and zero-point Energies=          -1514.394338
 Sum of electronic and thermal Energies=             -1514.355701
 Sum of electronic and thermal Enthalpies=           -1514.354757
 Sum of electronic and thermal Free Energies=        -1514.466563
E(RB-LYP/BS2) =  -1514.57278423

0 1
 C                 -1.20880500    2.32829900    0.10916600
 C                 -1.17648200    3.73192100    0.12979100
 C                  0.06063200    4.40423200    0.15858300
 C                  1.25843000    3.66503400    0.11603600
 C                  1.21272300    2.26196400    0.09700000
 N                 -0.01756800    1.60112100    0.17895600
 H                  0.09075300    5.49572800    0.17855900
 H                 -2.11055000    4.29727500    0.11143700
 H                  2.22176800    4.17847100    0.08480100
 C                 -2.33485500    1.45860700   -0.02280700
 C                  2.28485000    1.32605400   -0.03234900
 N                 -1.99624500    0.14684400   -0.06885400
 N                  1.85993300    0.04364500   -0.09271600
 Co                -0.06754400   -0.20871100   -0.08697300
 C                 -3.06511200   -0.80680700   -0.20493000
 C                 -3.85877200   -1.14743700    0.92095600
 C                 -3.33245800   -1.39000700   -1.47422800
 C                 -4.85114600   -2.13717200    0.77583400
 C                 -4.34063900   -2.36562700   -1.56687300
 C                 -5.09757400   -2.77331100   -0.45127100
 H                 -5.45106200   -2.40907600    1.65114200
 H                 -4.54782000   -2.81189600   -2.54529500
 C                  2.85024700   -0.99173400   -0.18940700
 C                  3.16759100   -1.54696400   -1.45624500
 C                  3.48800100   -1.45657000    0.98896400
 C                  4.10176800   -2.59678600   -1.51056600
 C                  4.41031600   -2.51521900    0.88153600
 C                  4.72351800   -3.10726600   -0.35432400
 H                  4.35458000   -3.02363100   -2.48690500
 H                  4.89701900   -2.88267800    1.79130000
 C                 -3.70306600   -0.44989300    2.26149400
 H                 -2.74141400    0.07064900    2.34486300
 H                 -4.50440100    0.29752400    2.40651500
 H                 -3.78070000   -1.16901400    3.09284000
 C                 -2.59509600   -0.94707900   -2.72304000
 H                 -2.53667500    0.15182900   -2.78642500
 H                 -1.55412100   -1.30591400   -2.72719400
 H                 -3.10347700   -1.32547400   -3.62413300
 C                 -6.14318000   -3.86698900   -0.57550800
 H                 -6.66512600   -3.81860000   -1.54596300
 H                 -5.68411500   -4.87037800   -0.50468600
 H                 -6.89867000   -3.79567000    0.22387700
 C                  2.55718600   -0.99060800   -2.72757600
 H                  1.45805600   -1.06101200   -2.70925600
 H                  2.78918500    0.08251400   -2.84615200
 H                  2.93956200   -1.52548600   -3.61095200
 C                  3.21529800   -0.81305700    2.33729800
 H                  3.87571500    0.05734900    2.50660500
 H                  2.17960700   -0.45168900    2.41094900
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 H                  3.40166200   -1.52587200    3.15648400
 C                  5.69108300   -4.27434900   -0.44171100
 H                  5.15463900   -5.24120300   -0.43735700
 H                  6.28471600   -4.23817200   -1.37046300
 H                  6.38941600   -4.28428800    0.41104200
 C                 -3.75505000    1.95991400   -0.14622700
 H                 -3.77103000    2.99130500   -0.52900000
 H                 -4.33822900    1.32798300   -0.83302700
 H                 -4.28289400    1.95770000    0.82440200
 C                  3.74136400    1.71566200   -0.11799200
 H                  3.84788300    2.78515600   -0.35103100
 H                  4.27755400    1.52445800    0.82881800
 H                  4.25943400    1.13875100   -0.90063900
 C                 -0.15345100   -2.28611600   -0.39799800
 H                 -1.15746500   -2.57144100   -0.72060100
 H                  0.65493800   -2.56935600   -1.07531500
 C                  0.11769200   -2.08168800    0.96641600
 H                  1.16697600   -2.12353500    1.26536700
 H                 -0.09148500   -0.27558200   -1.57238200
 C                 -0.83921600   -2.34754000    2.11069700
 H                 -1.87926100   -2.24997600    1.77283800
 H                 -0.71786900   -3.41078600    2.41033100
 C                 -0.57197300   -1.46467500    3.34816600
 H                  0.44782100   -1.63379900    3.73523200
 H                 -0.65339400   -0.39657100    3.08783300
 H                 -1.28270300   -1.68301700    4.16318700
```

[LCoH(butene)] isomer 2

