Supplementary Information

Insertion and isomerisation of internal olefins at alkylaluminium hydride: catalysis with zirconocene dichloride

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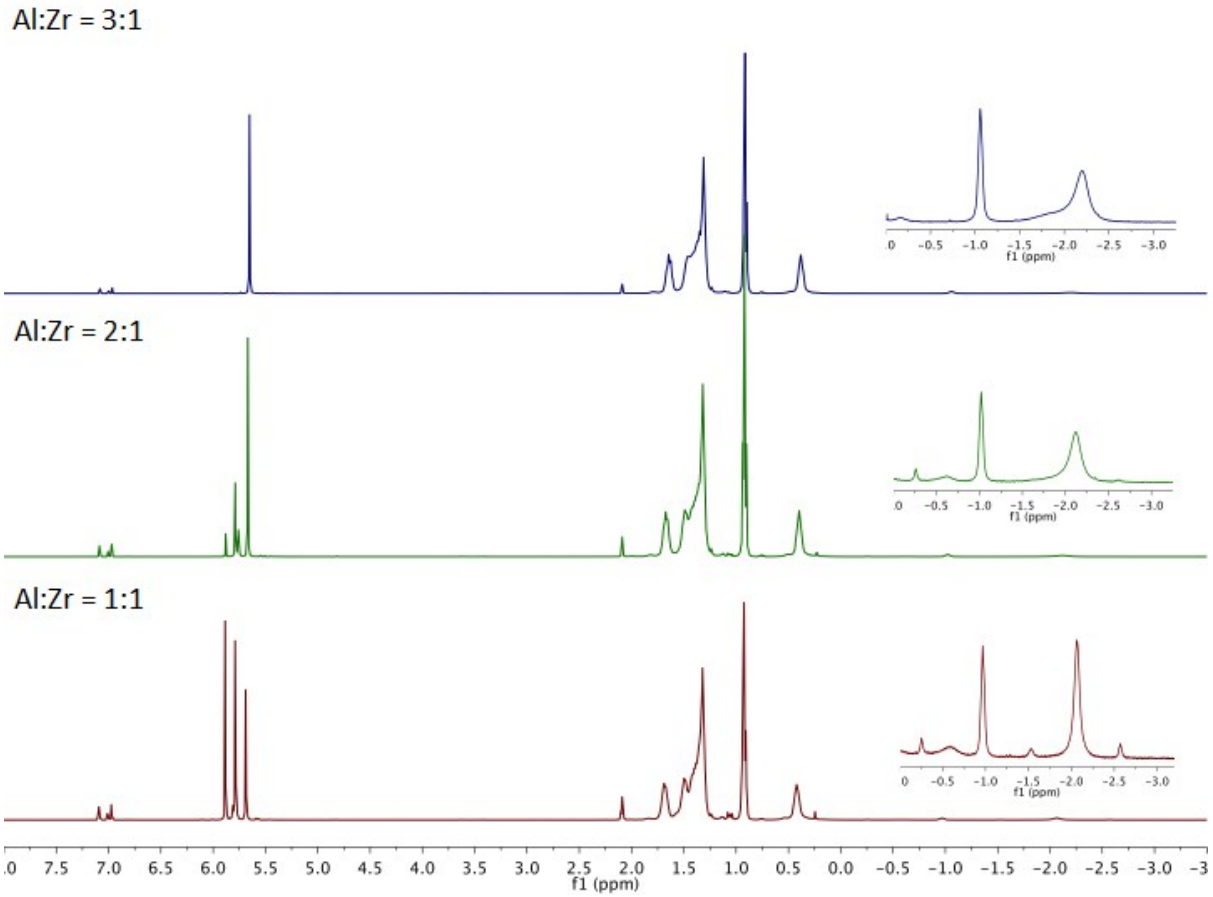


Figure S1. ^{1}H NMR spectra of $[Cp_2ZrCl_2]$ + $[Al(Oct)_2H]$ at different Al/Zr ratios.

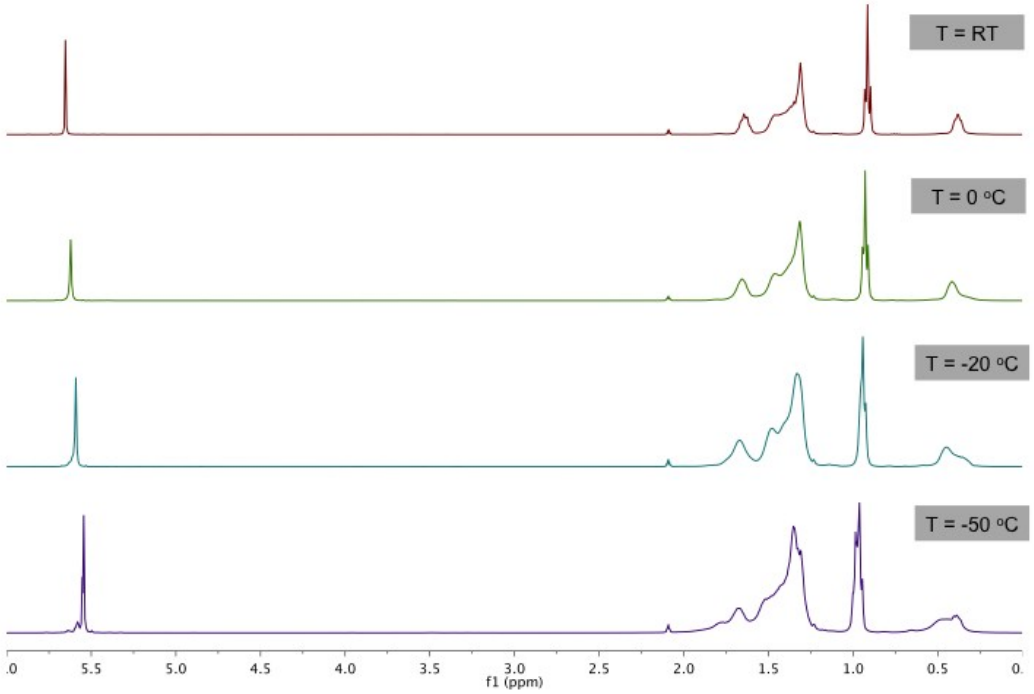


Figure S2. VT ^{1}H NMR spectroscopy of [Cp_2ZrCl_2] + 3 [$Al(Oct)_2H$] in toluene-d_8.

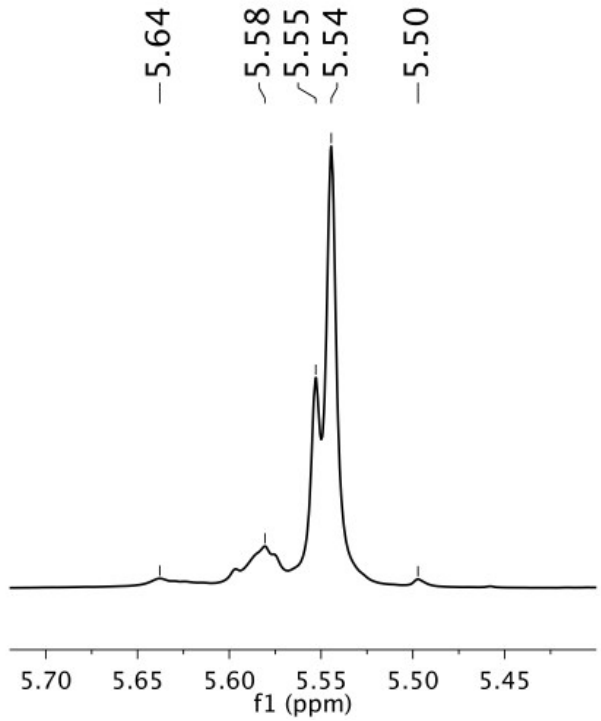


Figure S3. ^{1}H NMR spectrum of [Cp_2ZrCl_2] + 3 [$Al(Oct)_2H$] in the cyclopentadienyl*H* region (-50 °C, toluene-d_8).

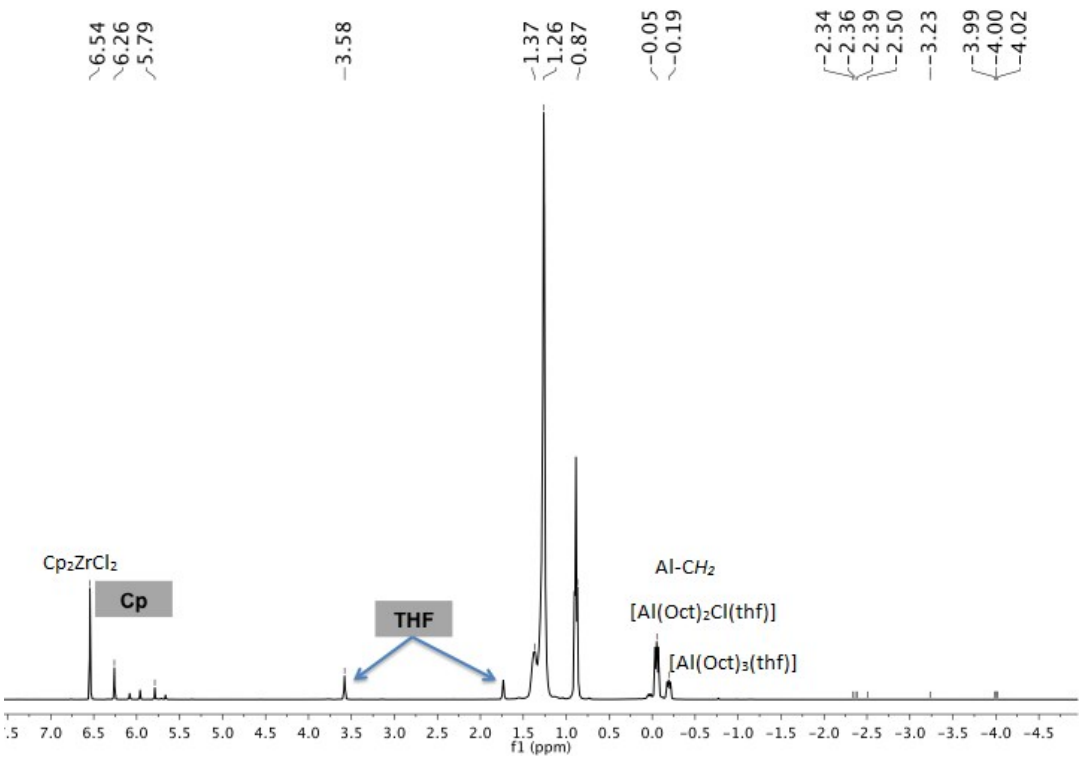


Figure S4. ^{1}H NMR spectrum of $[Cp_2ZrCl_2]$ + $[Al(Oct)_2H]$ (1:1) in THF-d_8 (-50 °C).

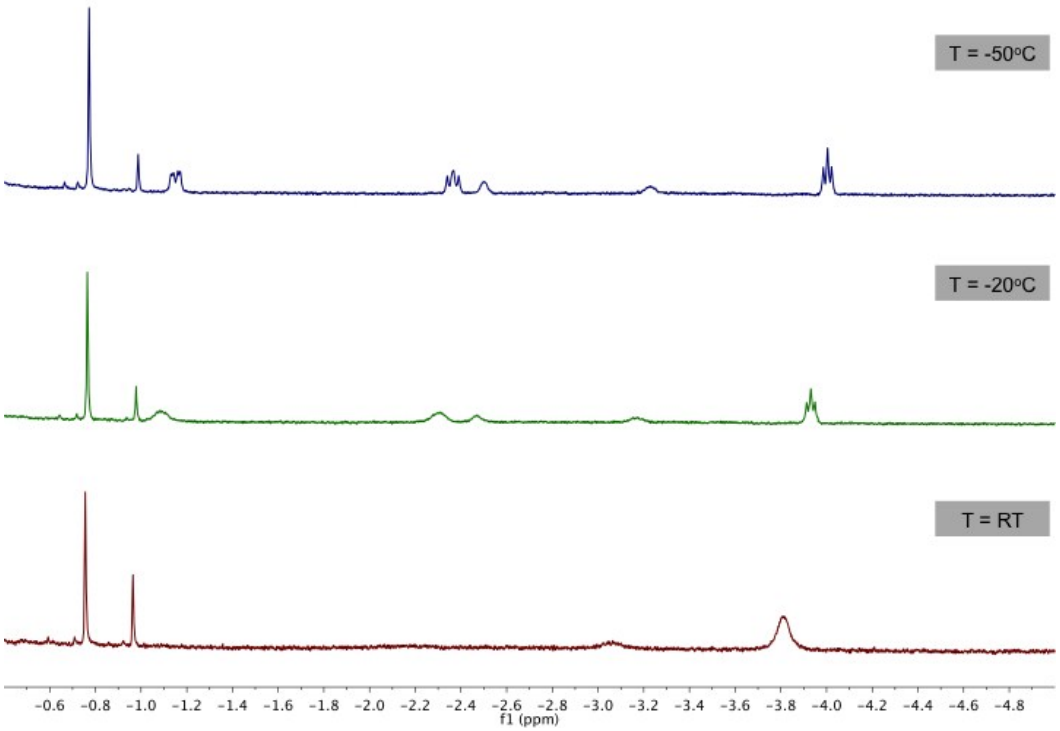


Figure S5. VT ^{1}H NMR spectroscopy of $[Cp_2ZrCl_2]$ + $[Al(Oct)_2H]$ (1:1) in the Zr-hydride region (THF-d_8).

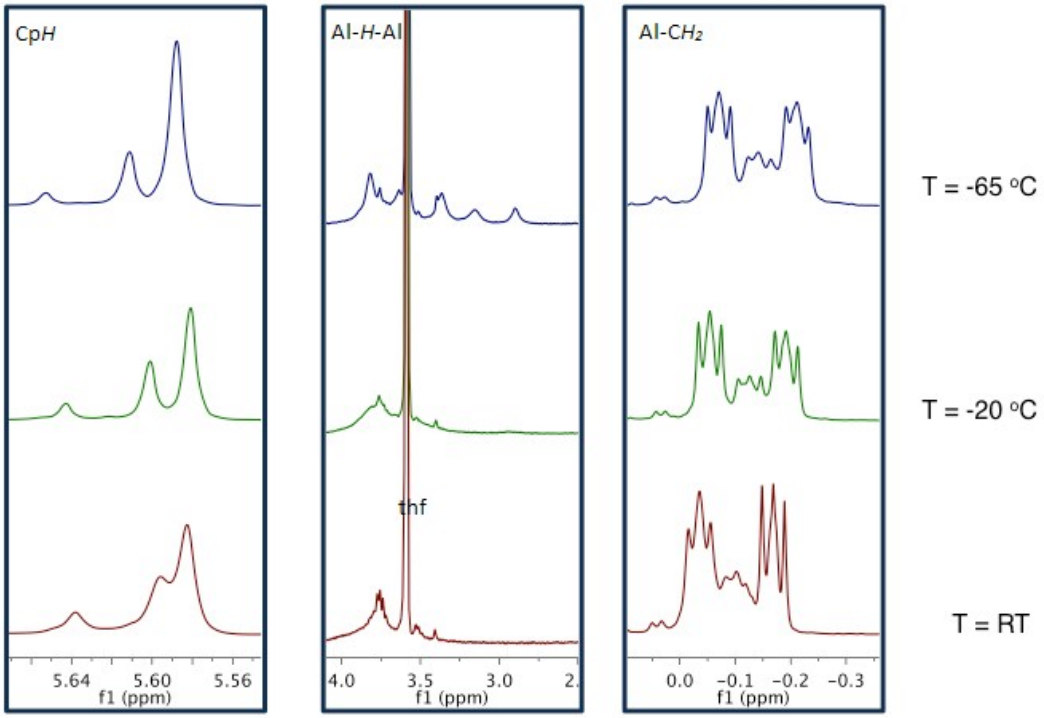


Figure S6. VT ^{1}H NMR spectroscopy of [Cp_2ZrCl_2] + [$Al(Oct)_2H$] (1:3) in the CpH, Al-H-Al and $AlCH_2$ regions (THF-d_8).

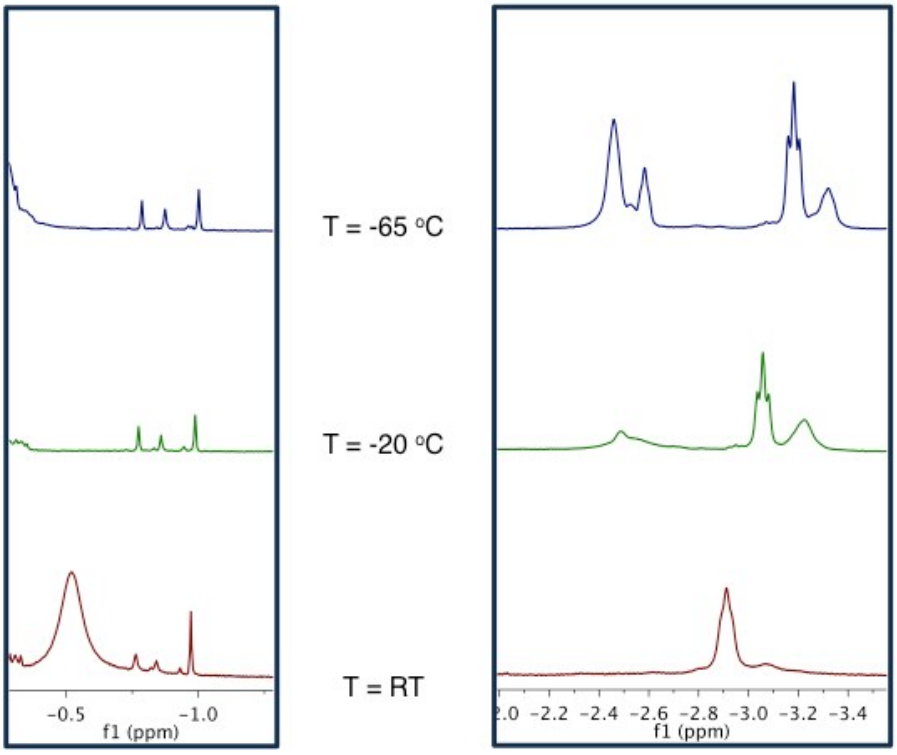


Figure S7. VT ^{1}H NMR spectroscopy of [Cp_2ZrCl_2] + [$Al(Oct)_2H$] (1:3) in the Zr-H region (THF-d_8).

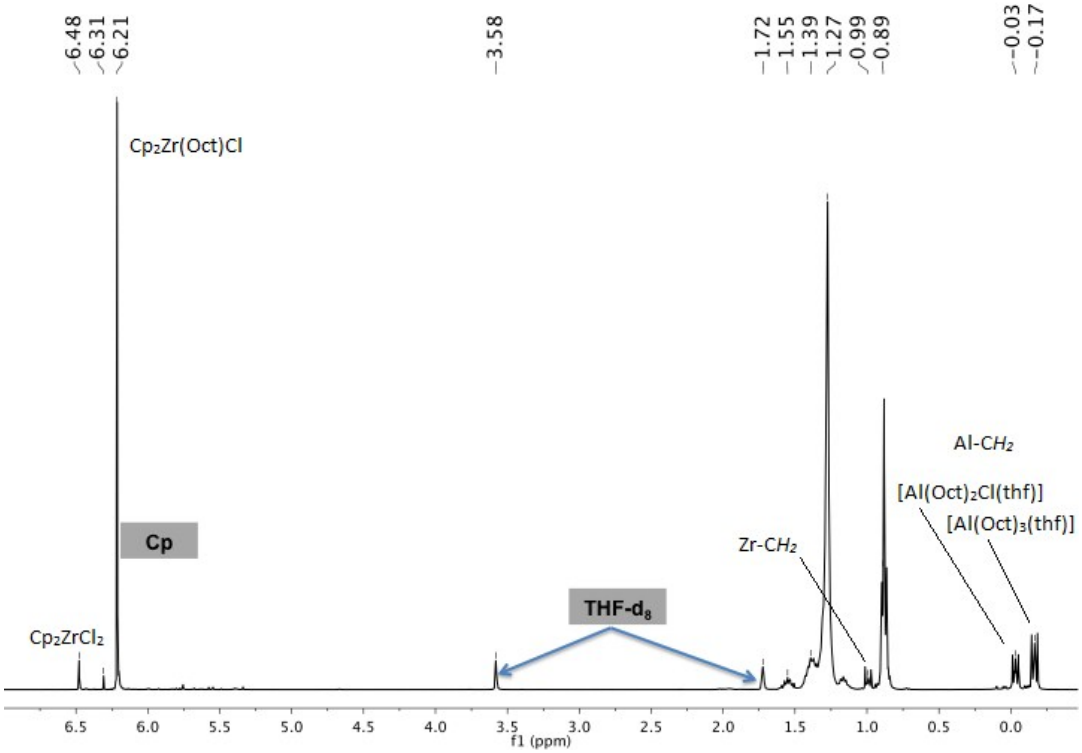


Figure S8. ^{1}H NMR spectrum from the reaction of [Cp_2ZrCl_2] / [$Al(Oct)_2H$] / 1-octene (1:1:1) in THF-d_8.

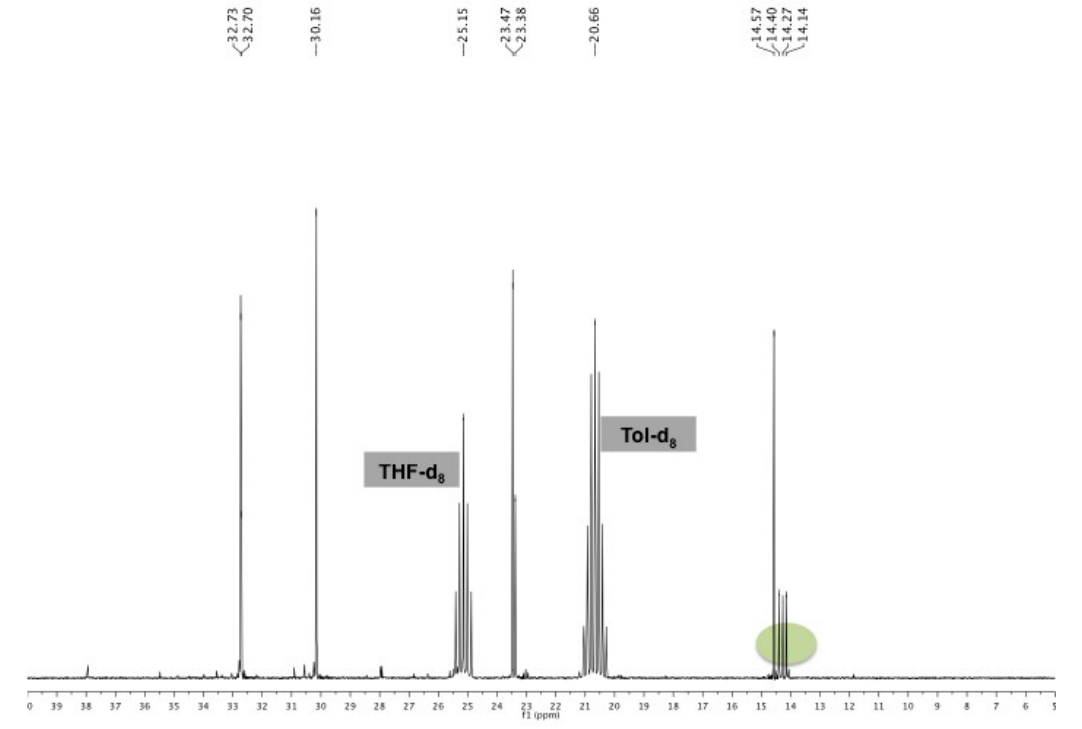


Figure S9. ^{13}C NMR of 1-d_1-*n*-octane obtained by quenching the [Cp_2ZrCl_2]/[$Al(Oct)_2H$]/internal octene reaction mixture with D_2O (reaction solvent THF-d_8, extracted into toluene-d_8 following D_2O quench).

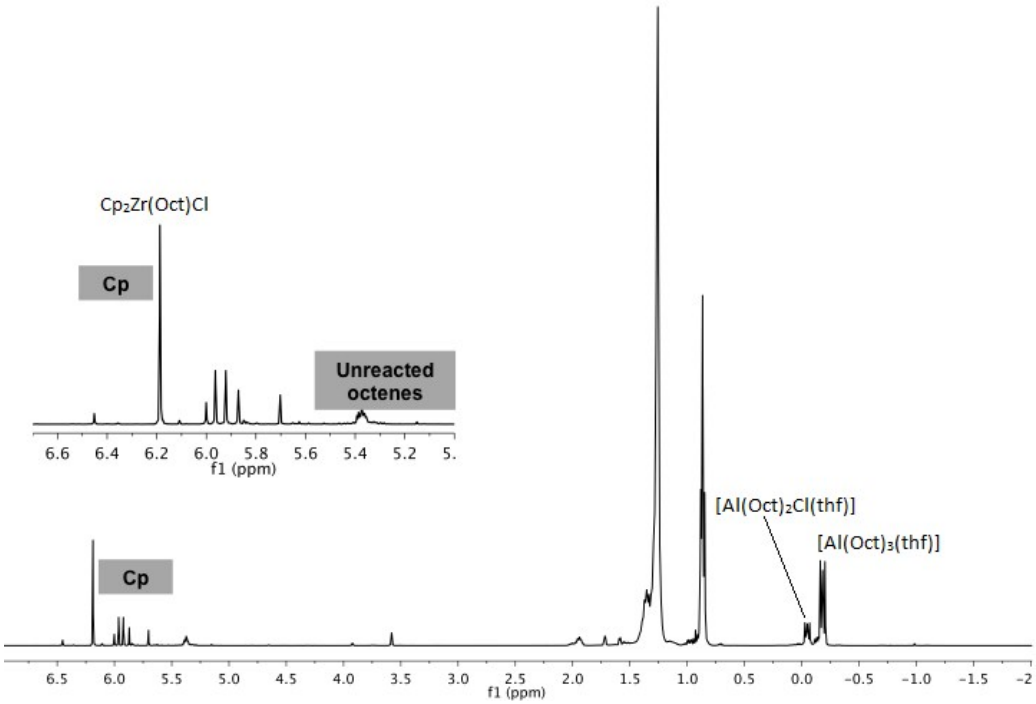


Figure S10. ^{1}H NMR following reaction (40 °C, 96 hr) of internal octenes with [Cp_2ZrCl_2] and [$Al(Oct)_2H$] in THF-d_8 (octene : Al-H : Zr = 4:4:1).

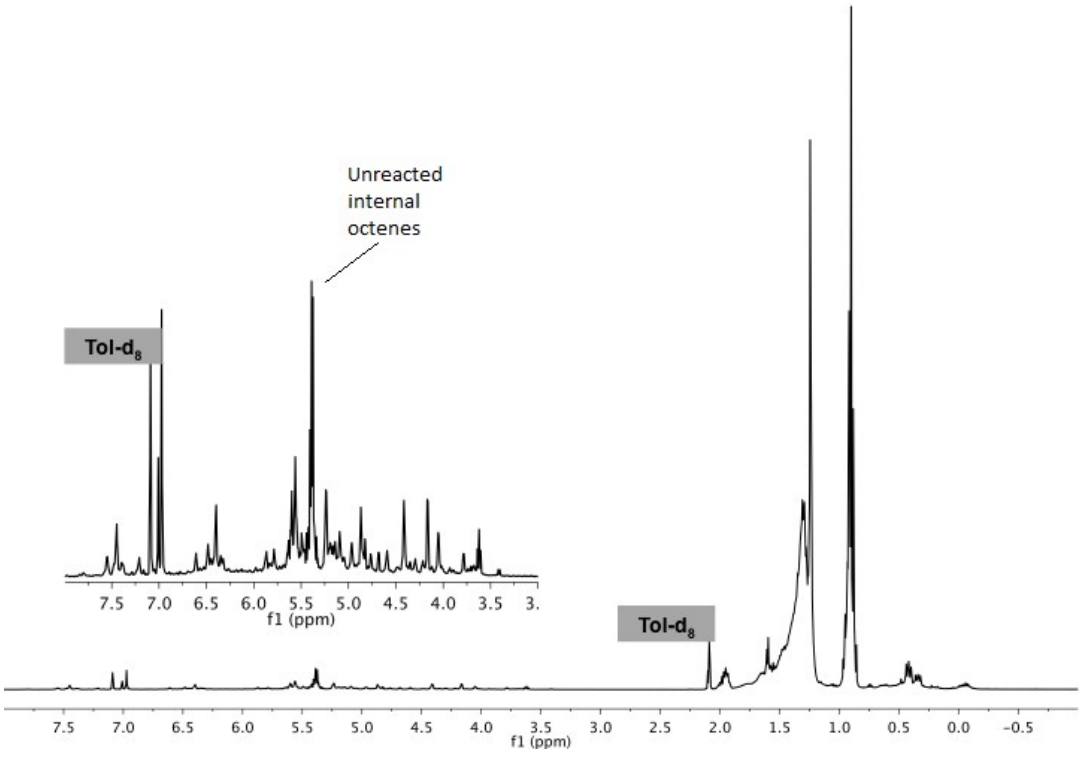


Figure S11. ^{1}H NMR following reaction (80 °C, 3 days) of internal octenes with [Cp_2ZrCl_2] and [$Al(Oct)_2H$] in toluene-d_8 (octene : Al-H : Zr = 1:1:1).

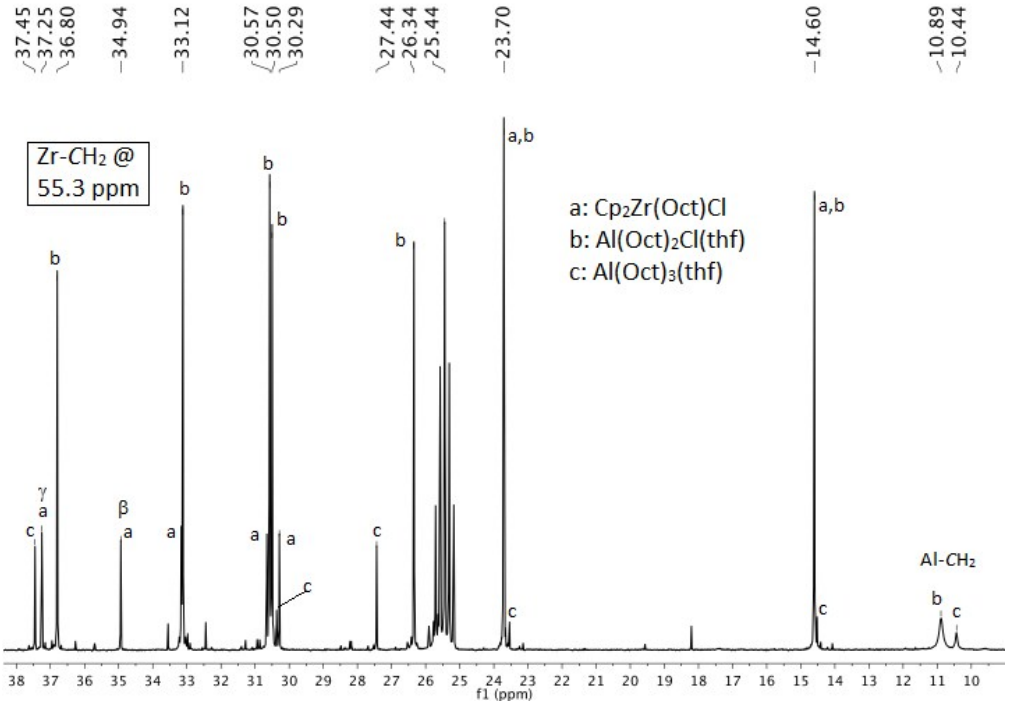


Figure S12. ^{13}C NMR spectrum from the reaction of $[Cp_2ZrCl_2]$ / $[Al(Oct)_2H]$ / 1-octene (1:1:1) in THF-d_8.

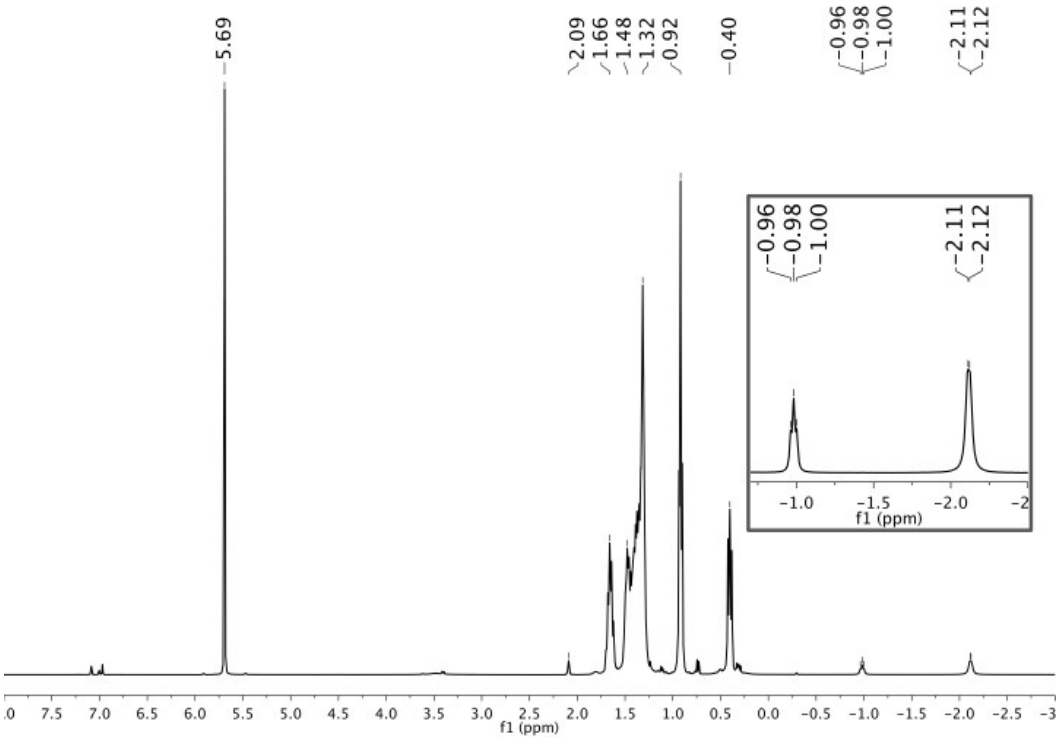


Figure S13. ^{1}H NMR spectrum of complex **4**, prepared by reacting $[Cp_2ZrCl_2]$ with 3 equivalents of $[Al(Oct)_2H]$ in toluene-d_8.

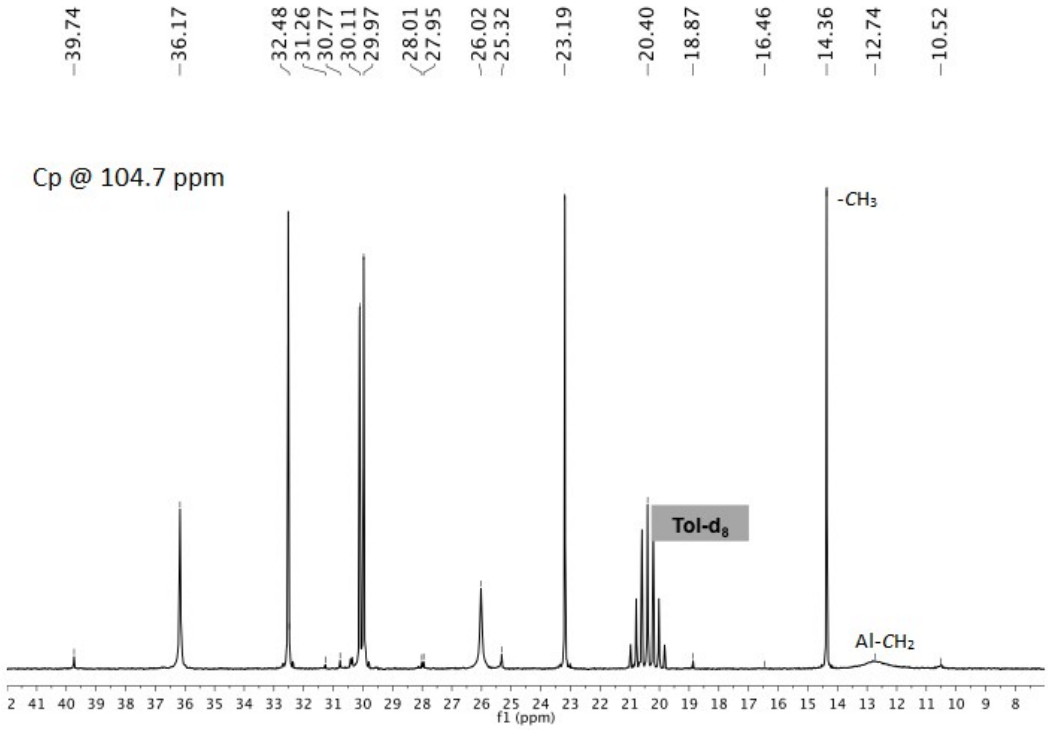


Figure S14. ^{13}C NMR spectrum of complex **4**, prepared by reacting [Cp_2ZrCl_2] with 3 equivalents of [$Al(Oct)_2H$] in toluene-d_8.