```
BLYP/BS1:
 Zero-point correction=                           0.621244 (Hartree/Particle)
 Thermal correction to Energy=                    0.659115
 Thermal correction to Enthalpy=                  0.660060
 Thermal correction to Gibbs Free Energy=         0.551385
 Sum of electronic and zero-point Energies=          -1514.396948
 Sum of electronic and thermal Energies=             -1514.359076
 Sum of electronic and thermal Enthalpies=           -1514.358132
 Sum of electronic and thermal Free Energies=        -1514.466807
E(RB-LYP/BS2) =  -1514.57625460

0 1
 C                 -1.17784700    2.46712300   -0.15454400
 C                 -1.14559600    3.86652400   -0.26342400
 C                  0.09035100    4.54000400   -0.29460900
 C                  1.29132200    3.80719500   -0.23064200
 C                  1.25144300    2.40816800   -0.12330400
 N                  0.01997300    1.75033900   -0.05928700
 H                  0.11786500    5.62864500   -0.37739700
 H                 -2.08004100    4.42799800   -0.32726900
 H                  2.25333500    4.32220600   -0.27176700
 C                 -2.30079200    1.58532200   -0.11711200
 C                  2.32936000    1.47222300   -0.06221500
 N                 -1.93908800    0.28228800   -0.04909900
 N                  1.90733000    0.18629000   -0.01812500
 Co                -0.02504700   -0.07398700   -0.16723000
 C                 -2.98262700   -0.69465700    0.07081600
 C                 -3.43181300   -1.05912800    1.36442900
 C                 -3.53155200   -1.29433500   -1.09108100
 C                 -4.41319500   -2.06214000    1.47486700
 C                 -4.51129300   -2.29045000   -0.92815100
 C                 -4.95746500   -2.69839000    0.34404500
 H                 -4.76229100   -2.35009200    2.47222300
 H                 -4.93721200   -2.75979800   -1.82130700
 C                  2.91326800   -0.83192900    0.07807900
 C                  3.50535400   -1.35711700   -1.09661200
 C                  3.30429800   -1.29056500    1.36180900
 C                  4.45552100   -2.38746800   -0.96329400
 C                  4.25416000   -2.32506100    1.44288000
```

C	4.83216100	-2.89717800	0.29316200
H	4.90914800	-2.80419500	-1.86888700
H	4.55469000	-2.68812500	2.43149800
C	-2.90472200	-0.34603600	2.59692100
H	-1.81487100	-0.19680100	2.54384800
H	-3.35104500	0.66037100	2.69759800
H	-3.14694400	-0.90970600	3.51157300
C	-3.07747900	-0.86028500	-2.47091400
H	-3.38702000	0.17774300	-2.68886400
H	-1.97897500	-0.87709100	-2.54840700
H	-3.50631000	-1.51152700	-3.24855000
C	-5.98241700	-3.80949400	0.49009900
H	-6.69667200	-3.81298700	-0.35000800
H	-5.49757300	-4.80316000	0.50836500
H	-6.55548600	-3.70946000	1.42647100
C	3.14012200	-0.80729900	-2.46180600
H	2.07021200	-0.55777100	-2.51222600
H	3.69864600	0.12160300	-2.68123600
H	3.38010700	-1.53200500	-3.25550700
C	2.75330500	-0.63537900	2.61521100
H	3.19329000	0.36773800	2.76416800
H	1.66403400	-0.48986800	2.54781900
H	2.98308700	-1.23731500	3.50843800
C	5.81981100	-4.04521700	0.40588500
H	5.30134700	-5.02195100	0.40691200
H	6.52711900	-4.05348800	-0.43972700
H	6.40283500	-3.98640000	1.33986900
C	-3.74163000	2.03398000	-0.14957700
H	-3.81371300	3.13094500	-0.15628800
H	-4.26418400	1.65199300	-1.04437800
H	-4.30128600	1.66102800	0.72482400
C	3.78829200	1.86049700	-0.04304100
H	3.90414700	2.94761200	0.07312400
H	4.32226300	1.36925400	0.78699900
H	4.30466200	1.56125200	-0.97252800
C	-0.05964300	-2.03195300	0.90798100
H	0.92986700	-2.22119100	1.32724300
H	-0.87291500	-1.89263000	1.62060400
C	-0.33107000	-2.38558300	-0.41229800
H	-1.37836900	-2.40917100	-0.72239700
H	-0.01380000	-0.28512400	-1.66743300
C	0.60213600	-3.16842900	-1.31386300
H	1.64992900	-2.91283200	-1.10605500
H	0.49196600	-4.23834000	-1.03591000
C	0.29114500	-3.02854900	-2.81731400
H	-0.74419100	-3.34432700	-3.03587700
H	0.39551800	-1.98202700	-3.14132000
H	0.97017100	-3.65264900	-3.42255400

Transition structure CoH(butene) to Co(*n*-Bu)