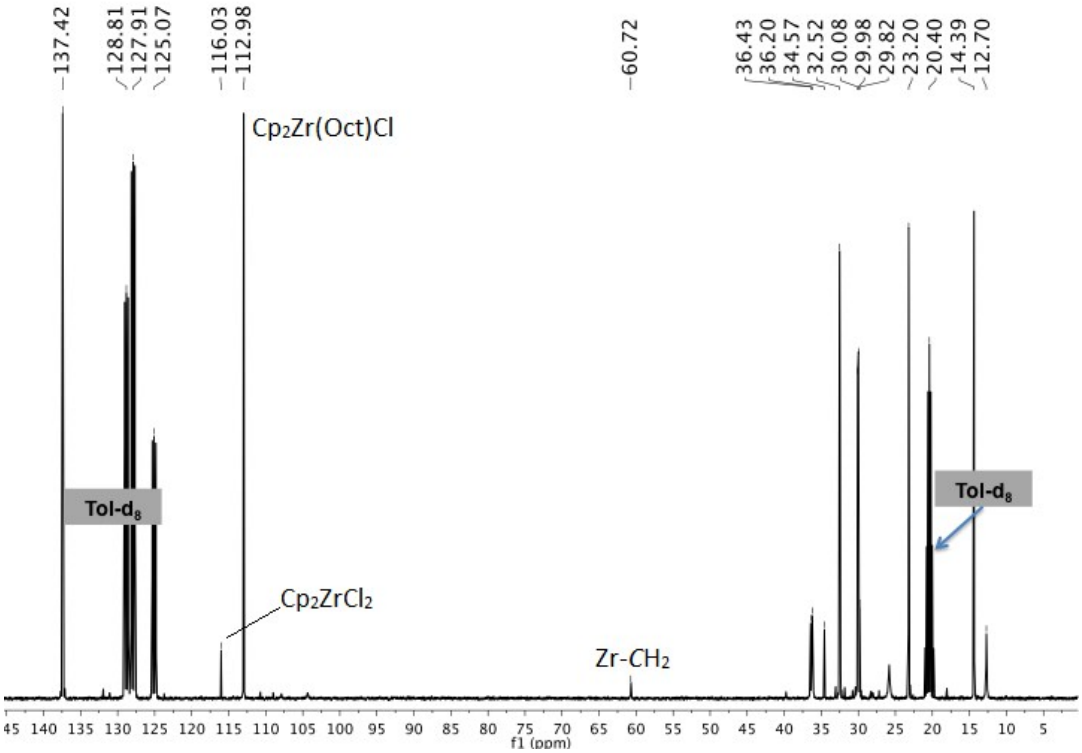


Figure S15. ^{13}C NMR spectrum from the reaction of [Cp_2ZrCl_2] / [$Al(Oct)_2H$] / 1-octene (1:1:1) in Toluene-d_8.

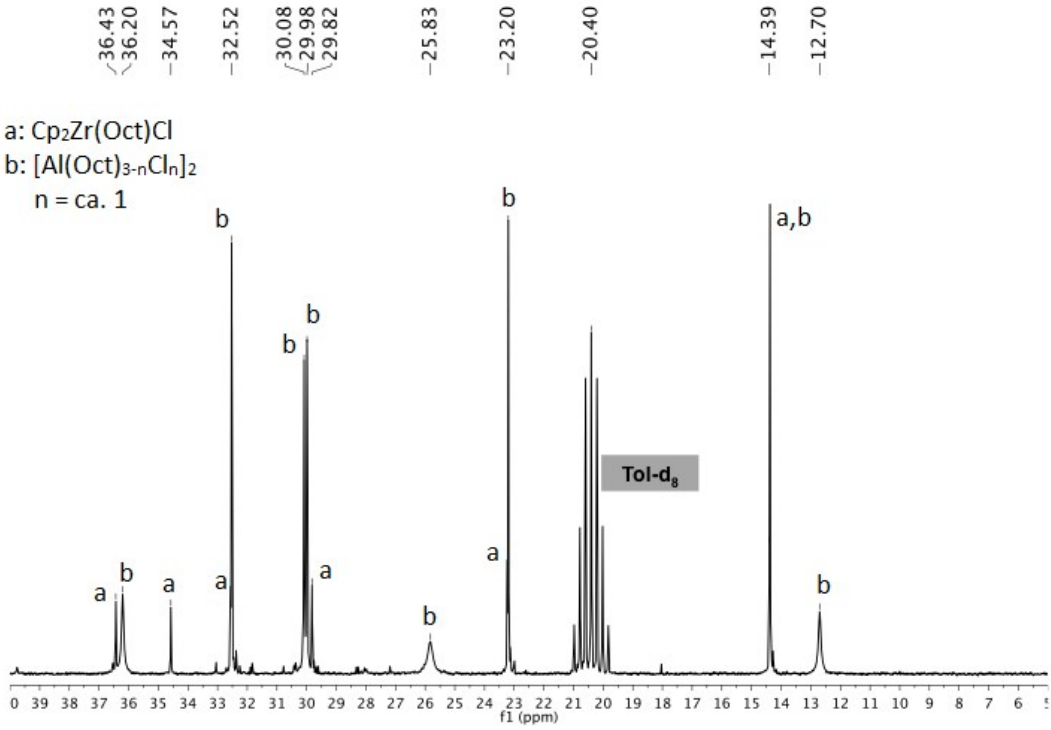


Figure S16. ^{13}C NMR spectrum from the reaction of $[Cp_2ZrCl_2]$ / $[Al(Oct)_2H]$ / 1-octene (1:1:1) in Toluene-d_8 (*n*-alkyl region).

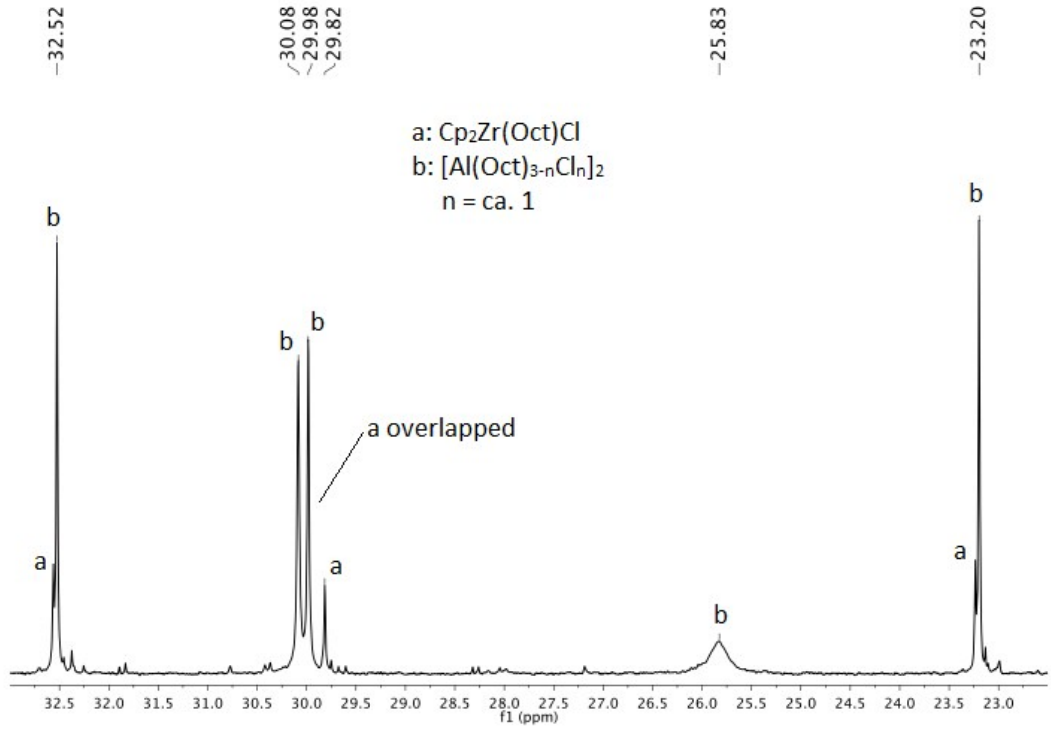


Figure S17. ^{13}C NMR spectrum from the reaction of $[Cp_2ZrCl_2]$ / $[Al(Oct)_2H]$ / 1-octene (1:1:1) in Toluene-d_8 (expansion of *n*-alkyl region).

Theoretical ^{1}H NMR shielding values

The theoretical ^{1}H NMR shielding values for complexes **4**, **6–8** (R = *n*-Pr) and two other complexes, $[Cp_2Zr(H)(\mu\text{-}Cl,H)AlPr_2]$ and $[Cp_2Zr(Cl)(\mu\text{-}H)_2AlPr_2]$, were calculated with the GIAO-DFT[1] method. The *n*-octyl groups were replaced with *n*-propyl and calculations were performed at the B3LYP/BS2//M06/BS1 level of theory (the B3LYP functional was employed to calculate shielding values in order to maintain consistency with our previous NMR calculations on Al-hydride clusters[2]). Chemical shifts were obtained by referencing to the calculated shielding value for tetramethylsilane.

The calculated shifts for each complex are illustrated in Figure S18. Complex **4** is predicted to lead to signals at -2.0 ppm for the two outer hydrides and -1.0 ppm for the inner hydride. This is in reasonable agreement with the measured ^{1}H NMR spectrum for **4** (R = octyl, Figure 1 main article). Complex **6** optimised to a structure with two bridging hydrides and one terminal Zr–hydride. We have not seen evidence for a hydride signal around 1.0 ppm as predicted, although such a signal could be easily masked by the large alkyl group resonances. Furthermore, the calculated NMR shifts reflect a static situation, whereas in solution dynamic exchange of the hydrides is possible. The bridging hydrides for **6** are more consistent with experimental observations. As such, it is possible that a structure such as **6** could give rise to a hydride signal in the region between -1.0 to -2.5 ppm as observed experimentally. Complex **7** optimised to a structure in which the chloro ligand is not interacting with zirconium. Both **7** and **8** are predicted to lead to Zr–H–Zr signals at ca. -4 ppm. There are no experimentally observed signals this far upfield, which may indicate that structures with Zr–H–Zr bridging are not present. The chemical shifts predicted for $[Cp_2Zr(H)(\mu\text{-}Cl,H)AlPr_2]$ and $[Cp_2Zr(Cl)(\mu\text{-}H)_2AlPr_2]$ appear to be too far downfield to account for the additional hydride signals observed.

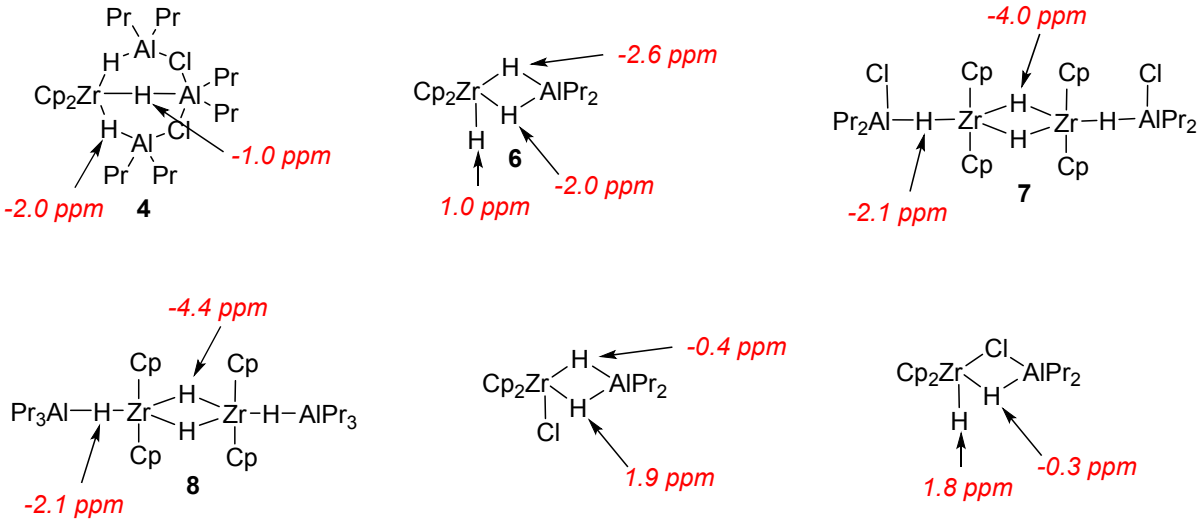


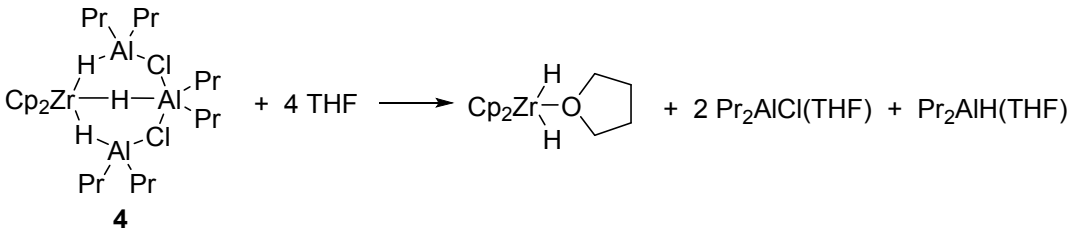
Figure S18. Calculated (B3LYP/BS2//M06/BS1) ^{1}H NMR chemical shifts for putative Zr/Al hydride clusters (relative to tetramethylsilane).

[1] (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.

[2] N. M. Weliange; D. S. McGuinness; M. G. Gardiner; J. Patel, *Dalton Trans.* **2015**, *44*, 15286.

THF coordination to Zr/Al hydride clusters

As discussed in the text, a rationale for trying the reaction in THF was that coordinating solvents might break up the stable Zr/Al hydride cluster(s). It appears however that such clusters persist in THF, albeit they are more reactive towards olefin. The thermodynamics of THF coordination to such clusters has been approximated by calculating the reaction free energy of the following reaction:



There are two isomers of $Cp_2ZrH_2(THF)$, with THF between the hydride ligands (most stable) and with the two hydrides adjacent to one another. The calculated free energy (M06/BS2//M06/BS1) for each reaction is 79 kJ·mol^{-1} and 99 kJ·mol^{-1} respectively. This would seemingly indicate that hydride bridged Zr/Al clusters are quite stable and will not be easily broken apart by additional ligation.

Spin states of binuclear Zr complexes

For the binuclear (Zr·····Zr) complexes postulated herein a number of spin states can be computed, these being a closed shell singlet (css), a triplet, and an open shell singlet (oss, a biradical where each Zr centre has one unpaired electron of opposite spin). The relative energies of these spin states that are indicated in the text are those resulting from use of the M06 functional (27% 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. Harvey's studies have suggested hybrid functionals with around 15% HF exchange may be most appropriate for comparing spin state splittings.[3] 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 and oss.

A related issue raised by a referee is that biradicals such as the oss exhibit significant multi-reference character and as such DFT may not lead to accurate energies for such species. This is a valid point, and the applicability of UDFT methods to oss biradicals has been studied.[4] In cases where the single electrons are located at different centres (as is the present case), the errors can be small. In complex **10**, the $\langle S^2 \rangle$ values for the oss before (0.972) and after (0.091) annihilation of the first spin contaminant indicate contamination of the singlet is predominately from the triplet state. In this case it is possible to obtain a spin corrected energy for the oss, as proposed by Yamaguchi.[5] This value for the energy of oss **10** is included below, although as the energies of the triplet and uncorrected oss are very similar, it leads to very little change in the relative energies.

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[3] 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).

[4] See for instance: J. Gräfenstein; E. Kraka; M. Filatov; D. Cremer, *Int. J. Mol. Sci.* **2002**, *3*, 360, and references therein.

[5] K. Yamaguchi; F. Jensen; A. Dorigo; K. N. Houk, *Chem. Phys. Lett.* **1988**, *149*, 537.

The use of DFT methods for systems with multi-configurational character has been extensively discussed, and we refer to the papers of Truhlar and references therein.[6] 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.

With the above considerations in mind, we have evaluated the energies of complexes **10** and **11** with a variety of different density functionals, both local and hybrid (DF/BS2//DF/BS1). The results are presented in Table S1. The M06L functional was included (0% HF) for comparison to M06 (29% HF), and noting that this functional has been reported to perform well for transition metal systems.[7] The BLYP, B1LYP and BHandHLYP functionals include 0%, 25% and 50% HF exchange respectively. Furthermore, Truhlar[6b] has demonstrated the accuracy of BLYP for transition metal dimers, including Zr_2. For complex **10** M06, M06L and BLYP lead to very similar relative energies. At the other extreme, BHandHLYP predicts the triplet and oss are lower in energy than the css. Given that high amounts of HF exchange is known to overestimate the stability of high spin states, and leads to poor results in multi-reference systems, these values are probably unreliable. The B1LYP functional leads to relative energies between M06(L)/BLYP and BHandHLYP. It can be seen that inclusion of spin correction to the oss **10** leads to only a minor stabilisation of this state.