```
Zero-point correction=                           0.621706 (Hartree/Particle)
 Thermal correction to Energy=                    0.659368
 Thermal correction to Enthalpy=                  0.660312
 Thermal correction to Gibbs Free Energy=         0.552024
 Sum of electronic and zero-point Energies=          -1514.390106
 Sum of electronic and thermal Energies=             -1514.352444
 Sum of electronic and thermal Enthalpies=           -1514.351500
 Sum of electronic and thermal Free Energies=        -1514.459789
E(RB-LYP/BS2) =  -1514.57094843
```

0 1

C	-1.30446700	2.91633400	-0.17933400
C	-1.33064500	4.31851700	-0.24639600
C	-0.12440100	5.04445900	-0.25763400
C	1.10526900	4.36245200	-0.18470600

C	1.12593300	2.96019400	-0.11942700
N	-0.07620800	2.24247500	-0.14768800
H	-0.14289300	6.13537100	-0.30619500
H	-2.28850700	4.84176700	-0.28100000
H	2.04424700	4.91979900	-0.17325300
C	-2.39292700	1.99263100	-0.10393000
C	2.24095200	2.07489500	0.00708100
N	-1.98062200	0.70980100	0.02166900
N	1.87092500	0.77482700	0.09728500
Co	-0.04634400	0.42047400	-0.06873900
C	-2.97776400	-0.31311600	0.14323000
C	-3.40019000	-0.70124700	1.43947300
C	-3.50365400	-0.93803100	-1.01560300
C	-4.33421600	-1.74715800	1.55520600
C	-4.43344400	-1.98105800	-0.84732200
C	-4.85398500	-2.40870400	0.42665900
H	-4.66428900	-2.05067300	2.55441100
H	-4.84158700	-2.47020300	-1.73820800
C	2.91082600	-0.20356000	0.22720300
C	3.55207300	-0.71147200	-0.92888500
C	3.27676500	-0.64955600	1.52236400
C	4.53628000	-1.70510800	-0.76647200
C	4.26337300	-1.64593200	1.63326300
C	4.89728500	-2.19601000	0.50207500
H	5.02895900	-2.10833300	-1.65772400
H	4.54721200	-1.99750700	2.63093300
C	-2.88563700	0.03162700	2.66458800
H	-1.79054600	0.14825000	2.62901500
H	-3.30420200	1.05270500	2.72557300
H	-3.16288900	-0.50084600	3.58785300
C	-3.08785800	-0.48034000	-2.40107700
H	-3.48002600	0.52740300	-2.62768700
H	-1.99178600	-0.41384900	-2.48770800
H	-3.46764500	-1.16940000	-3.17166300
C	-5.82537900	-3.56616800	0.57897800
H	-6.51413400	-3.63084600	-0.27956700
H	-5.29199200	-4.53281100	0.64203300
H	-6.42945500	-3.46818900	1.49603100
C	3.19381100	-0.18805300	-2.30677500
H	2.11338500	0.00383900	-2.38713600
H	3.70655800	0.76786300	-2.52034200
H	3.49072000	-0.90384600	-3.08922800
C	2.64961900	-0.02294500	2.75335400
H	2.99685500	1.01738600	2.89039600
H	1.55321800	0.02543000	2.65928100
H	2.91195600	-0.58826800	3.66138700
C	5.92582300	-3.30391500	0.64702900
H	5.44452800	-4.29941000	0.66177700
H	6.64250800	-3.30121500	-0.19062400
H	6.49577400	-3.20576400	1.58584900
C	-3.84987900	2.38440500	-0.14876800
H	-3.96813700	3.47577800	-0.08788300
H	-4.33405500	2.04343200	-1.08170400
H	-4.41311600	1.93031800	0.68319600
C	3.68050600	2.52721900	0.05558900
H	3.74580900	3.61457100	0.20593100
H	4.22613300	2.03335000	0.87599300
H	4.22062400	2.28351400	-0.87714800
C	-0.04155000	-1.52560200	0.90297300
H	0.92858500	-1.72363500	1.36331600
H	-0.90419300	-1.55372000	1.56937600
C	-0.22098800	-1.86105700	-0.47330500
H	-1.25746500	-2.00720300	-0.79410400
H	-0.05852900	-0.43733800	-1.41615100
C	0.77744900	-2.70549100	-1.25424600
H	1.80573900	-2.41265200	-1.00219900
H	0.65537100	-3.74427700	-0.88498700
C	0.56278700	-2.69173500	-2.77957400

```
 H                -0.45743600   -3.02568200   -3.03859800
 H                 0.69404700   -1.67613200   -3.18616300
 H                 1.27730500   -3.36063100   -3.28784900
```

[LCo(*n*-Bu)] (oss)

```
UBLYP/BS1:
 Zero-point correction=                           0.623450 (Hartree/Particle)
 Thermal correction to Energy=                    0.661855
 Thermal correction to Enthalpy=                  0.662799
 Thermal correction to Gibbs Free Energy=         0.551227
 Sum of electronic and zero-point Energies=          -1514.409147
 Sum of electronic and thermal Energies=             -1514.370742
 Sum of electronic and thermal Enthalpies=           -1514.369798
 Sum of electronic and thermal Free Energies=        -1514.481370
E(UB-LYP/BS2) =  -1515.03259701

0 1
 C                -1.49918600    3.05059200   -0.21293000
 C                -1.63419500    4.44962700   -0.29970200
 C                -0.46954900    5.24502600   -0.33478500
 C                 0.80936100    4.65345700   -0.27024900
 C                 0.90495900    3.25113800   -0.18325500
 N                -0.24161700    2.48474300   -0.17928000
 H                -0.55950100    6.33195800   -0.40146800
 H                -2.62482100    4.90791000   -0.33227000
 H                 1.71138400    5.26878400   -0.28147100
 C                -2.51121800    2.01684000   -0.14347000
 C                 2.07287100    2.39967600   -0.09017500
 N                -2.00036600    0.77788600    0.01255900
 N                 1.77254300    1.09393400    0.05590500
 Co               -0.09759200    0.65129800    0.12496600
 C                -2.86470900   -0.36706900    0.04458400
 C                -3.41942000   -0.79204700    1.27453900
 C                -3.06789700   -1.10127100   -1.14779300
 C                -4.18015900   -1.97548300    1.28876700
 C                -3.83900500   -2.27577400   -1.08451700
 C                -4.39687200   -2.73569700    0.12393400
 H                -4.60861500   -2.31388700    2.23818600
 H                -4.00133100   -2.84888800   -2.00350800
 C                 2.80954400    0.10304600    0.08829800
 C                 3.16861500   -0.54676400   -1.11751700
 C                 3.37176200   -0.28312900    1.32716600
 C                 4.07873900   -1.61606000   -1.05432000
 C                 4.27903100   -1.35914900    1.34044000
 C                 4.63293700   -2.04968300    0.16621900
 H                 4.35335700   -2.12972100   -1.98169100
 H                 4.71077200   -1.67121600    2.29714500
 C                -3.18301800    0.01369700    2.53638100
 H                -2.10620500    0.20719000    2.67827400
 H                -3.68000900    0.99938900    2.49173700
 H                -3.56757000   -0.51738100    3.42101300
 C                -2.45620400   -0.62571100   -2.45098400
 H                -2.80672600    0.38558300   -2.72129200
 H                -1.35682000   -0.56168800   -2.36917900
 H                -2.70644400   -1.30963300   -3.27695600
 C                -5.18322400   -4.03398700    0.17573500
 H                -4.52410400   -4.89329100    0.39926300
 H                -5.95765800   -4.00626700    0.96008600
 H                -5.67801000   -4.24516700   -0.78661800
 C                 2.57595600   -0.08896700   -2.43636800
 H                 1.47328100   -0.06636500   -2.38864500
 H                 2.89714100    0.93667900   -2.69143800
 H                 2.87956700   -0.75599700   -3.25805000
 C                 3.00331500    0.45832900    2.59706900
 H                 3.38948400    1.49369500    2.58791900
 H                 1.90833300    0.52947500    2.70735100
```