Table S1. Relative free energies (DF/BS2//DF/BS1, kJ·mol^{-1}, 298 K) for different spin states of complexes **10** and **11**.[a]

Spin state	M06	$M06_{sc}$[b]	M06L	BLYP	B1LYP	BHandHLYP
			$[Cp_2Zr(\mu\text{-}Pr,Cl)ZrCp_2]$ **10**			
css	0	0	0	0	0	0
oss	21	19	24	21	-5	-35
triplet	22	22	23	22	-5	-36
			$[Cp_2Zr]_2$ **11**			
css	0		0	0		
oss	-30		-27	-12		
triplet	-34		-27	-10		

[a] free energies relative to the css in each case. [b] After spin correction to the energy of the oss, see text.

For complex **11** the high spin states are more stable, even with local functionals. Again the M06 and M06L values are very similar, while BLYP predicts the different spin states are closer in energy. It can be noted in all cases that the triplet and oss are very close in energy. Given the uncertainty in which of these is more stable, the free energy surface shown in Figure 3 has only been calculated with css and triplet species and corresponding MECPs.

While benchmarking of these DFT results would be desirable, this is a non-trivial task. The binuclear complexes are not easily simplified, as the cyclopentadienyl ligand cannot be replace with realistic smaller models, and at any rate are non-innocent in the reaction. In particular, accurately assessing the spin state splitting between the triplet and oss would likely require very high levels of theory. For this reason we instead draw on the work of Truhlar which shows that local density

[6] (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.

[7] D. G. Gusev, *Organometallics* **2013**, *32*, 4239.

functionals like BLYP perform well for binuclear Zr.[6b] The observation that the M06 functional used throughout is in reasonably good agreement with BLYP and M06L is encouraging.

The goal of the theoretical studies in the present work was to show that reductive elimination from mononuclear Zr-dialkyls and alkylhydrides is favourable, leading to more stable products. Despite the uncertainty in ground spin states of the dimers, this theory seems to show that reductive elimination would lead to such complexes. An accurate assessment of spin state energies for such species would be the subject of a much more demanding theoretical study.

Optimised geometries and energies (Hartrees) of all stationary points

Propene

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M06/BS1:
 E(RM06) =  -117.799195084
 Zero-point correction=                           0.079553 (Hartree/Particle)
 Thermal correction to Energy=                    0.083638
 Thermal correction to Enthalpy=                  0.084582
 Thermal correction to Gibbs Free Energy=         0.054580
 Sum of electronic and zero-point Energies=           -117.719642
 Sum of electronic and thermal Energies=              -117.715557
 Sum of electronic and thermal Enthalpies=            -117.714613
 Sum of electronic and thermal Free Energies=         -117.744615
E(RM06/BS2) =  -117.836559676

 C                 -1.34753600    0.08138600   -0.16528800
 H                 -0.89321800   -0.81668100   -0.58600600
 H                 -2.42834500    0.06665000   -0.04010900
 C                 -0.61200200    1.13536500    0.17547400
 H                 -1.10892200    2.01417400    0.59455100
 C                  0.87034300    1.22083700    0.03205800
 H                  1.16388000    2.05938600   -0.61493300
 H                  1.35817400    1.39000700    1.00245900
 H                  1.28276700    0.29963100   -0.39820700
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Propane

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M06/BS1:
 E(RM06) =  -119.032431946
 Zero-point correction=                           0.103365 (Hartree/Particle)
 Thermal correction to Energy=                    0.107902
 Thermal correction to Enthalpy=                  0.108846
 Thermal correction to Gibbs Free Energy=         0.077703
 Sum of electronic and zero-point Energies=           -118.929066
 Sum of electronic and thermal Energies=              -118.924530
 Sum of electronic and thermal Enthalpies=            -118.923586
 Sum of electronic and thermal Free Energies=         -118.954729
E(RM06/BS2) =  -119.068818876

 C                 -1.45930100    1.94885500   -0.00025400
 H                 -1.11232400    2.50152400    0.88423600
 H                 -1.11259300    2.50080700   -0.88529600
 H                 -2.55611600    1.97526200   -0.00009600
 C                 -0.92032500    0.52738200    0.00022100
 H                 -1.30321300   -0.01374400    0.87854400
 H                 -1.30340600   -0.01443300   -0.87759500
 C                  0.59921900    0.49315200    0.00008900
 H                  0.98949400   -0.53224700    0.00062200
 H                  1.00365000    1.00393600   -0.88507000
 H                  1.00385000    1.00492900    0.88458400
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Cp_2ZrHPr

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M06/BS1
 E(RM06) =  -552.842819158
 Zero-point correction=                           0.266694 (Hartree/Particle)
 Thermal correction to Energy=                    0.281830
 Thermal correction to Enthalpy=                  0.282774
 Thermal correction to Gibbs Free Energy=         0.223091
 Sum of electronic and zero-point Energies=           -552.576125
 Sum of electronic and thermal Energies=              -552.560990
 Sum of electronic and thermal Enthalpies=            -552.560045
 Sum of electronic and thermal Free Energies=         -552.619728
E(RM06/BS2) =  -553.017705864

 C                 -2.17618900   -0.92078000   -0.74258100
 C                 -2.45466600    0.45338300   -0.94364900
 C                 -2.17536600    1.14467700    0.25813500
 C                 -1.68571700   -1.07246800    0.57483500
 C                 -1.68871800    0.20742100    1.19551600
 H                 -2.28700900   -1.70830300   -1.47850900
 H                 -2.80856700    0.90363700   -1.86703800
 H                 -2.28157400    2.21232800    0.41844500
 H                 -1.36817400   -2.00366900    1.03459100
 H                 -1.39523800    0.42340500    2.21800700
 Zr                 0.05446900    0.28038200   -0.60537900
 C                  2.56093600    0.64928900   -0.57676800
 C                  2.07677000    1.13021900    0.66317300
 C                  1.57059200    0.02798300    1.38829200
 C                  2.37050600   -0.75237500   -0.61516700
 C                  1.74211200   -1.13573700    0.59425000
 H                  2.98467600    1.25886800   -1.36957000
 H                  2.06840400    2.16733300    0.98341100
 H                  1.13191700    0.06431500    2.38061900
 H                  2.63069600   -1.41220600   -1.43446100
 H                  1.44621900   -2.14474600    0.86528400
 C                  0.09472300    2.36987800   -1.54972000
 H                 -0.81980200    2.96830600   -1.41603400
 H                  0.94109400    3.00961400   -1.25367900
 C                  0.23420600    2.00081900   -3.03270000
 H                 -0.60152200    1.35516800   -3.35872700
 H                  1.14332300    1.39695700   -3.20766900
 C                  0.28372500    3.22319300   -3.94583800
 H                  0.38173700    2.94675800   -5.00482400
 H                 -0.62907000    3.82442400   -3.83425800
 H                  1.13420100    3.86684800   -3.68179600
 H                  0.13247900   -0.94654800   -2.02013400
```

Cp_2ZrPr_2

```
M06/BS1
 E(RM06) =  -670.687359819
 Zero-point correction=                           0.353043 (Hartree/Particle)
 Thermal correction to Energy=                    0.372770
 Thermal correction to Enthalpy=                  0.373714
 Thermal correction to Gibbs Free Energy=         0.305215
 Sum of electronic and zero-point Energies=           -670.334317
 Sum of electronic and thermal Energies=              -670.314590
 Sum of electronic and thermal Enthalpies=            -670.313646
 Sum of electronic and thermal Free Energies=         -670.382145
E(RM06/BS2) =  -670.898842154

 C                 -2.23454300    0.10852000   -1.17107700
 C                 -2.04596400    1.27718000   -0.39507500
 C                 -1.72389500    0.87822800    0.92077000
 C                 -2.04434100   -1.01308200   -0.33402200
 C                 -1.71347200   -0.54176400    0.95778500
```

H	-2.46390200	0.08205800	-2.23188300
H	-2.10574300	2.29908200	-0.75714200
H	-1.51456400	1.53813500	1.75744300
H	-2.11078500	-2.05366400	-0.63400800
H	-1.50671000	-1.15703400	1.82832400
Zr	0.23013000	0.13412100	-0.48402600
C	2.35917000	1.38761500	0.18682800
C	1.51958000	1.33166000	1.32320100
C	1.43204500	-0.02472400	1.73463200
C	2.76638300	0.07115000	-0.11894000
C	2.20192000	-0.80205400	0.84119200
H	2.61647100	2.27937300	-0.37461700
H	1.04220800	2.17839400	1.80760900
H	0.86705200	-0.39614600	2.58436000
H	3.38034200	-0.22455300	-0.96467000
H	2.31046400	-1.88216800	0.86030400
C	0.52895400	1.63728100	-2.19655000
H	0.71581600	2.64264700	-1.77302000
H	1.51230500	1.31586400	-2.60272800
C	0.61192800	-1.84402900	-1.60032300
H	1.69967500	-1.90161900	-1.78905600
H	0.39437400	-2.68757400	-0.91581500
C	-0.11035100	-2.06738000	-2.92695000
H	-1.20435300	-2.03227100	-2.78904900
H	0.12374400	-1.24220000	-3.62194100
C	0.25687000	-3.38740400	-3.59573100
H	-0.26052000	-3.52620000	-4.55540600
H	1.33802100	-3.44038800	-3.78692500
H	-0.00092400	-4.23734400	-2.94753000
C	-0.45315900	1.77163900	-3.35578500
H	-1.42114600	2.15361800	-2.98971200
H	-0.67213300	0.78229400	-3.79295400
C	0.04908200	2.69140000	-4.46271700
H	-0.67393800	2.78580400	-5.28505100
H	0.24744100	3.69957200	-4.07127300
H	0.99139100	2.31479400	-4.88545900

TS Cp_2Zr---H---Pr reductive elimination

M06/BS1
E(RM06) = -552.794519403
Zero-point correction= 0.264854 (Hartree/Particle)
Thermal correction to Energy= 0.279546
Thermal correction to Enthalpy= 0.280491
Thermal correction to Gibbs Free Energy= 0.222160
Sum of electronic and zero-point Energies= -552.529666
Sum of electronic and thermal Energies= -552.514973
Sum of electronic and thermal Enthalpies= -552.514029
Sum of electronic and thermal Free Energies= -552.572359
E(RM06/BS2) = -552.971509363

C	-2.01508500	-0.38737600	-1.20332500
C	-2.22629400	0.93528000	-0.75350900
C	-2.02930900	0.97322800	0.65937800
C	-1.66358900	-1.18079800	-0.09204000
C	-1.68164700	-0.34663800	1.05938700
H	-2.05537200	-0.72900100	-2.23317000
H	-2.49505700	1.78653400	-1.37452000
H	-2.18767000	1.82529200	1.31073000
H	-1.41840500	-2.23794500	-0.11554000
H	-1.47111000	-0.66831400	2.07570200
Zr	0.19697400	0.51558600	-0.28380600
C	2.63743100	0.76287500	-0.06588800
C	2.10385700	1.33521900	1.12450200
C	1.50585100	0.29450200	1.86547900
C	2.38693100	-0.64207100	-0.04276600
C	1.67573700	-0.91872900	1.14827100

H	3.18905300	1.29661000	-0.83377100
H	2.14862300	2.37944400	1.41570200
H	0.98318100	0.40693800	2.81123100
H	2.70461200	-1.36784100	-0.78188900
H	1.30504700	-1.89289000	1.45668200
C	0.57153600	1.53291800	-2.30219500
H	0.29543500	2.36030900	-1.53020100
H	1.62873300	1.72120500	-2.53461800
C	-0.27074200	1.74231500	-3.55076000
H	-1.32469400	1.50473000	-3.34460700
H	0.06034400	1.01572700	-4.30821900
C	-0.15776500	3.15514000	-4.10127700
H	-0.73679800	3.27379800	-5.02577300
H	-0.52937600	3.89201200	-3.37562700
H	0.88752300	3.41054100	-4.32409700
H	0.58871900	0.14777300	-2.15991100

Cp_2Zr-----HPr post-reductive elimination complex

```
M06/BS1:
 E(RM06) =  -552.803067858
 Zero-point correction=                           0.270076 (Hartree/Particle)
 Thermal correction to Energy=                    0.285233
 Thermal correction to Enthalpy=                  0.286178
 Thermal correction to Gibbs Free Energy=         0.227025
 Sum of electronic and zero-point Energies=           -552.532992
 Sum of electronic and thermal Energies=              -552.517835
 Sum of electronic and thermal Enthalpies=            -552.516890
 Sum of electronic and thermal Free Energies=         -552.576043
E(RM06/BS2) =  -552.981055031
```

C	-1.98255900	-0.49553200	-1.22057800
C	-2.14832700	0.85894300	-0.85845300
C	-1.93628100	0.99733200	0.54597300
C	-1.64714800	-1.23464900	-0.06713200
C	-1.62171800	-0.31515300	1.02919700
H	-2.04211200	-0.89809700	-2.22904400
H	-2.38815000	1.67260700	-1.54034400
H	-2.11465900	1.88459300	1.14131700
H	-1.47307400	-2.30396500	-0.01948600
H	-1.44403400	-0.57969500	2.06794800
Zr	0.24975900	0.36296900	-0.30330500
C	2.63509700	0.53382900	-0.08591200
C	2.13514500	1.34433800	0.98399300
C	1.48507800	0.48332800	1.88975000
C	2.31806700	-0.84100500	0.19277200
C	1.59436400	-0.84723200	1.41017400
H	3.23548400	0.88681500	-0.92065800
H	2.24475800	2.41758300	1.09334400
H	0.94881100	0.79160300	2.78310500
H	2.63424300	-1.71144900	-0.36942100
H	1.16494900	-1.72499000	1.88660200
C	0.70404800	1.45076000	-2.56717400
H	0.41429900	2.07417100	-1.66142300
H	1.74005700	1.74568300	-2.77998700
C	-0.22531400	1.82975900	-3.71297600
H	-1.21275500	1.37226400	-3.55488700
H	0.16752300	1.39783300	-4.64423700
C	-0.36470500	3.33685800	-3.84625500
H	-1.00030900	3.60974100	-4.69668400
H	-0.81102200	3.76952600	-2.93917100
H	0.61392300	3.81496100	-3.99149200
H	0.72873700	0.32064600	-2.47250000

Cp_2Zr

```
M06/BS1:
 E(RM06) =  -433.759209902
 Zero-point correction=                           0.163708 (Hartree/Particle)
 Thermal correction to Energy=                    0.174032
 Thermal correction to Enthalpy=                  0.174976
 Thermal correction to Gibbs Free Energy=         0.126284
 Sum of electronic and zero-point Energies=           -433.595502
 Sum of electronic and thermal Energies=              -433.585178
 Sum of electronic and thermal Enthalpies=            -433.584234
 Sum of electronic and thermal Free Energies=         -433.632926
E(RM06/BS2) =  -433.896154413

 C                 -1.92606600   -1.96142300   -0.82393100
 C                 -2.03103500   -0.55834700   -0.74427700
 C                 -1.79233500   -0.14988500    0.58957900
 C                 -1.61815900   -2.47382200    0.47871400
 C                 -1.52864700   -1.33322700    1.36372900
 H                 -2.06120900   -2.55180900   -1.72631400
 H                 -2.21640600    0.10606300   -1.58507600
 H                 -1.85159200    0.86696800    0.96364600
 H                 -1.61345000   -3.51867100    0.76989600
 H                 -1.42138500   -1.37355700    2.44275400
 Zr                 0.33796300   -1.23244000   -0.02528600
 C                  2.79469600   -0.49706500    0.07769300
 C                  2.13180400   -0.12555200    1.27009700
 C                  1.65491800   -1.32963200    1.89440000
 C                  2.74867100   -1.89945300   -0.06043100
 C                  2.04669000   -2.44817000    1.06454300
 H                  3.22649900    0.19172400   -0.64486100
 H                  2.04136600    0.88311400    1.65996100
 H                  1.20539100   -1.39760800    2.87973300
 H                  3.18479500   -2.46503100   -0.87950100
 H                  1.97837400   -3.49901600    1.32442900
```

TS Cp_2ZrPr_2 β-H to α' transfer

```
M06/BS1:
 E(RM06) =  -670.646885358
 Zero-point correction=                           0.350347 (Hartree/Particle)
 Thermal correction to Energy=                    0.368894
 Thermal correction to Enthalpy=                  0.369838
 Thermal correction to Gibbs Free Energy=         0.305088
 Sum of electronic and zero-point Energies=           -670.296538
 Sum of electronic and thermal Energies=              -670.277992
 Sum of electronic and thermal Enthalpies=            -670.277048
 Sum of electronic and thermal Free Energies=         -670.341797
E(RM06/BS2) =  -670.861488677

 C                 -2.14520200   -0.41108200   -1.21166200
 C                 -1.96004500    0.89187200   -0.67171900
 C                 -1.67176200    0.75410800    0.70008200
 C                 -1.99589800   -1.34511500   -0.16033900
 C                 -1.67559100   -0.63225700    1.01464800
 H                 -2.38916600   -0.64343000   -2.24373000
 H                 -2.01893900    1.82671000   -1.22207900
 H                 -1.45997300    1.56378700    1.39267800
 H                 -2.08516500   -2.42182700   -0.24502200
 H                 -1.48239000   -1.06874900    1.99036200
 Zr                 0.28866800   -0.25784200   -0.53762500
 C                  2.50303000    1.01518800   -0.24718500
 C                  1.62622300    1.43006600    0.78137200
 C                  1.41389600    0.31845000    1.64062400
 C                  2.79611000   -0.35004800   -0.05400700
 C                  2.12715200   -0.78382200    1.12161500
```

H	2.85246700	1.63293900	-1.06784400
H	1.20654800	2.42506600	0.90214900
H	0.79379700	0.31327300	2.53240400
H	3.41506900	-0.96819600	-0.69751700
H	2.15444500	-1.78465800	1.53884300
C	0.50697900	1.28714900	-2.56330600
H	0.37633100	2.13682900	-1.87283500
H	1.53154800	1.38877300	-2.95740600
C	0.71843700	-2.43926700	-1.09779600
H	1.64065100	-2.85590000	-0.68330500
H	-0.09482400	-3.17048900	-1.05461900
C	0.83396700	-1.71148100	-2.37322000
H	0.59302100	-0.15210600	-2.43559700
H	1.86889300	-1.58939300	-2.72604700
C	-0.07881200	-2.15547400	-3.50165100
H	-0.13429700	-1.43172200	-4.32728600
H	0.26682100	-3.11219100	-3.92216900
H	-1.10326900	-2.32090000	-3.13907000
C	-0.48111600	1.42445200	-3.71745900
H	-1.49493900	1.13113700	-3.40190700
H	-0.21114800	0.72160000	-4.52141400
C	-0.52736300	2.83824100	-4.27867100
H	-1.21067000	2.92042400	-5.13443500
H	-0.86459000	3.55117000	-3.51158900
H	0.46852800	3.16354100	-4.61075700

$Cp_2Zr(C_3H_6)$---HPr post elimination complex