```
 H                  3.41662400   -0.04764700    3.48340300
 C                  5.56012900   -3.25127500    0.21390200
 H                  6.19493800   -3.23647000    1.11481500
 H                  4.98596100   -4.19588000    0.23160400
 H                  6.21971600   -3.28995100   -0.66929800
 C                 -3.98423400    2.32563700   -0.23552200
 H                 -4.33477200    2.86389000    0.66474500
 H                 -4.19503800    2.97667200   -1.10167400
 H                 -4.57585000    1.40542300   -0.33367700
 C                  3.47574700    2.94718200   -0.16543000
 H                  3.66775000    3.65705100    0.65952300
 H                  4.21775900    2.13946600   -0.10743500
 H                  3.63312900    3.50125900   -1.10822300
 C                  0.05509600   -1.15033000    0.91346200
 H                  0.93090100   -1.16506300    1.58465500
 H                 -0.83669000   -1.41215700    1.50870500
 C                  0.25620100   -2.20477700   -0.20079000
 H                 -0.70556800   -2.40397900   -0.70667300
 H                  0.94992100   -1.83455100   -0.97585700
 C                  0.83995300   -3.54146600    0.32164100
 H                  1.78621000   -3.32618000    0.85048900
 H                  0.14898000   -3.97354100    1.07007800
 C                  1.10433200   -4.55874200   -0.80583700
 H                  0.17627200   -4.79623100   -1.35590300
 H                  1.82889600   -4.15074100   -1.53318200
 H                  1.51604400   -5.50618600   -0.41581600
```

$[Al_3(\mu\text{-}H)_3Pr_6]$ (**3**, R = Pr)

```
BLYP/BS1
 Zero-point correction=                           0.574042 (Hartree/Particle)
 Thermal correction to Energy=                    0.609285
 Thermal correction to Enthalpy=                  0.610229
 Thermal correction to Gibbs Free Energy=         0.501071
 Sum of electronic and zero-point Energies=          -1439.353762
 Sum of electronic and thermal Energies=             -1439.318519
 Sum of electronic and thermal Enthalpies=           -1439.317575
 Sum of electronic and thermal Free Energies=        -1439.426734
E(RB-LYP/BS2) =  -1440.24786272

0 1
 Al                 0.55642000    1.82507800    0.16543200
 Al                -1.60764400   -0.39819300    0.64158700
 C                 -2.63551900   -0.85139200    2.27322300
 C                 -3.14911800   -2.31699400    2.28070700
 H                 -3.49858300   -0.16183700    2.36566600
 H                 -2.01584200   -0.67314300    3.17328700
 H                 -3.77652000   -2.50060700    1.38734100
 H                 -2.29288800   -3.01359200    2.19737300
 C                 -2.27365600   -0.35330600   -1.22635400
 C                 -3.37520700    0.71320600   -1.46826800
 H                 -2.65931800   -1.35050600   -1.51625400
 H                 -1.42812600   -0.16230200   -1.91531900
 H                 -4.26779200    0.47208600   -0.86024100
 H                 -3.02824300    1.70222100   -1.11639500
 C                  1.80047300    2.34110700    1.62013900
 C                  3.25273200    2.58350000    1.12797300
 H                  1.80514200    1.53605900    2.38148100
 H                  1.43461300    3.24332000    2.14860200
 H                  3.59708500    1.71802700    0.53115700
 H                  3.27394300    3.45153300    0.44184500
 C                 -0.15308400    2.88157600   -1.35325400
 C                 -1.16397400    3.98490900   -0.94064000
 H                 -0.64609000    2.18157300   -2.05559500
 H                  0.67532400    3.34046600   -1.92802200
 H                 -1.95673700    3.55229800   -0.29988500
 H                 -0.65559800    4.74488300   -0.31724600
 H                 -0.81445600    1.10172400    0.91733600
```

H	-0.19275100	-1.36596600	0.70716900
H	1.21524000	0.39373300	-0.51730700
Al	1.28716800	-1.28580000	-0.16396600
C	2.74269300	-1.50277000	1.16358700
C	4.16303200	-1.30736000	0.56798800
H	2.58600700	-0.77041100	1.97982100
H	2.68264800	-2.49812600	1.64634100
H	4.36429700	-2.09581800	-0.18186000
H	4.21543900	-0.34859600	0.01709800
C	0.98280600	-2.25617000	-1.86768700
C	0.06527100	-3.50046900	-1.72406000
H	0.53949500	-1.56562000	-2.61091400
H	1.95587700	-2.56856500	-2.29621000
H	0.50396100	-4.21281200	-0.99852600
H	-0.90948500	-3.19724300	-1.29762700
C	-1.83007300	4.67956500	-2.14723000
H	-2.38677300	3.94734400	-2.75800200
H	-1.07198700	5.14868200	-2.79839600
C	4.25629400	2.81865400	2.27612500
H	4.28881300	1.94281300	2.94796700
H	3.96407800	3.69310900	2.88366500
C	5.27864800	-1.32273100	1.63386200
H	5.12931200	-0.50874400	2.36498500
H	5.27741500	-2.27585700	2.19124000
C	-0.18227900	-4.23234800	-3.05978900
H	-0.66095200	-3.55704400	-3.79046400
H	0.76846900	-4.57944600	-3.50081900
C	-3.78754400	0.83599100	-2.95007700
H	-2.92133000	1.12632300	-3.57067000
H	-4.16429300	-0.12750800	-3.33591700
C	-3.96222000	-2.67069800	3.54417400
H	-3.35125200	-2.53449600	4.45367600
H	-4.84651000	-2.01608900	3.63662900
H	-4.57763900	1.59358700	-3.09543900
H	-2.53853000	5.46468400	-1.82943600
H	-0.83758300	-5.11165500	-2.93016000
H	-4.31480100	-3.71696100	3.52540200
H	5.27883900	2.99296200	1.89781900
H	6.27842300	-1.19328700	1.18333800

[LCo(μ-H)$_2$AlPr$_2$] (**7b**, R = Pr)