```
M06/BS1:
 E(RM06) =  -670.673814149
 Zero-point correction=                           0.352943 (Hartree/Particle)
 Thermal correction to Energy=                    0.372845
 Thermal correction to Enthalpy=                  0.373789
 Thermal correction to Gibbs Free Energy=         0.304617
 Sum of electronic and zero-point Energies=           -670.320871
 Sum of electronic and thermal Energies=              -670.300970
 Sum of electronic and thermal Enthalpies=            -670.300025
 Sum of electronic and thermal Free Energies=         -670.369197
E(RM06/BS2) =  -670.886572990
```

C	-2.02699800	-0.48105400	-1.28177900
C	-1.83343800	0.76643400	-0.61834600
C	-1.72374600	0.50745900	0.76696500
C	-2.04149100	-1.49566400	-0.29422400
C	-1.83664600	-0.89118100	0.96500700
H	-2.16311300	-0.62761800	-2.34931400
H	-1.79704200	1.74562800	-1.08916000
H	-1.55579100	1.25061500	1.54121200
H	-2.16599000	-2.55747000	-0.47375000
H	-1.76964200	-1.40916400	1.91772700
Zr	0.30520000	-0.49086800	-0.37113700
C	2.54709400	0.74364700	-0.36053900
C	1.67201600	1.37380300	0.56373200
C	1.44508700	0.45808200	1.62846800
C	2.83780900	-0.54736000	0.11838000
C	2.15842300	-0.73321600	1.34744800
H	2.90904500	1.16912400	-1.29251000
H	1.27463700	2.38249000	0.48880300
H	0.83098800	0.64114800	2.50539400
H	3.44310800	-1.29088400	-0.39050000
H	2.17620600	-1.63198000	1.95544500
C	0.51332500	1.55165800	-3.03030500
H	0.49972700	2.20457200	-2.14461000
H	1.47854800	1.71055800	-3.53344300
C	0.76999600	-2.69530800	-0.79448100
H	1.67765800	-3.07948400	-0.31967200
H	-0.04689200	-3.42096700	-0.73228800

```
 C                  0.89344900   -1.95129500   -2.05016600
 H                  0.50864700    0.48774500   -2.71661900
 H                  1.92697300   -1.75564100   -2.36944100
 C                  0.01273700   -2.32787200   -3.22206500
 H                 -0.09454800   -1.51343400   -3.95792200
 H                  0.40917000   -3.20012800   -3.76853400
 H                 -1.00133900   -2.60151600   -2.89529800
 C                 -0.65119200    1.86133300   -3.95615100
 H                 -1.60262200    1.65356500   -3.44129700
 H                 -0.62333100    1.18350300   -4.82229400
 C                 -0.63185700    3.30671500   -4.42664600
 H                 -1.46918400    3.53032300   -5.09868700
 H                 -0.69381700    3.99854500   -3.57435400
 H                  0.29875800    3.53398700   -4.96503700
```

$Cp_2Zr(C_3H_6)$ (metallacyclopropane complex)

```
M06/BS1:
 E(RM06) =  -551.635931704
 Zero-point correction=                           0.247438 (Hartree/Particle)
 Thermal correction to Energy=                    0.261525
 Thermal correction to Enthalpy=                  0.262469
 Thermal correction to Gibbs Free Energy=         0.206599
 Sum of electronic and zero-point Energies=           -551.388494
 Sum of electronic and thermal Energies=              -551.374407
 Sum of electronic and thermal Enthalpies=            -551.373462
 Sum of electronic and thermal Free Energies=         -551.429333
E(RM06/BS2) =  -551.809363182

 C                 -1.90414200   -0.33241000   -1.33497800
 C                 -1.69360700    0.80056700   -0.50313700
 C                 -1.78020200    0.37498000    0.84890400
 C                 -2.11216200   -1.45214200   -0.49050000
 C                 -2.03727700   -1.01686000    0.85098800
 H                 -1.91345200   -0.34338400   -2.41986400
 H                 -1.51697800    1.81852800   -0.83959000
 H                 -1.66314000    1.00549500    1.72535200
 H                 -2.28554300   -2.47229300   -0.81562500
 H                 -2.13298900   -1.64804700    1.73023200
 Zr                 0.28836200   -0.65546200   -0.15523800
 C                  2.40644100    0.70210000   -0.53076300
 C                  1.59772800    1.37756200    0.42084500
 C                  1.55269800    0.58125500    1.59910100
 C                  2.85187500   -0.50263500    0.05740100
 C                  2.33414500   -0.58053800    1.36799300
 H                  2.63231100    1.03877900   -1.53813200
 H                  1.11560200    2.34149500    0.28482800
 H                  1.03239900    0.83132300    2.51904000
 H                  3.45279300   -1.26337600   -0.43063700
 H                  2.48979100   -1.39858500    2.06519500
 C                  0.77411400   -2.79251100   -0.71729100
 H                  1.70240000   -3.20359800   -0.30629400
 H                 -0.03239100   -3.53364600   -0.69924600
 C                  0.86491700   -1.96170700   -1.93921900
 H                  1.89238000   -1.74715200   -2.25920600
 C                 -0.00723100   -2.31142100   -3.12396400
 H                 -0.07544200   -1.48811300   -3.85141100
 H                  0.37961700   -3.19033900   -3.66663100
 H                 -1.03375000   -2.56225800   -2.81957700
```

$Cp_2ZrPrCl$

```
M06/BS1:
 E(RM06) =  -1012.50939473
 Zero-point correction=                           0.261860 (Hartree/Particle)
```

```
 Thermal correction to Energy=                    0.278273
 Thermal correction to Enthalpy=                  0.279217
 Thermal correction to Gibbs Free Energy=         0.217589
 Sum of electronic and zero-point Energies=          -1012.247534
 Sum of electronic and thermal Energies=             -1012.231122
 Sum of electronic and thermal Enthalpies=           -1012.230178
 Sum of electronic and thermal Free Energies=        -1012.291806
E(RM06/BS2) =  -1012.71612526

 C                 -2.08082800    0.20602600   -1.28780100
 C                 -1.88698200    1.41854700   -0.58526000
 C                 -1.64357900    1.10586700    0.77025200
 C                 -1.98566400   -0.85915300   -0.36077200
 C                 -1.70429600   -0.30726100    0.90944000
 H                 -2.23779900    0.11380100   -2.35807100
 H                 -1.86560100    2.40938100   -1.02784300
 H                 -1.45880900    1.81939600    1.56722900
 H                 -2.09139300   -1.91524900   -0.58389200
 H                 -1.58309100   -0.86375600    1.83332300
 Zr                 0.32927700    0.18217600   -0.49223300
 C                  2.43973700    1.29570300    0.40963500
 C                  1.54052700    1.15032300    1.49038400
 C                  1.39307100   -0.23971700    1.75065800
 C                  2.82538500    0.00562100   -0.01591700
 C                  2.18972100   -0.94399900    0.82066800
 H                  2.72969600    2.23033000   -0.05899800
 H                  1.06545700    1.95816000    2.03802800
 H                  0.78787800   -0.68026300    2.53634300
 H                  3.46452500   -0.21709700   -0.86491200
 H                  2.28051600   -2.02228700    0.74318600
 C                  0.60273300   -1.84592500   -1.53193000
 H                  1.68438800   -1.87078100   -1.76131400
 H                  0.42990100   -2.68998000   -0.83836000
 C                 -0.15834900   -2.08346200   -2.83380800
 H                 -1.24201600   -2.15438500   -2.64586700
 H                 -0.02825900   -1.21982500   -3.50636700
 C                  0.29420900   -3.34810500   -3.55509600
 H                 -0.25968900   -3.51043100   -4.49000100
 H                  1.36296400   -3.29431500   -3.80538400
 H                  0.15097300   -4.23432200   -2.92019000
 Cl                 0.85404200    1.55619000   -2.45049200
```

Complex **10**, $Cp_2Zr(\mu\text{-}Pr)(\mu\text{-}Cl)ZrCp_2$ (Closed shell singlet)

```
M06/BS1:
 E(RM06) =  -1446.35108460
 Zero-point correction=                           0.431880 (Hartree/Particle)
 Thermal correction to Energy=                    0.458117
 Thermal correction to Enthalpy=                  0.459061
 Thermal correction to Gibbs Free Energy=         0.378509
 Sum of electronic and zero-point Energies=          -1445.919204
 Sum of electronic and thermal Energies=             -1445.892967
 Sum of electronic and thermal Enthalpies=           -1445.892023
 Sum of electronic and thermal Free Energies=        -1445.972576
E(RM06/BS2) =  -1446.69298361

 C                 -2.46533900   -0.88831100   -0.23153700
 C                 -2.45063300    0.47229600    0.14021900
 C                 -1.82120400    0.58192400    1.39905200
 C                 -1.86398400   -1.63864800    0.81435700
 C                 -1.47788100   -0.72925300    1.82370700
 H                 -2.87581700   -1.29903800   -1.14696100
 H                 -2.79792100    1.31004100   -0.45644400
 H                 -1.63871000    1.50472100    1.94205300
 H                 -1.74911100   -2.71626400    0.84566100
 H                 -1.00100700   -0.99223600    2.76253000
```

Zr	0.01362700	-0.23946600	-0.13396100
C	2.48889000	0.36669200	-0.06445300
C	1.83564000	1.15782000	0.92155100
C	1.38063300	0.28930500	1.93268300
C	2.44286900	-0.98178700	0.35514200
C	1.73254100	-1.03960000	1.57260000
H	2.96681600	0.74984100	-0.95846800
H	1.70356300	2.23450900	0.88810800
H	0.83467200	0.58517000	2.82292400
H	2.86100100	-1.83319000	-0.17136600
H	1.50947300	-1.93832800	2.14121300
C	0.24439100	-2.04518200	-1.62442800
H	0.13433500	-1.96677000	-2.78901100
H	1.31919100	-2.28580100	-1.59267500
C	-0.48812700	-3.38429500	-1.44905400
H	-0.23625300	-3.79353800	-0.45678200
H	-1.58152000	-3.23946800	-1.43893600
C	-0.13692400	-4.41508400	-2.51578400
H	-0.64835900	-5.37404800	-2.35531600
H	-0.41388700	-4.05378600	-3.51932700
H	0.94586100	-4.60977000	-2.53026100
C	-2.47970700	0.15799500	-3.38356600
C	-2.25368900	-1.16637700	-3.81392300
C	-1.59706900	-1.12122200	-5.06514700
C	-1.97627300	1.04294300	-4.37861700
C	-1.44171200	0.24576000	-5.42056000
H	-2.95533000	0.46002300	-2.45963200
H	-2.49823600	-2.07204900	-3.26509100
H	-1.27741300	-1.98006700	-5.64893800
H	-2.01496200	2.12674900	-4.34581400
H	-0.99139800	0.61871700	-6.33517500
Zr	0.04075700	-0.08737400	-3.45885300
C	2.53537100	-0.39323900	-3.34165900
C	2.03858500	-1.20162800	-4.40852800
C	1.55662600	-0.32780900	-5.41148400
C	2.36562800	0.96375000	-3.70346600
C	1.74505900	1.01062400	-4.96858500
H	2.99366000	-0.76672600	-2.43392100
H	2.06004200	-2.28663500	-4.45212600
H	1.11970000	-0.63103900	-6.35768500
H	2.60825200	1.82780200	-3.09295800
H	1.46039200	1.90994900	-5.50740600
Cl	-0.10575200	1.84163800	-1.68314900

Complex **10**, $Cp_2Zr(\mu\text{-}Pr)(\mu\text{-}Cl)ZrCp_2$ (open shell singlet)

```
M06/BS1:
 E(UM06) =  -1446.33521163
 Zero-point correction=                           0.429476 (Hartree/Particle)
 Thermal correction to Energy=                    0.456761
 Thermal correction to Enthalpy=                  0.457705
 Thermal correction to Gibbs Free Energy=         0.372229
 Sum of electronic and zero-point Energies=          -1445.905736
 Sum of electronic and thermal Energies=             -1445.878451
 Sum of electronic and thermal Enthalpies=           -1445.877506
 Sum of electronic and thermal Free Energies=        -1445.962983
E(UM06/BS2) =  -1446.67876557
```

C	-2.54326100	-0.92820900	0.18668800
C	-2.54378800	0.47151200	0.37121000
C	-1.99001000	0.75766300	1.64097000
C	-1.98672100	-1.53169100	1.34669700
C	-1.65389300	-0.48397100	2.24894900
H	-2.89183400	-1.45850200	-0.69576300
H	-2.86634800	1.21334100	-0.35338500
H	-1.85973300	1.74465200	2.07405700

H	-1.87267700	-2.59696600	1.52339400
H	-1.23671500	-0.61486600	3.24212700
Zr	-0.09394900	-0.27470600	0.34866500
C	2.40043700	0.14307200	0.20249300
C	1.89946000	0.86581600	1.32028400
C	1.45384400	-0.09049100	2.27077700
C	2.27050700	-1.23774400	0.46579600
C	1.67161500	-1.39161600	1.73751900
H	2.78704700	0.58608100	-0.71082800
H	1.88583100	1.94502200	1.43244000
H	1.03356200	0.13446000	3.24572200
H	2.53665900	-2.04798900	-0.20861300
H	1.43268700	-2.33412200	2.22267500
C	-0.05752600	-1.72380400	-1.51625000
H	-0.92058300	-1.37010800	-2.11524900
H	0.90656200	-1.46112900	-1.99703900
C	-0.15620300	-3.23906800	-1.40363800
H	0.42752900	-3.57339400	-0.52712800
H	-1.20111100	-3.50803100	-1.17075100
C	0.30916100	-4.01389200	-2.63071600
H	0.19430700	-5.10004200	-2.50958600
H	-0.25091000	-3.71047000	-3.52996100
H	1.37336300	-3.81165500	-2.83071100
C	-2.44851600	0.16780700	-3.72365600
C	-2.29513100	-1.16444800	-4.17513700
C	-1.64516500	-1.13498100	-5.42817300
C	-1.91459000	1.03952800	-4.71407600
C	-1.42600400	0.22785400	-5.76866800
H	-2.87842300	0.47597000	-2.77564300
H	-2.58398200	-2.06096100	-3.63168000
H	-1.36853400	-1.99901000	-6.02608300
H	-1.90093600	2.12374200	-4.67082400
H	-0.96887000	0.58935900	-6.68441600
Zr	0.03635200	-0.17319400	-3.81169200
C	2.53772300	-0.57219900	-3.65649600
C	2.03137000	-1.30586300	-4.76775800
C	1.58143800	-0.35874300	-5.72239700
C	2.39681700	0.80557100	-3.92809500
C	1.79026400	0.94763700	-5.19617400
H	2.96249200	-1.00142100	-2.75280100
H	2.03039100	-2.38536600	-4.88111300
H	1.16168700	-0.59384200	-6.69533700
H	2.64651400	1.61773200	-3.25265600
H	1.54522700	1.88523700	-5.68640100
Cl	-0.04807300	1.47068100	-1.74082200

Complex **10**, $Cp_2Zr(\mu\text{-}Pr)(\mu\text{-}Cl)ZrCp_2$ (triplet)

```
M06/BS1:
 E(UM06) =  -1446.33478620
 Zero-point correction=                           0.429503 (Hartree/Particle)
 Thermal correction to Energy=                    0.456711
 Thermal correction to Enthalpy=                  0.457655
 Thermal correction to Gibbs Free Energy=         0.371766
 Sum of electronic and zero-point Energies=          -1445.905283
 Sum of electronic and thermal Energies=             -1445.878076
 Sum of electronic and thermal Enthalpies=           -1445.877131
 Sum of electronic and thermal Free Energies=        -1445.963020
E(UM06/BS2) =  -1446.67799009
```

C	-2.53429500	-0.93191400	0.19555300
C	-2.53095500	0.46716200	0.38305600
C	-1.99224300	0.74838100	1.66075000
C	-1.99447900	-1.54064600	1.36074600
C	-1.66881600	-0.49621400	2.26979700
H	-2.87290600	-1.45793200	-0.69318700