```
Zero-point correction=                           0.706164 (Hartree/Particle)
 Thermal correction to Energy=                    0.748536
 Thermal correction to Enthalpy=                  0.749481
 Thermal correction to Gibbs Free Energy=         0.634496
 Sum of electronic and zero-point Energies=          -1837.159164
 Sum of electronic and thermal Energies=             -1837.116791
 Sum of electronic and thermal Enthalpies=           -1837.115847
 Sum of electronic and thermal Free Energies=        -1837.230831
E(RB-LYP/BS2) =  -1837.47928416
```

```
0 1
 C                 -2.10319900    1.26366300   -0.95306200
 C                 -2.18151200    2.31654700   -1.88026400
 C                 -0.99888900    2.88205500   -2.39228200
 C                  0.25176100    2.40299400   -1.95878100
 C                  0.30721300    1.34775400   -1.03308100
 N                 -0.86446200    0.77250700   -0.55722500
 H                 -1.05125900    3.69914600   -3.11487400
 H                 -3.15623400    2.69163800   -2.19788400
 H                  1.17478300    2.84667700   -2.33664400
 C                 -3.15504900    0.58017300   -0.25730700
 C                  1.44844400    0.72591100   -0.42442400
 N                 -2.70151500   -0.38827500    0.56518700
 N                  1.11780600   -0.25990800    0.43264800
 Co                -0.78196700   -0.66556700    0.57966000
 C                 -3.69744200   -1.09422500    1.32954100
```

C	-3.95747400	-0.68404700	2.66052900
C	-4.44702500	-2.12503400	0.71611700
C	-4.98867500	-1.33094900	3.36572600
C	-5.46388300	-2.74431000	1.46569900
C	-5.75065100	-2.36561900	2.78992100
H	-5.20041800	-1.01773000	4.39336600
H	-6.04054500	-3.55124600	1.00207700
C	2.20990800	-0.93932800	1.07705700
C	2.91418300	-1.95141300	0.38180000
C	2.58245000	-0.54287700	2.38351300
C	4.01108500	-2.55510600	1.02282100
C	3.68628300	-1.17742500	2.98126400
C	4.41332000	-2.18599100	2.32001300
H	4.55746000	-3.34443800	0.49702700
H	3.98312000	-0.87593400	3.99108900
C	-3.17589000	0.45348400	3.28682300
H	-2.09376000	0.24595600	3.26616300
H	-3.32070600	1.39745500	2.73152300
H	-3.49014000	0.61738800	4.32938300
C	-4.15611800	-2.55715800	-0.70900600
H	-4.55643900	-1.84061600	-1.44867000
H	-3.07135200	-2.62759200	-0.88453900
H	-4.61194900	-3.53731700	-0.91849200
C	-6.81877800	-3.08446200	3.59305800
H	-7.62097900	-3.47184300	2.94357500
H	-6.39013800	-3.94802600	4.13300900
H	-7.27518000	-2.41978200	4.34496500
C	2.48947200	-2.38718400	-1.00736400
H	1.41191800	-2.61670000	-1.03316800
H	2.66054100	-1.60005700	-1.76269700
H	3.04909900	-3.28125400	-1.32220400
C	1.81685700	0.54720100	3.10660000
H	1.81656000	1.49212900	2.53544800
H	0.75914600	0.26277400	3.23397900
H	2.25475100	0.74332000	4.09775000
C	5.57203900	-2.88726700	3.00548900
H	5.22242300	-3.77228100	3.56815900
H	6.31871500	-3.24067900	2.27558500
H	6.07959800	-2.22236000	3.72350200
C	-4.61214900	0.95813700	-0.38067700
H	-4.71862800	1.94687600	-0.84985300
H	-5.18031800	0.23234800	-0.98809600
H	-5.09241200	0.98882300	0.60989100
C	2.87065700	1.16319400	-0.68193800
H	2.89393000	2.14210200	-1.18201500
H	3.43293300	1.24079500	0.26177200
H	3.41511100	0.44378700	-1.31820100
Al	-0.65066400	-2.94400600	1.58303500
C	-2.15267400	-4.23953600	1.82090200
C	0.96694300	-3.80138000	2.38124200
C	-2.70853100	-4.29618300	3.26784300
H	-2.99167600	-4.12625700	1.11963000
H	-1.69436500	-5.22479600	1.58758000
H	1.78514700	-3.11369100	2.63531500
H	0.59211100	-4.19043700	3.35352600
C	-3.75050800	-5.41681900	3.47546300
H	-1.87911200	-4.44403900	3.98676700
C	2.65276700	-5.76077700	2.31758900
H	-4.60183900	-5.28088000	2.78653200
H	-4.14587500	-5.43058000	4.50806500
H	-3.31034100	-6.40877100	3.26917000
H	3.49926500	-5.08390400	2.52267900
H	3.03442100	-6.61617700	1.73060500
H	2.29331600	-6.14813800	3.28739800
H	-0.66736300	-2.18775200	-0.02422600
H	-3.17105200	-3.32859000	3.52416900
H	-0.77063200	-1.25308200	2.09847800
C	1.52712600	-5.00459500	1.57925400

```
 H                  1.91545300   -4.65785100    0.60462300
 H                  0.71353800   -5.71821000    1.34583700
```

[$Pr_2Al(\mu\text{-}H,Me)AlPr_2$]

```
BLYP/BS1:
 Zero-point correction=                           0.409490 (Hartree/Particle)
 Thermal correction to Energy=                    0.434357
 Thermal correction to Enthalpy=                  0.435301
 Thermal correction to Gibbs Free Energy=         0.350917
 Sum of electronic and zero-point Energies=           -998.821248
 Sum of electronic and thermal Energies=              -998.796380
 Sum of electronic and thermal Enthalpies=            -998.795436
 Sum of electronic and thermal Free Energies=         -998.879821
E(RB-LYP/BS2) =  -999.460890455

0 1
 C                  2.56350900   -1.04214100   -0.97887700
 H                  3.15342000   -0.69265900   -1.84987400
 H                  1.94544300   -1.87893600   -1.35982200
 C                  1.98424100    2.23377000    0.20249000
 H                  1.13198300    2.78163900    0.65177400
 H                  2.73155700    2.13987800    1.01727700
 C                 -2.23937300    1.78673900    0.06415300
 H                 -1.54373800    2.57388400    0.41630800
 H                 -2.73107700    2.21330800   -0.83300100
 C                 -2.04594100   -1.50925900   -1.12617800
 H                 -1.26069500   -2.17723200   -1.53169400
 H                 -2.48398900   -2.06246100   -0.27022500
 H                  0.08389900    0.64624300   -1.50447900
 Al                 1.38766600    0.42933400   -0.36106500
 Al                -1.22522100    0.16563900   -0.45717200
 C                  3.53658900   -1.57668900    0.10628900
 H                  4.16387300   -0.74893600    0.48973500
 H                  2.96228800   -1.94829800    0.97687800
 C                  2.59098500    3.08789500   -0.94214800
 H                  3.45293000    2.55747200   -1.39099600
 H                  1.84911600    3.20006200   -1.75606900
 C                 -3.31638000    1.52994000    1.15202700
 H                 -4.02841300    0.75857300    0.80075500
 H                 -2.84321500    1.10878600    2.06152100
 C                 -3.14465200   -1.28985700   -2.19996700
 H                 -3.93379100   -0.62669600   -1.79680300
 H                 -2.71827000   -0.75430300   -3.07011600
 C                  3.04859700    4.48938500   -0.48569000
 H                  2.20150800    5.05970000   -0.06543900
 H                  3.82004200    4.41335000    0.30086600
 C                  4.45594200   -2.70787400   -0.40131200
 H                  3.85925700   -3.56493800   -0.75997700
 H                  5.07620500   -2.35932500   -1.24558000
 C                 -3.79268700   -2.60217800   -2.68977800
 H                 -3.03468700   -3.27124000   -3.13367900
 H                 -4.26215700   -3.14431200   -1.84991100
 C                 -4.10497800    2.79661700    1.54734900
 H                 -3.42634300    3.57312300    1.94177700
 H                 -4.62250500    3.22308100    0.67026100
 C                  0.10407400   -0.45330400    1.15640500
 H                  0.91998100   -0.09480500    1.81674600
 H                 -0.78210300   -0.21688200    1.77919800
 H                  0.18955800   -1.55122000    1.11635700
 H                 -4.57071800   -2.41815700   -3.45159600
 H                 -4.86472100    2.58464700    2.32030000
 H                  3.47200000    5.07632300   -1.31987900
 H                  5.13410300   -3.07346900    0.38991400
```

[$LCo(\mu\text{-}H)_2Al_2(\mu\text{-}Me)Pr_4$] (**9**)