```
 H                -2.84012700    1.21161300   -0.34470800
 H                -1.86444500    1.73368600    2.09837100
 H                -1.88748700   -2.60689900    1.53611800
 H                -1.26314100   -0.63091100    3.26733600
 Zr               -0.08466500   -0.28799000    0.39124700
 C                 2.41222600    0.10181800    0.26766900
 C                 1.90804900    0.84042600    1.37421000
 C                 1.44393700   -0.10272400    2.32890900
 C                 2.26675600   -1.27524600    0.54281100
 C                 1.65441500   -1.41081600    1.80995800
 H                 2.81329500    0.53171500   -0.64584100
 H                 1.90569700    1.92056000    1.47731400
 H                 1.01494900    0.13548700    3.29698000
 H                 2.53072300   -2.09373200   -0.12203300
 H                 1.40000300   -2.34592200    2.30153800
 C                -0.03606600   -1.69683600   -1.50935700
 H                -0.89544500   -1.30731400   -2.09054500
 H                 0.93216700   -1.42243300   -1.97497100
 C                -0.15441500   -3.21194800   -1.42548100
 H                 0.41913600   -3.56999300   -0.55136100
 H                -1.20408200   -3.47101800   -1.20222100
 C                 0.30771900   -3.97524800   -2.66093500
 H                 0.18283700   -5.06190700   -2.55403800
 H                -0.24702300   -3.65535000   -3.55785000
 H                 1.37432000   -3.78023600   -2.85453900
 C                -2.44120300    0.18058900   -3.73529900
 C                -2.29421200   -1.16008600   -4.16239600
 C                -1.65886100   -1.15640700   -5.42364900
 C                -1.91532800    1.03191400   -4.74710400
 C                -1.43972000    0.19913100   -5.79206900
 H                -2.85922300    0.50837100   -2.78857500
 H                -2.57756500   -2.04537000   -3.59814300
 H                -1.39200700   -2.03232900   -6.00843600
 H                -1.90024900    2.11681700   -4.72573600
 H                -0.99253800    0.54236700   -6.71970800
 Zr                0.04312100   -0.16831300   -3.84829700
 C                 2.54464600   -0.52181100   -3.70021100
 C                 2.04827100   -1.29628900   -4.78832800
 C                 1.57817300   -0.38614300   -5.76820700
 C                 2.38104000    0.84535200   -4.01300200
 C                 1.76883600    0.93842000   -5.28247800
 H                 2.98244400   -0.91675800   -2.78731900
 H                 2.06572900   -2.37841200   -4.87077700
 H                 1.15486900   -0.65763200   -6.73020900
 H                 2.61937900    1.68054700   -3.36205500
 H                 1.50471700    1.85611700   -5.79990100
 Cl               -0.01659700    1.42254700   -1.73264900
```

Complex **11**, Zr_2Cp_4 (closed shell singlet)

```
M06/BS1:
 E(RM06) =  -867.611775273
 Zero-point correction=                           0.330767 (Hartree/Particle)
 Thermal correction to Energy=                    0.351300
 Thermal correction to Enthalpy=                  0.352244
 Thermal correction to Gibbs Free Energy=         0.282850
 Sum of electronic and zero-point Energies=           -867.281008
 Sum of electronic and thermal Energies=              -867.260476
 Sum of electronic and thermal Enthalpies=            -867.259531
 Sum of electronic and thermal Free Energies=         -867.328926
E(RM06/BS2) =  -867.884183797

 C                -0.36879800   -0.07233800   -1.30921700
 C                 0.94633600    0.53004800   -1.33681300
 C                 1.34789600    0.67589000    0.04605800
 C                -0.72192000   -0.33762800    0.03188400
 C                 0.32446000    0.13307600    0.86362000
```

```
 H                -0.97297000   -0.30168500   -2.18242900
 H                 1.24822500    1.19079000   -2.19963200
 H                 2.27247400    1.12072400    0.39796800
 H                -1.63620400   -0.81819200    0.36607600
 H                 0.34636200    0.06885300    1.94802600
 Zr                1.33150200   -1.67278900   -0.52755100
 C                 3.39376100   -2.90703800    0.27904500
 C                 2.78467200   -2.28129800    1.39961400
 C                 1.53477800   -2.91434200    1.63688500
 C                 2.49717600   -3.89184400   -0.19408700
 C                 1.34298200   -3.90311800    0.64535700
 H                 4.36781900   -2.66533100   -0.13235900
 H                 3.21142800   -1.47407600    1.98925300
 H                 0.83189200   -2.66049300    2.42543300
 H                 2.65705500   -4.55043600   -1.04358900
 H                 0.49468400   -4.57497000    0.56386600
 C                 1.20819100   -1.49595900   -4.06860400
 C                 1.66780200   -2.27884200   -2.94132600
 C                 3.05050200   -2.60335900   -3.22130800
 C                 2.28384300   -1.30360900   -4.96304700
 C                 3.41095300   -1.99216000   -4.44945600
 H                 0.20204400   -1.10600800   -4.19440700
 H                 0.93285600   -2.89946100   -2.35035300
 H                 3.70337200   -3.20193700   -2.59487700
 H                 2.25102800   -0.72912300   -5.88349800
 H                 4.39224500   -2.03202300   -4.91397600
 Zr                2.87495700   -0.23916200   -2.76708000
 C                 4.62750000    0.58396700   -1.13790500
 C                 5.29337000   -0.07105600   -2.20831700
 C                 5.11235100    0.70441700   -3.38514200
 C                 4.00435800    1.73591500   -1.67029600
 C                 4.30211400    1.81730300   -3.06362200
 H                 4.59676000    0.24929100   -0.10642200
 H                 5.86069800   -0.99550100   -2.13664100
 H                 5.50175100    0.46597600   -4.37106800
 H                 3.40636200    2.45473500   -1.11598700
 H                 3.99950600    2.60971300   -3.74035800
```

Complex **11** (open shell singlet)

```
M06/BS1:
 E(UM06) =  -867.622241787
 Zero-point correction=                           0.330870 (Hartree/Particle)
 Thermal correction to Energy=                    0.351672
 Thermal correction to Enthalpy=                  0.352616
 Thermal correction to Gibbs Free Energy=         0.281458
 Sum of electronic and zero-point Energies=           -867.291372
 Sum of electronic and thermal Energies=              -867.270570
 Sum of electronic and thermal Enthalpies=            -867.269625
 Sum of electronic and thermal Free Energies=         -867.340784
E(UM06/BS2) =  -867.894080832

 C                -0.37118600   -0.07492900   -1.36995100
 C                 0.91438000    0.56994400   -1.29742300
 C                 1.20551500    0.73077200    0.10644800
 C                -0.81051000   -0.37233000   -0.06463800
 C                 0.15734500    0.13343900    0.84501100
 H                -0.90643700   -0.32202100   -2.28161100
 H                 1.31838200    1.19601400   -2.13119700
 H                 2.08246000    1.21742900    0.52280500
 H                -1.72985600   -0.88541900    0.19852400
 H                 0.10491500    0.06147700    1.92782300
 Zr                1.34800800   -1.62437800   -0.46257000
 C                 3.42945800   -2.85798400    0.24053800
 C                 2.88347300   -2.21260100    1.38261600
 C                 1.63706400   -2.82927800    1.68380200
 C                 2.50603300   -3.84999700   -0.16799100
```

```
 C                  1.39703000   -3.84374500    0.72161500
 H                  4.37823500   -2.62945200   -0.23497300
 H                  3.34891900   -1.40712500    1.94451200
 H                  0.97905200   -2.56628900    2.50713900
 H                  2.61966200   -4.51351600   -1.02187800
 H                  0.54182900   -4.51070800    0.68919300
 C                  1.15563500   -1.43032500   -4.05970300
 C                  1.65747000   -2.28765900   -3.01697800
 C                  3.00339400   -2.64047700   -3.39983700
 C                  2.18008200   -1.19903900   -4.99853500
 C                  3.31599800   -1.95294700   -4.59637600
 H                  0.15955100   -1.00037300   -4.10185300
 H                  0.98092800   -2.88471000   -2.35585900
 H                  3.66336900   -3.30988600   -2.85556600
 H                  2.10998700   -0.56864400   -5.87900400
 H                  4.26805800   -1.98798100   -5.11835600
 Zr                 2.95655100   -0.29892200   -2.76991400
 C                  4.64446900    0.50869900   -1.08436300
 C                  5.33714100   -0.19472800   -2.10601400
 C                  5.22406200    0.55452200   -3.31016500
 C                  4.09016300    1.67283900   -1.67003200
 C                  4.44737100    1.71195800   -3.04498700
 H                  4.55561900    0.20663900   -0.04520200
 H                  5.87918600   -1.12882200   -1.98458900
 H                  5.65498300    0.28571900   -4.27046500
 H                  3.48891800    2.41973300   -1.15710700
 H                  4.19946900    2.49701800   -3.75166300
```

Complex **11** (triplet)

```
M06/BS1:
 E(UM06) =  -867.623302564
 Zero-point correction=                           0.330720 (Hartree/Particle)
 Thermal correction to Energy=                    0.351545
 Thermal correction to Enthalpy=                  0.352490
 Thermal correction to Gibbs Free Energy=         0.280277
 Sum of electronic and zero-point Energies=           -867.292583
 Sum of electronic and thermal Energies=              -867.271757
 Sum of electronic and thermal Enthalpies=            -867.270813
 Sum of electronic and thermal Free Energies=         -867.343026
E(UM06/BS2) =  -867.894661847

 C                 -0.37992900   -0.09116600   -1.36458500
 C                  0.90191900    0.56205700   -1.29271400
 C                  1.19068200    0.73075300    0.11290900
 C                 -0.82030700   -0.38160000   -0.05939400
 C                  0.14243600    0.13069000    0.85135200
 H                 -0.91237300   -0.34702600   -2.27550100
 H                  1.31126300    1.17618400   -2.13096600
 H                  2.05789800    1.23430300    0.52963500
 H                 -1.73497600   -0.90358000    0.20377100
 H                  0.08633000    0.06248400    1.93420800
 Zr                 1.36094400   -1.61177100   -0.44304400
 C                  3.43149800   -2.88081900    0.22677600
 C                  2.90587200   -2.22162700    1.37256200
 C                  1.65528100   -2.82496600    1.68939700
 C                  2.49508300   -3.86567000   -0.16604500
 C                  1.39611600   -3.84187600    0.73280900
 H                  4.37395300   -2.65854200   -0.26555300
 H                  3.39063900   -1.42504100    1.93039100
 H                  1.01099600   -2.55650900    2.52168300
 H                  2.59019600   -4.53113800   -1.02064700
 H                  0.53277900   -4.49889500    0.70919600
 C                  1.15809000   -1.40993700   -4.06847800
 C                  1.65084900   -2.28001500   -3.03200100
 C                  2.99545700   -2.64385400   -3.41579700
 C                  2.18460500   -1.18439400   -5.00449100
```

C	3.31448400	-1.94964100	-4.60791600
H	0.16689800	-0.96871300	-4.10870000
H	0.97188900	-2.86348000	-2.36369300
H	3.64457200	-3.33174600	-2.88183800
H	2.12264500	-0.54221900	-5.87739400
H	4.26578800	-1.98885600	-5.13094800
Zr	2.97657400	-0.32157600	-2.75996300
C	4.63864800	0.54024300	-1.07566300
C	5.34036100	-0.18688200	-2.07691200
C	5.23624900	0.53924600	-3.29719600
C	4.09151900	1.69311200	-1.68796700
C	4.45685000	1.70204300	-3.05919300
H	4.54024200	0.25879700	-0.03114700
H	5.89212800	-1.11098900	-1.92766100
H	5.67811600	0.25479200	-4.24786700
H	3.48405400	2.44886500	-1.19609900
H	4.20985500	2.47087900	-3.78409200

Complex **11** singlet to triplet MECP

E (M06/BS1) = -867.6106967

C	-0.36588600	-0.04790600	-1.30741800
C	0.95531100	0.54010500	-1.35929700
C	1.38615100	0.67543600	0.01346300
C	-0.69615000	-0.31294500	0.04159300
C	0.37323300	0.14344500	0.85045700
H	-0.98613600	-0.26964900	-2.17164400
H	1.24080200	1.20115900	-2.23032100
H	2.32627200	1.09688700	0.34978600
H	-1.61186300	-0.77694300	0.39449400
H	0.41673000	0.07977900	1.93403700
Zr	1.30802500	-1.68176900	-0.57625200
C	3.37017500	-2.90109100	0.24590000
C	2.75291000	-2.28645800	1.36885000
C	1.51194900	-2.93408900	1.60765400
C	2.48066700	-3.89318100	-0.22978900
C	1.32815900	-3.91672600	0.61337400
H	4.34665500	-2.65637900	-0.15509500
H	3.16950300	-1.47403700	1.95898400
H	0.80458500	-2.68537700	2.39372300
H	2.64619200	-4.55551000	-1.07496600
H	0.48398500	-4.59335800	0.52786300
C	1.23522300	-1.45156700	-4.11296400
C	1.60959600	-2.23993800	-2.95191400
C	2.99798200	-2.60794600	-3.15766300
C	2.36164300	-1.31526400	-4.95653200
C	3.43540700	-2.03172200	-4.37838400
H	0.25041900	-1.02982900	-4.29301900
H	0.81846200	-2.84964100	-2.41700000
H	3.60215300	-3.21533300	-2.49433500
H	2.39431500	-0.75409900	-5.88559100
H	4.43560800	-2.11325900	-4.79460400
Zr	2.86052700	-0.23234700	-2.75246500
C	4.63883900	0.56686300	-1.13030300
C	5.29138400	-0.08342100	-2.21198300
C	5.11059300	0.70419800	-3.38017300
C	4.01864200	1.72608800	-1.64871000
C	4.30780900	1.81504500	-3.04462100
H	4.62472000	0.22861100	-0.10010200
H	5.85146500	-1.01316800	-2.15256400
H	5.48636100	0.46718300	-4.37194500
H	3.43232000	2.44755200	-1.08512200
H	4.00143400	2.61252200	-3.71417900

TS11-12 (singlet)

```
M06/BS1:
 E(RM06) =  -867.595248696
 Zero-point correction=                           0.327615 (Hartree/Particle)
 Thermal correction to Energy=                    0.347566
 Thermal correction to Enthalpy=                  0.348511
 Thermal correction to Gibbs Free Energy=         0.280500
 Sum of electronic and zero-point Energies=           -867.267634
 Sum of electronic and thermal Energies=              -867.247682
 Sum of electronic and thermal Enthalpies=            -867.246738
 Sum of electronic and thermal Free Energies=         -867.314749
E(RM06/BS2) =  -867.866424779

 C                 -0.23457900   -0.13772100   -1.36446000
 C                  1.12698800    0.36560200   -1.35823600
 C                  1.40392800    0.57126600    0.04604500
 C                 -0.73225600   -0.26016900   -0.03230200
 C                  0.28181500    0.18867800    0.83556500
 H                 -0.79427500   -0.38602000   -2.26474200
 H                  1.43008300    1.09081500   -2.66514900
 H                  2.35655700    0.89913100    0.45448600
 H                 -1.71997000   -0.60391100    0.26023100
 H                  0.21806500    0.22565300    1.92059400
 Zr                 1.20836200   -1.76783200   -0.45262700
 C                  3.35612000   -2.81902700    0.23847100
 C                  2.78257000   -2.20888800    1.39099300
 C                  1.60216100   -2.92014500    1.74319300
 C                  2.49376400   -3.88822000   -0.13295400
 C                  1.41914600   -3.95077700    0.80034500
 H                  4.29608300   -2.55190100   -0.23092300
 H                  3.19171200   -1.35954100    1.93145200
 H                  0.94241300   -2.69049900    2.57451000
 H                  2.64297800   -4.57381500   -0.96332200
 H                  0.59887200   -4.66312500    0.78765100
 C                  1.16478800   -1.47418200   -4.14240400
 C                  1.57635200   -2.36052900   -3.09865100
 C                  2.96116800   -2.66735800   -3.31123000
 C                  2.28063000   -1.20172400   -4.95397300
 C                  3.38475600   -1.94287000   -4.44422700
 H                  0.17090700   -1.05917000   -4.27364700
 H                  0.86997800   -2.97133300   -2.50992400
 H                  3.56605700   -3.34530400   -2.71844800
 H                  2.29217400   -0.54126200   -5.81507500
 H                  4.39269200   -1.93605900   -4.84900200
 Zr                 2.85805100   -0.24796000   -2.67794800
 C                  4.68098300    0.57482500   -1.11029800
 C                  5.31969500   -0.05276300   -2.20872000
 C                  5.06315800    0.72723400   -3.36676200
 C                  4.00697900    1.71850600   -1.59601100
 C                  4.24046700    1.81910800   -2.99709200
 H                  4.70105200    0.22968600   -0.08090200
 H                  5.91147400   -0.96383000   -2.16964700
 H                  5.41367500    0.50823800   -4.37199700
 H                  3.40077300    2.40352500   -1.01128900
 H                  3.87982500    2.60558900   -3.65035500
```

TS11-12 triplet

```
M06/BS1:
 E(UM06) =  -867.603198683
 Zero-point correction=                           0.327965 (Hartree/Particle)
 Thermal correction to Energy=                    0.347880
 Thermal correction to Enthalpy=                  0.348824
 Thermal correction to Gibbs Free Energy=         0.279451
 Sum of electronic and zero-point Energies=           -867.275234
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```
 Sum of electronic and thermal Energies=             -867.255319
 Sum of electronic and thermal Enthalpies=           -867.254374
 Sum of electronic and thermal Free Energies=        -867.323748
E(UM06/BS2) =  -867.873758521

 C                 -0.42266400   -0.06743300   -1.34498300
 C                  0.84470000    0.59154800   -1.29835600
 C                  1.22039700    0.69649600    0.07861900
 C                 -0.80001300   -0.39634700   -0.02669900
 C                  0.21134300    0.08188800    0.84948100
 H                 -0.99612500   -0.29073700   -2.23801300
 H                  1.26556900    1.16325200   -2.14929200
 H                  2.12158000    1.16731800    0.46154000
 H                 -1.70508700   -0.92081300    0.26348600
 H                  0.21991400   -0.02765200    1.93029500
 Zr                 1.29428900   -1.72776800   -0.53053800
 C                  3.36077500   -2.94402300    0.26771100
 C                  2.75191300   -2.32892400    1.39138100
 C                  1.50288800   -2.97115600    1.61723600
 C                  2.47836200   -3.93849400   -0.21341600
 C                  1.32955100   -3.96417800    0.62193200
 H                  4.31997600   -2.67093400   -0.16426000
 H                  3.17392000   -1.52110100    1.98364800
 H                  0.79880100   -2.73591600    2.41064200
 H                  2.63242700   -4.56576100   -1.08594300
 H                  0.48074400   -4.63122100    0.51697300
 C                  1.23673500   -1.37349900   -3.91471900
 C                  1.74645600   -2.12527300   -2.79674300
 C                  3.05093400   -2.57676100   -3.24048000
 C                  2.20762200   -1.28166800   -4.93943200
 C                  3.33363600   -2.03181700   -4.52619000
 H                  0.27166700   -0.87225600   -3.94196300
 H                  0.54913500   -2.76236900   -1.97193300
 H                  3.73773500   -3.18938700   -2.66140800
 H                  2.10041800   -0.75093700   -5.88080900
 H                  4.24315600   -2.18101500   -5.10333800
 Zr                 3.07326400   -0.25503000   -2.79108000
 C                  4.76814000    0.68891600   -1.16975500
 C                  5.46111900   -0.04336500   -2.16893300
 C                  5.29389500    0.64165000   -3.40593600
 C                  4.16295600    1.80635300   -1.79213400
 C                  4.48757900    1.78933300   -3.17570100
 H                  4.69357500    0.42001600   -0.11883000
 H                  6.03744900   -0.95070200   -2.01121300
 H                  5.71424200    0.34065800   -4.36110000
 H                  3.54948600    2.55599300   -1.29763600
 H                  4.20370900    2.53503500   -3.91088500
```

Complex **12** triplet

```
M06/BS1:
 E(UM06) =  -867.631608269
 Zero-point correction=                           0.329123 (Hartree/Particle)
 Thermal correction to Energy=                    0.349458
 Thermal correction to Enthalpy=                  0.350402
 Thermal correction to Gibbs Free Energy=         0.280432
 Sum of electronic and zero-point Energies=           -867.302485
 Sum of electronic and thermal Energies=              -867.282150
 Sum of electronic and thermal Enthalpies=            -867.281206
 Sum of electronic and thermal Free Energies=         -867.351177
E(UM06/BS2) =  -867.901483469

 C                 -0.41049900   -0.02972900   -1.41430500
 C                  0.88643800    0.54859100   -1.31210200
 C                  1.23201100    0.57930600    0.07438300
 C                 -0.84506300   -0.37491900   -0.11726900
 C                  0.16645400    0.00798200    0.79783300
```

H	-0.96266000	-0.20504300	-2.33131400
H	1.33078200	1.16188100	-2.12658900
H	2.15312800	0.97279200	0.49546900
H	-1.78199700	-0.86307700	0.12624400
H	0.14335400	-0.14158200	1.87361200
Zr	1.16836600	-1.87138500	-0.62818300
C	3.35808000	-2.83561900	0.15336200
C	2.74049200	-2.23752900	1.27847700
C	1.57002500	-2.98273200	1.58179000
C	2.55881200	-3.93647500	-0.24814300
C	1.46301100	-4.03605300	0.64436200
H	4.26728800	-2.49177000	-0.33356600
H	3.10139700	-1.36619700	1.81891100
H	0.87229200	-2.77667600	2.38863400
H	2.74006100	-4.58351700	-1.09986200
H	0.66817700	-4.77056400	0.59503600
C	1.28578500	-1.43456900	-3.92774200
C	1.78979500	-2.21671000	-2.82716800
C	3.13268300	-2.54933600	-3.24401700
C	2.26998300	-1.25356700	-4.93032400
C	3.42834700	-1.95389800	-4.50123700
H	0.29303500	-0.99103600	-3.97555600
H	-0.32395300	-2.94402000	-0.98677900
H	3.83794800	-3.14680400	-2.66840100
H	2.15733100	-0.70900100	-5.86359400
H	4.36486500	-2.02982200	-5.04918900
Zr	3.05814000	-0.20529300	-2.79121700
C	4.78132500	0.67489400	-1.17984100
C	5.46414300	-0.01414200	-2.21257700
C	5.26839800	0.70642700	-3.42450300
C	4.15134800	1.80615000	-1.75718000
C	4.45821100	1.83918400	-3.14621600
H	4.73474000	0.37666100	-0.13547100
H	6.04293800	-0.92659500	-2.09912800
H	5.67509600	0.43873200	-4.39529000
H	3.54525700	2.53724200	-1.22716500
H	4.15730800	2.60524100	-3.85297000

Complex **12** singlet

M06/BS1:
E(RM06) = -867.628953413
Zero-point correction= 0.329045 (Hartree/Particle)
Thermal correction to Energy= 0.349329
Thermal correction to Enthalpy= 0.350274
Thermal correction to Gibbs Free Energy= 0.281480
Sum of electronic and zero-point Energies= -867.299909
Sum of electronic and thermal Energies= -867.279624
Sum of electronic and thermal Enthalpies= -867.278680
Sum of electronic and thermal Free Energies= -867.347473
E(RM06/BS2) = -867.898455141

C	-0.23287400	-0.10189900	-1.36832000
C	1.13581200	0.40171400	-1.29421900
C	1.33140900	0.53965900	0.13512900
C	-0.81061000	-0.21649100	-0.06967800
C	0.16087100	0.17967100	0.86471700
H	-0.77819800	-0.27525300	-2.29285500
H	2.04154100	1.20387000	-3.82584600
H	2.25065600	0.88409900	0.60657200
H	-1.81533800	-0.56086400	0.16738300
H	0.04281300	0.18466700	1.94587200
Zr	1.13810600	-1.77149400	-0.38753900
C	3.35907900	-2.67661400	0.22089600
C	2.75373000	-2.08176300	1.37193600
C	1.64125700	-2.88892200	1.76226200
C	2.59769700	-3.83286800	-0.09874100

C	1.55530700	-3.96448200	0.84755900
H	4.26697800	-2.35246300	-0.27597800
H	3.11547100	-1.20949900	1.90784800
H	0.99727000	-2.72444100	2.62005600
H	2.78275900	-4.50662200	-0.93159300
H	0.79753600	-4.74436400	0.85095800
C	1.08348700	-1.57212600	-4.02207600
C	1.71880600	-2.37028300	-3.02902200
C	3.07780100	-2.55219000	-3.43500400
C	2.04647900	-1.22967200	-4.99740600
C	3.26596400	-1.85005100	-4.64479800
H	0.05003700	-1.24415600	-4.01525400
H	1.16502000	-3.01191200	-2.30721500
H	3.82731200	-3.13370900	-2.90647600
H	1.87497600	-0.59145500	-5.85646200
H	4.20171000	-1.76926000	-5.19063100
Zr	2.77580100	-0.15475300	-2.76732800
C	4.55843000	0.37661800	-1.05420400
C	5.21180600	-0.23843900	-2.15101900
C	5.11785700	0.63944000	-3.26102700
C	4.05111600	1.62527100	-1.49482200
C	4.40785600	1.79278000	-2.85400200
H	4.47499700	-0.02873100	-0.05096500
H	5.71722200	-1.20062400	-2.14182600
H	5.51446400	0.45676400	-4.25567100
H	3.47186500	2.32733400	-0.90442000
H	4.15189100	2.64043600	-3.47807600

Complex **12** triplet to singlet MECP

E (M06/BS1) = -867.6275392

C	-0.37041800	-0.01421600	-1.44595100
C	0.91733700	0.56653500	-1.26651100
C	1.18311800	0.58415400	0.13824800
C	-0.87028000	-0.38447000	-0.17806000
C	0.08048300	0.00126000	0.79537300
H	-0.87073800	-0.17952500	-2.39376600
H	1.39942000	1.21274200	-2.03540300
H	2.07846800	0.97919000	0.60987200
H	-1.81387200	-0.88390500	0.00803900
H	-0.00569100	-0.15667900	1.86697100
Zr	1.22327200	-1.81518900	-0.63981700
C	3.43535100	-2.74007400	0.14856800
C	2.80732600	-2.14775300	1.27192100
C	1.65129100	-2.91201600	1.57787700
C	2.65774400	-3.85911200	-0.24503400
C	1.56433900	-3.97340600	0.64664100
H	4.35410900	-2.40086900	-0.32252700
H	3.15327400	-1.27064300	1.81167400
H	0.94830000	-2.71414400	2.38189100
H	2.85178400	-4.50842200	-1.09210300
H	0.78327900	-4.72270700	0.60028500
C	1.25617900	-1.48311900	-3.94133500
C	1.80813600	-2.21979100	-2.81641600
C	3.15348000	-2.51503400	-3.26594300
C	2.20687700	-1.34894200	-4.98943700
C	3.39114900	-1.99030300	-4.56822600
H	0.23396200	-1.11573100	-4.00018100
H	-0.24871200	-2.92955300	-0.96998100
H	3.89963600	-3.05771100	-2.68692700
H	2.05761300	-0.84469400	-5.94181000
H	4.31638000	-2.05951900	-5.13610100
Zr	2.98625800	-0.17314400	-2.90948900
C	4.63711700	0.52262500	-1.16736200
C	5.33427500	-0.12470400	-2.22854100
C	5.25909300	0.70850800	-3.38228700

C	4.11621300	1.73772300	-1.68270500
C	4.50635100	1.85790300	-3.04081200
H	4.54514100	0.16454400	-0.14618900
H	5.87308100	-1.06556900	-2.16210600
H	5.71615700	0.50782300	-4.34644800
H	3.52648500	2.46410600	-1.12922600
H	4.25990600	2.68125700	-3.70545000

TS12-13

M06/BS1:

E(RM06) =	-867.609365736
Zero-point correction=	0.324496 (Hartree/Particle)
Thermal correction to Energy=	0.344418
Thermal correction to Enthalpy=	0.345362
Thermal correction to Gibbs Free Energy=	0.277136
Sum of electronic and zero-point Energies=	-867.284870
Sum of electronic and thermal Energies=	-867.264948
Sum of electronic and thermal Enthalpies=	-867.264004
Sum of electronic and thermal Free Energies=	-867.332230

E(RM06/BS2) = -867.878190836

C	-0.21081200	-0.07259400	-1.35792200
C	1.15224700	0.43211500	-1.31051900
C	1.40960900	0.53049000	0.10755300
C	-0.73395600	-0.23939100	-0.05615100
C	0.27930600	0.11420500	0.86468800
H	-0.78191800	-0.25167400	-2.26291600
H	2.22886300	1.18861300	-4.29030200
H	2.33982300	0.87632500	0.55681800
H	-1.73033000	-0.59497500	0.19859200
H	0.19882200	0.08550000	1.94888200
Zr	1.23567100	-1.82072200	-0.41661600
C	3.35529900	-2.98794400	0.32657300
C	2.73773900	-2.37677700	1.45097200
C	1.51168000	-3.06155700	1.69680800
C	2.51172800	-4.02395600	-0.13005700
C	1.37554900	-4.07816100	0.71373300
H	4.30544400	-2.69796400	-0.11453100
H	3.14418600	-1.56245200	2.04384900
H	0.81804100	-2.85613700	2.50696100
H	2.68202600	-4.64728600	-1.00249800
H	0.54936300	-4.77582800	0.61724600
C	1.15412100	-1.53099500	-3.83159600
C	1.79695300	-2.13227300	-2.69668700
C	3.14278500	-2.38452100	-3.14372600
C	2.06773500	-1.41024500	-4.90847600
C	3.29933700	-1.93966400	-4.48737200
H	0.12138800	-1.19878500	-3.86266600
H	0.72060800	-2.83326900	-1.96280100
H	3.92939800	-2.83402600	-2.54244100
H	1.85399700	-0.96896200	-5.87582100
H	4.21149100	-1.98898300	-5.07713300
Zr	2.78091000	0.03563900	-2.91910600
C	4.53918000	0.57956500	-1.17769400
C	5.21996900	-0.02902400	-2.25930300
C	5.12840800	0.83774000	-3.37494300
C	4.03552200	1.82830800	-1.62480900
C	4.40727200	1.99161700	-2.97850900
H	4.44807900	0.17362200	-0.17326300
H	5.72360800	-0.99110000	-2.23920400
H	5.53299900	0.65112700	-4.36543500
H	3.44696500	2.52713300	-1.03914600
H	4.15706600	2.83418900	-3.61231800

Complex **13**

```
M06/BS1:
 E(RM06) =  -867.659697720
 Zero-point correction=                           0.325981 (Hartree/Particle)
 Thermal correction to Energy=                    0.346263
 Thermal correction to Enthalpy=                  0.347207
 Thermal correction to Gibbs Free Energy=         0.278248
 Sum of electronic and zero-point Energies=          -867.333717
 Sum of electronic and thermal Energies=             -867.313435
 Sum of electronic and thermal Enthalpies=           -867.312491
 Sum of electronic and thermal Free Energies=        -867.381450
E(RM06/BS2) =  -867.927580267

 C                  0.06732200    0.12084100   -1.30952400
 C                  1.47994600    0.33864100   -1.19901800
 C                  1.73627000    0.27634600    0.20667700
 C                 -0.51832300   -0.02138400   -0.02763100
 C                  0.52416200    0.05488500    0.92050800
 H                 -0.48959400    0.05294200   -2.24267100
 H                  2.04317000    1.06354100   -4.38013300
 H                  2.71481500    0.38127100    0.67506900
 H                 -1.56906000   -0.19319400    0.18331500
 H                  0.41616200   -0.03364500    1.99900400
 Zr                 1.05443900   -1.99372700   -0.45450800
 C                  3.06989400   -3.06616800    0.57993800
 C                  2.24811000   -2.66621800    1.66114500
 C                  1.06310200   -3.43560600    1.61688200
 C                  2.40139300   -4.10768000   -0.11571000
 C                  1.16153500   -4.33273200    0.52318500
 H                  4.04374700   -2.65036400    0.33398900
 H                  2.47717400   -1.88692400    2.38192400
 H                  0.21507100   -3.34658600    2.28957200
 H                  2.76537200   -4.61807000   -1.00103500
 H                  0.40102800   -5.04222500    0.21661300
 C                  1.36244000   -1.73298700   -3.72220000
 C                  2.02163500   -2.18471200   -2.53255600
 C                  3.39503700   -2.30476000   -2.91620300
 C                  2.28283600   -1.62575700   -4.79425000
 C                  3.55631800   -1.96357600   -4.28896500
 H                  0.30597900   -1.48251800   -3.80149400
 H                 -0.68560300   -2.67013500   -0.66230300
 H                  4.21009900   -2.61368900   -2.26136700
 H                  2.05505000   -1.30960000   -5.80726000
 H                  4.48828100   -1.96430300   -4.84957600
 Zr                 2.88186100    0.09826900   -3.00397700
 C                  4.81224200    0.78940300   -1.54837500
 C                  5.38067300    0.35472400   -2.76902600
 C                  4.98021900    1.25602000   -3.78260400
 C                  4.08057600    1.97858400   -1.80476100
 C                  4.18484100    2.26647100   -3.18425500
 H                  4.92551500    0.30100900   -0.58390300
 H                  5.99530800   -0.52987500   -2.90702400
 H                  5.22263100    1.18039700   -4.83868200
 H                  3.51592800    2.54692500   -1.07318500
 H                  3.71507000    3.09358800   -3.70441200
```

Complex **14**

```
M06/BS1:
 E(RM06) =  -867.653982558
 Zero-point correction=                           0.327281 (Hartree/Particle)
 Thermal correction to Energy=                    0.347146
 Thermal correction to Enthalpy=                  0.348090
 Thermal correction to Gibbs Free Energy=         0.279389
 Sum of electronic and zero-point Energies=          -867.326702
```

```
 Sum of electronic and thermal Energies=             -867.306836
 Sum of electronic and thermal Enthalpies=           -867.305892
 Sum of electronic and thermal Free Energies=        -867.374594
E(RM06/BS2) =  -867.922469698

 C                  1.57925600    0.42975000    0.33257600
 C                  2.83663400    0.15515000   -0.31404500
 C                  3.56223900   -0.59482700    0.66475400
 C                  1.50950200   -0.20706800    1.58993900
 C                  2.75096900   -0.86617100    1.79774800
 H                  0.75203300    0.96408400   -0.13409400
 H                  1.37141000   -0.50419200   -3.79191600
 H                  4.55619200   -1.01630800    0.53331000
 H                  0.66423500   -0.20769500    2.27479000
 H                  3.03545700   -1.42467300    2.68675100
 Zr                 1.76497900   -1.95491500   -0.24500600
 C                  1.18249900   -4.24952100    0.62585900
 C                  0.22380900   -3.37037700    1.18424900
 C                 -0.56249900   -2.85347700    0.12689700
 C                  0.97000400   -4.29817300   -0.77770900
 C                 -0.10849200   -3.43708800   -1.08526900
 H                  1.94455200   -4.79653900    1.17418500
 H                  0.12988200   -3.11418900    2.23559600
 H                 -1.37237700   -2.13587700    0.22380900
 H                  1.55163400   -4.87797300   -1.48650600
 H                 -0.50606200   -3.23296200   -2.07456200
 C                  2.85827000   -2.63390000   -3.15194200
 C                  3.36110900   -2.38917400   -1.82575400
 C                  4.61881600   -1.72020500   -2.05417500
 C                  3.72552000   -2.08987500   -4.12125200
 C                  4.83898800   -1.54409400   -3.43549800
 H                  1.89732100   -3.08307800   -3.39192700
 H                  1.06710000   -0.97721300   -1.78208100
 H                  5.30096800   -1.36470200   -1.28621800
 H                  3.56277100   -2.08137000   -5.19578600
 H                  5.69912100   -1.06397800   -3.89654600
 Zr                 2.85079500   -0.13949800   -2.70375500
 C                  3.45035400    2.31557000   -2.35405100
 C                  4.40941300    1.75532300   -3.22287700
 C                  3.75110600    1.41842600   -4.44224300
 C                  2.19459100    2.28836000   -3.01013500
 C                  2.38784100    1.76542000   -4.31484700
 H                  3.63037000    2.65764600   -1.34142700
 H                  5.46531800    1.62016400   -3.00727900
 H                  4.21708200    0.97789100   -5.31923100
 H                  1.24972300    2.62921300   -2.59612000
 H                  1.62024000    1.62953700   -5.06700000
```

Complex **15**

```
M06/BS1:
 E(UM06) =  -867.614353679
 Zero-point correction=                           0.327668 (Hartree/Particle)
 Thermal correction to Energy=                    0.348670
 Thermal correction to Enthalpy=                  0.349614
 Thermal correction to Gibbs Free Energy=         0.276276
 Sum of electronic and zero-point Energies=           -867.286686
 Sum of electronic and thermal Energies=              -867.265684
 Sum of electronic and thermal Enthalpies=            -867.264740
 Sum of electronic and thermal Free Energies=         -867.338078
E(UM06/BS2) =  -867.887404604