```
BLYP/BS1:
 Zero-point correction=                           0.927117 (Hartree/Particle)
 Thermal correction to Energy=                    0.984310
 Thermal correction to Enthalpy=                  0.985254
 Thermal correction to Gibbs Free Energy=         0.837682
 Sum of electronic and zero-point Energies=          -2356.202023
 Sum of electronic and thermal Energies=             -2356.144830
 Sum of electronic and thermal Enthalpies=           -2356.143885
 Sum of electronic and thermal Free Energies=        -2356.291457
E(RB-LYP/BS2) =  -2356.87091297

0 1
 C                 -2.05493400    1.43855500   -0.92171700
 C                 -2.09518000    2.52819200   -1.80508400
 C                 -0.89443100    3.03334200   -2.33812300
 C                  0.33023800    2.45534000   -1.95833200
 C                  0.34468900    1.36997500   -1.06512700
 N                 -0.84675000    0.84661300   -0.57310200
 H                 -0.91167000    3.87662200   -3.03150000
 H                 -3.05586600    2.97496700   -2.06901400
 H                  1.26997200    2.84983400   -2.34897600
 C                 -3.14287600    0.79084900   -0.24885100
 C                  1.46107300    0.67442000   -0.49427100
 N                 -2.74385300   -0.22704600    0.53053900
 N                  1.09682600   -0.31059100    0.34837500
 Co                -0.82115500   -0.58575900    0.57357400
 C                 -3.74561100   -0.98455400    1.22451500
 C                 -4.04384600   -0.66236900    2.56945000
 C                 -4.45507100   -1.99203300    0.52862100
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 C                 -5.37126700   -2.77497000    1.25542200
 C                 -5.61577400   -2.55416700    2.62541900
 H                 -5.19476400   -1.24308800    4.30023100
 H                 -5.90682500   -3.57656800    0.73697700
 C                  2.18255600   -1.00272100    0.99349100
 C                  2.80508700   -2.08273500    0.32721400
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 C                  3.89601900   -2.71106000    0.95674500
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 C                  4.38981000   -2.27422300    2.19998800
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 H                 -3.85853600    1.48952300    2.70410600
 H                 -3.69360800    0.64670300    4.26657900
 C                 -4.28019400   -2.15835400   -0.96939600
 H                 -4.73445000   -1.31064600   -1.51219000
 H                 -3.21669100   -2.19331900   -1.25092400
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C	-2.48398900	-4.84128000	-0.14134500
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H	-2.17729100	-4.90395800	-1.20588800
H	1.51664400	-4.15602500	1.05593200
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Al	-0.67624800	-2.15802600	3.31389200
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H	-1.31551100	-2.18784400	5.75301600
C	2.41615300	-4.89775200	4.76500300
H	0.51573200	-4.10765900	5.47369400
C	-1.36433400	0.42024500	6.83501800
H	2.91790000	-5.11791100	3.80617800
H	2.35588600	-5.83801500	5.34252000
H	3.05998000	-4.19538000	5.32400500
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H	-0.85663000	1.34011400	7.17730800
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H	-0.74445700	-0.88786300	2.17077600
H	0.40918700	-5.01851100	3.96403400
C	-2.01764600	-3.77444400	2.80035300
H	-1.99253800	-3.74044900	3.90713200
H	-3.05070400	-3.51425100	2.53001500
H	-1.88593700	-4.86048900	2.63959000
C	-0.78751300	-0.10077900	5.50074600
H	-0.87463200	0.69888100	4.74087900
H	0.29826300	-0.27703200	5.62297400
C	0.92067100	-5.64841600	-0.40797200
H	0.91139500	-5.00113500	-1.30442400
H	0.10581600	-6.37761700	-0.56496400