 C                  1.25231500    0.23642300    0.13487100
 C                  2.55615300    0.12845400   -0.47495100
 C                  3.38969500   -0.39012700    0.56626500
 C                  1.30054700   -0.23704600    1.47353300
 C                  2.63354500   -0.63861600    1.73967200
```

H	0.35855000	0.62354200	-0.35527800
H	0.90916600	-0.09464600	-3.40516400
H	4.44286100	-0.64398400	0.45694200
H	0.46744000	-0.29479500	2.17099300
H	3.00521000	-1.04149900	2.67861200
Zr	1.78261800	-2.12423000	-0.12447600
C	1.40327800	-4.41143000	0.81065000
C	0.42018800	-3.58169400	1.40961000
C	-0.47302400	-3.14628700	0.39996800
C	1.10145600	-4.49548000	-0.57786400
C	-0.05502500	-3.71702200	-0.82708300
H	2.21491200	-4.91748200	1.32316900
H	0.37490000	-3.30572000	2.45956500
H	-1.32432600	-2.48653300	0.54028000
H	1.67209800	-5.04334400	-1.32082900
H	-0.53643600	-3.57520400	-1.79094900
C	2.59367000	-2.46961000	-3.26623100
C	3.16554200	-2.38054200	-1.95250400
C	4.48546400	-1.85129000	-2.18510200
C	3.50178300	-2.00810000	-4.25072200
C	4.69300500	-1.63738500	-3.57571100
H	1.57724800	-2.80386700	-3.48236900
H	0.78120100	-0.19318700	-2.63540800
H	5.23292800	-1.66720100	-1.41666400
H	3.32529100	-1.95285100	-5.32233100
H	5.60225800	-1.26746100	-4.04405600
Zr	2.99348000	-0.03076900	-2.76483400
C	3.62048500	2.38720600	-2.29298100
C	4.67596900	1.79987100	-3.02692900
C	4.18533700	1.48555000	-4.32671100
C	2.47037100	2.40200200	-3.11342400
C	2.81966100	1.85443100	-4.38478400
H	3.66520500	2.70905300	-1.25886100
H	5.68733800	1.63276400	-2.66744400
H	4.75774800	1.03639200	-5.13272600
H	1.49103500	2.77216600	-2.82188000
H	2.16903400	1.76947400	-5.24965200

Complex **14** to **15** MECP

E (M06/BS1) = -867.6134118

C	1.50242200	0.31527800	0.22763600
C	2.79967100	0.08729800	-0.37014800
C	3.55298500	-0.55357000	0.66720400
C	1.46938800	-0.21822500	1.54146700
C	2.74646200	-0.76968100	1.81307400
H	0.66329500	0.81067800	-0.26245500
H	0.96892600	-0.44077100	-3.29521000
H	4.57531100	-0.91519700	0.57750400
H	0.61839500	-0.21832700	2.21933200
H	3.05157900	-1.24881200	2.73997900
Zr	1.81148900	-2.07400200	-0.14354000
C	1.16533000	-4.32393400	0.73229400
C	0.20263200	-3.40755400	1.23458300
C	-0.55020300	-2.90583900	0.14327800
C	0.98877300	-4.39598400	-0.67744100
C	-0.06676100	-3.52561200	-1.03683300
H	1.87934100	-4.89115700	1.32017300
H	0.07779800	-3.12311300	2.27560100
H	-1.35783700	-2.18175600	0.20214900
H	1.58194100	-4.99520400	-1.36122800
H	-0.44014500	-3.35241500	-2.04309500
C	2.80542900	-2.53938400	-3.25491100
C	3.29070600	-2.41427300	-1.90477600
C	4.59864700	-1.82199600	-2.07471600
C	3.73422800	-2.01854900	-4.18560500

C	4.86236500	-1.57699500	-3.44884400
H	1.82371100	-2.92850600	-3.52849100
H	0.86135600	-0.56849500	-2.51672000
H	5.29278300	-1.58839200	-1.27204900
H	3.60995100	-1.95840000	-5.26458800
H	5.76734300	-1.14436300	-3.87123300
Zr	3.01695400	-0.10772700	-2.68768500
C	3.52447900	2.34980900	-2.33385800
C	4.48978300	1.84099700	-3.23250500
C	3.82424500	1.48324300	-4.43955400
C	2.25857800	2.27022200	-2.95959800
C	2.44596700	1.74788300	-4.27518300
H	3.71090700	2.68650700	-1.32054800
H	5.55556900	1.75170200	-3.04295200
H	4.29262300	1.06576700	-5.32639300
H	1.31356100	2.57677000	-2.51984200
H	1.67268900	1.59949900	-5.02306200

TS15-16

M06/BS1:
 E(UM06) = -867.609605715
 Zero-point correction= 0.326427 (Hartree/Particle)
 Thermal correction to Energy= 0.347094
 Thermal correction to Enthalpy= 0.348039
 Thermal correction to Gibbs Free Energy= 0.276549
 Sum of electronic and zero-point Energies= -867.283178
 Sum of electronic and thermal Energies= -867.262511
 Sum of electronic and thermal Enthalpies= -867.261567
 Sum of electronic and thermal Free Energies= -867.333057
E(UM06/BS2) = -867.880964945

C	1.68911800	0.32946800	0.30874400
C	2.97326300	0.07258600	-0.30381100
C	3.70700200	-0.62644400	0.71045400
C	1.64178200	-0.23843200	1.60789400
C	2.89860000	-0.84529700	1.85622000
H	0.86194000	0.86078600	-0.16491500
H	0.51076700	-0.47020500	-3.42613800
H	4.71548900	-1.01919100	0.60134900
H	0.79359000	-0.22799900	2.28911800
H	3.19097900	-1.35941900	2.76840800
Zr	1.91717900	-2.06234400	-0.12114100
C	1.06753700	-4.29220000	0.65735000
C	0.16654400	-3.32452400	1.17047400
C	-0.50599900	-2.71950700	0.07951300
C	0.93380600	-4.29539400	-0.75894700
C	-0.03834200	-3.33030400	-1.11238300
H	1.71942600	-4.93402700	1.24155500
H	0.03247100	-3.07233100	2.21868100
H	-1.25471800	-1.93511500	0.14618700
H	1.49841400	-4.91563400	-1.44777200
H	-0.36630200	-3.08885000	-2.12043600
C	2.85743000	-2.55821400	-3.19793300
C	3.38178100	-2.44576900	-1.85598100
C	4.68948000	-1.85716500	-2.05592400
C	3.76815500	-2.03710600	-4.14465300
C	4.91538700	-1.60163000	-3.43386000
H	1.87108200	-2.94788200	-3.45257500
H	0.59846200	-0.59886500	-2.67587100
H	5.40709700	-1.63516400	-1.27083500
H	3.61666700	-1.96384900	-5.21952700
H	5.80854100	-1.16376500	-3.87453900
Zr	3.07246300	-0.15540200	-2.60758600
C	3.25085600	2.37091800	-2.33796000
C	4.34762700	1.93763600	-3.12305200
C	3.83678300	1.44916600	-4.35717500

C	2.06626900	2.11785300	-3.06225400
C	2.42422600	1.54890200	-4.32042300
H	3.30885100	2.77121300	-1.33194600
H	5.39429400	1.98429400	-2.83695600
H	4.42722100	1.05568900	-5.17956200
H	1.05562400	2.32586600	-2.72053300
H	1.74183100	1.27507700	-5.12004900

Complex **16**

M06/BS1:

E(UM06) =	-867.615744954
Zero-point correction=	0.328526 (Hartree/Particle)
Thermal correction to Energy=	0.349678
Thermal correction to Enthalpy=	0.350622
Thermal correction to Gibbs Free Energy=	0.278817
Sum of electronic and zero-point Energies=	-867.287219
Sum of electronic and thermal Energies=	-867.266067
Sum of electronic and thermal Enthalpies=	-867.265123
Sum of electronic and thermal Free Energies=	-867.336928

E(UM06/BS2) = -867.885705465

C	2.09293200	0.42809600	0.42512600
C	3.36851100	0.03394400	-0.13894100
C	3.92116300	-0.84762300	0.86172100
C	1.88145900	-0.20591700	1.67377800
C	3.01715600	-1.00846100	1.94403400
H	1.37731200	1.09572100	-0.05503300
H	-0.58292800	-0.41585900	-3.65047600
H	4.87803900	-1.35872400	0.78841500
H	1.00000900	-0.11716900	2.30506900
H	3.17046500	-1.61683900	2.83246900
Zr	2.00976300	-1.94109900	-0.16574600
C	0.91098200	-4.10457600	0.50188700
C	0.06070700	-3.05988000	0.94859100
C	-0.45315200	-2.39118200	-0.19171200
C	0.90133100	-4.09658600	-0.91776300
C	0.05983800	-3.04548700	-1.34589500
H	1.46257800	-4.79565100	1.13257500
H	-0.14191900	-2.80229900	1.98423300
H	-1.13462900	-1.54467500	-0.18481300
H	1.46986000	-4.76038900	-1.56062800
H	-0.15564000	-2.77806600	-2.37645800
C	3.04838200	-2.45181200	-3.17509400
C	3.52325800	-2.48649600	-1.80686200
C	4.90157300	-2.07770000	-1.92022100
C	4.07307900	-2.01587200	-4.05097100
C	5.22843800	-1.77278700	-3.26851300
H	2.03219500	-2.69202700	-3.48924500
H	-0.44979700	-0.52792200	-2.92250700
H	5.59471900	-1.96853900	-1.08971800
H	3.98805900	-1.86971900	-5.12557400
H	6.19192600	-1.43511200	-3.64345900
Zr	3.48512900	-0.17198100	-2.41922500
C	2.91356700	2.29643600	-2.34303500
C	3.99860500	2.15712300	-3.24853900
C	3.53975400	1.41645500	-4.36682400
C	1.79159900	1.63701600	-2.89484600
C	2.18075600	1.07787100	-4.14321500
H	2.95144300	2.79618600	-1.38076600
H	4.99914800	2.55716100	-3.11194800
H	4.13274000	1.13538700	-5.23260800
H	0.80962800	1.55131900	-2.43815300
H	1.54713600	0.50265500	-4.81290000

Complex **17** triplet

```
M06/BS1:
 E(UM06) =  -866.445038115
 Zero-point correction=                           0.311259 (Hartree/Particle)
 Thermal correction to Energy=                    0.330952
 Thermal correction to Enthalpy=                  0.331896
 Thermal correction to Gibbs Free Energy=         0.262392
 Sum of electronic and zero-point Energies=           -866.133780
 Sum of electronic and thermal Energies=              -866.114086
 Sum of electronic and thermal Enthalpies=            -866.113142
 Sum of electronic and thermal Free Energies=         -866.182646
E(UM06/BS2) =  -866.711214397

 C                  2.08665700    0.41494200    0.41206900
 C                  3.37453600    0.04358800   -0.13931900
 C                  3.93436300   -0.81969200    0.87402900
 C                  1.87680500   -0.21270300    1.66494300
 C                  3.02571600   -0.98965500    1.95105900
 H                  1.35870400    1.06115400   -0.07844700
 H                  4.90138000   -1.31284900    0.81406100
 H                  0.98796100   -0.13674300    2.28754900
 H                  3.18464900   -1.58732500    2.84568200
 Zr                 2.05153600   -1.95343100   -0.16281200
 C                  0.85388900   -4.11093500    0.35218200
 C                  0.04844700   -3.06208000    0.86481800
 C                 -0.42538600   -2.29477100   -0.23048300
 C                  0.85886100   -4.00336100   -1.06391400
 C                  0.06653800   -2.88971200   -1.42423500
 H                  1.36858900   -4.86850700    0.93586800
 H                 -0.15284300   -2.86614800    1.91425000
 H                 -1.06766100   -1.42077700   -0.16924200
 H                  1.40270500   -4.64852000   -1.74588900
 H                 -0.12486700   -2.53921300   -2.43476100
 C                  3.14855200   -2.49089700   -3.15362100
 C                  3.59577800   -2.50265000   -1.77535800
 C                  4.96970500   -2.07076400   -1.86735700
 C                  4.18354300   -2.04819600   -4.01425900
 C                  5.31872400   -1.77748700   -3.21216900
 H                  2.14383200   -2.75331300   -3.48537600
 H                  5.64588800   -1.94257700   -1.02588500
 H                  4.11776000   -1.91579800   -5.09199300
 H                  6.28421700   -1.42879600   -3.57162800
 Zr                 3.52617800   -0.19725300   -2.41911300
 C                  2.80061800    2.23243400   -2.39794200
 C                  3.92738900    2.14848900   -3.25809000
 C                  3.55910500    1.36798700   -4.38269600
 C                  1.74162000    1.50244100   -2.98549100
 C                  2.21325700    0.95311200   -4.20878900
 H                  2.77142200    2.74740900   -1.44347300
 H                  4.89608700    2.60930200   -3.08737100
 H                  4.20053200    1.11350400   -5.22174100
 H                  0.74619200    1.36938700   -2.57072400
 H                  1.63934800    0.34016100   -4.89795300
```

Complex **17** singlet

```
M06/BS1:
 E(RM06) =  -866.454293517
 Zero-point correction=                           0.312266 (Hartree/Particle)
 Thermal correction to Energy=                    0.331634
 Thermal correction to Enthalpy=                  0.332578
 Thermal correction to Gibbs Free Energy=         0.265886
 Sum of electronic and zero-point Energies=           -866.142027
 Sum of electronic and thermal Energies=              -866.122660
 Sum of electronic and thermal Enthalpies=            -866.121715
```

```
 Sum of electronic and thermal Free Energies=         -866.188407
E(RM06/BS2) =  -866.719370290

 C                  2.27666800    0.39010700    0.59452000
 C                  3.53846600    0.03286100   -0.00741300
 C                  4.10191800   -0.88358500    0.95068100
 C                  2.07549100   -0.29574100    1.81258300
 C                  3.20803600   -1.11222100    2.03834100
 H                  1.53700500    1.05159800    0.14533400
 H                  5.06239300   -1.38381100    0.85324400
 H                  1.19220900   -0.24009800    2.44557500
 H                  3.38338700   -1.73851500    2.90915400
 Zr                 2.23669500   -1.97189300   -0.12562200
 C                  0.52783900   -3.84105800    0.03718700
 C                 -0.09266500   -2.69294100    0.57597900
 C                 -0.23093500   -1.74144300   -0.46463400
 C                  0.76721600   -3.60833700   -1.34165000
 C                  0.28878400   -2.30757500   -1.66091100
 H                  0.79000900   -4.74039000    0.58803500
 H                 -0.38325200   -2.55207600    1.61297900
 H                 -0.67501800   -0.75480700   -0.36218500
 H                  1.23081400   -4.30823100   -2.02924500
 H                  0.27572600   -1.85353200   -2.64547400
 C                  3.41850900   -2.58994200   -3.11467900
 C                  3.80452800   -2.57941300   -1.72423600
 C                  5.14880900   -2.06368400   -1.76885700
 C                  4.44382100   -2.07323000   -3.93654400
 C                  5.52961400   -1.72223700   -3.10030500
 H                  2.43898100   -2.89025600   -3.48544100
 H                  5.78825800   -1.89820300   -0.90516800
 H                  4.39632000   -1.93251100   -5.01440100
 H                  6.48877500   -1.32974800   -3.42819700
 Zr                 3.63366000   -0.26730300   -2.30388200
 C                  2.42956700    1.94418500   -2.35999400
 C                  3.43104800    2.03606100   -3.35969400
 C                  3.12496900    1.10552500   -4.37686800
 C                  1.49331500    0.95260900   -2.76065500
 C                  1.93715500    0.42799600   -4.00568900
 H                  2.38995800    2.53533300   -1.45101300
 H                  4.29462700    2.69544400   -3.33908300
 H                  3.71422100    0.91887900   -5.26991300
 H                  0.57966800    0.68894700   -2.23903200
 H                  1.44373900   -0.34700600   -4.58644700
```

Complex **17** triplet to singlet MECP

```
E (M06/BS1) = -866.4447288

 C                  2.11616200    0.42208800    0.43010400
 C                  3.40116600    0.04528100   -0.11730700
 C                  3.94712800   -0.83162200    0.88836700
 C                  1.88828300   -0.22141000    1.66986400
 C                  3.02688700   -1.01617900    1.95534100
 H                  1.39594800    1.07481600   -0.06259900
 H                  4.90570900   -1.34116700    0.82337300
 H                  0.99231200   -0.14763000    2.28259500
 H                  3.17231200   -1.62566400    2.84403900
 Zr                 2.07085400   -1.95350600   -0.16656000
 C                  0.83416900   -4.09064100    0.33228000
 C                  0.03880400   -3.03636000    0.84598400
 C                 -0.41642300   -2.25618400   -0.24698500
 C                  0.85380300   -3.97286400   -1.08282300
 C                  0.07666200   -2.84611200   -1.44236900
 H                  1.33943600   -4.85462900    0.91619300
 H                 -0.16010900   -2.84093400    1.89581600
 H                 -1.04413000   -1.37178300   -0.18261700
 H                  1.39089200   -4.62426200   -1.76406200
```

H	-0.10878300	-2.48975900	-2.45140400
C	3.17710900	-2.51018600	-3.14304900
C	3.62825300	-2.51374100	-1.76870200
C	4.99332000	-2.06221600	-1.86517600
C	4.19695600	-2.04568800	-4.00705800
C	5.33241400	-1.75299800	-3.21058400
H	2.17281300	-2.78141800	-3.46816600
H	5.66668300	-1.91266100	-1.02459600
H	4.12009200	-1.90997400	-5.08383500
H	6.29005900	-1.38945900	-3.57561600
Zr	3.53378400	-0.20131200	-2.40348000
C	2.76827600	2.20954000	-2.39667300
C	3.88932100	2.14225100	-3.26536900
C	3.52822600	1.35081500	-4.38280100
C	1.71648000	1.45851300	-2.97432700
C	2.19155200	0.91390000	-4.19829500
H	2.73652400	2.73366400	-1.44733300
H	4.85427000	2.61340200	-3.09989300
H	4.17241400	1.09608400	-5.21980100
H	0.72459300	1.31474600	-2.55597300
H	1.62610800	0.28501700	-4.88012500