Supporting Information

Construction of Oxygen-bridged Multimetallic Assembly: Dual Catalysts for Hydroamination Reactions

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^{1}H NMR of [Cp*$_2$(Me)Zr(μ-O)Zr(NMe$_2$)$_2$(μ-O)Zr(Me)Cp*$_2$] (2).

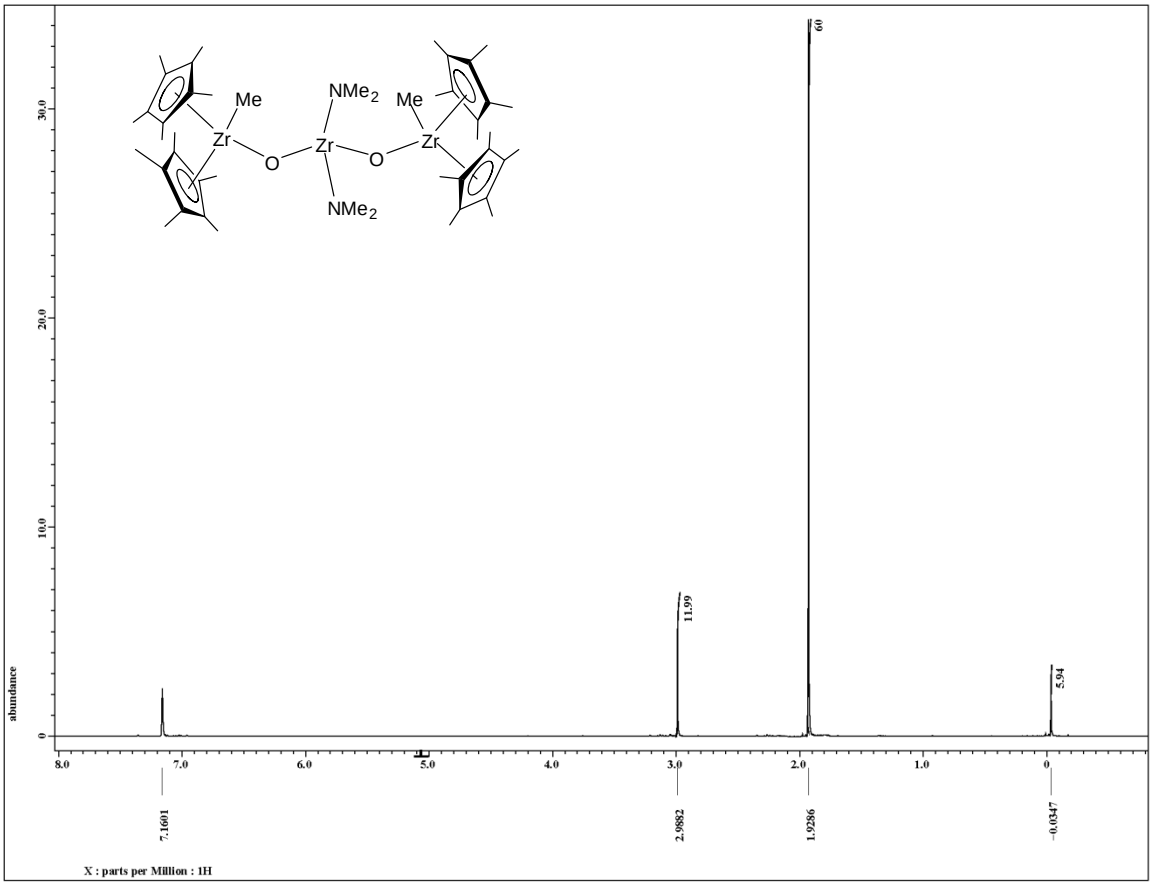


Fig. S1 ^{1}H NMR spectrum of complex **2** in C_6D_6.

^{13}C NMR of [Cp*$_2$(Me)Zr(μ-O)Zr(NMe$_2$)$_2$(μ-O)Zr(Me)Cp*$_2$] (2).

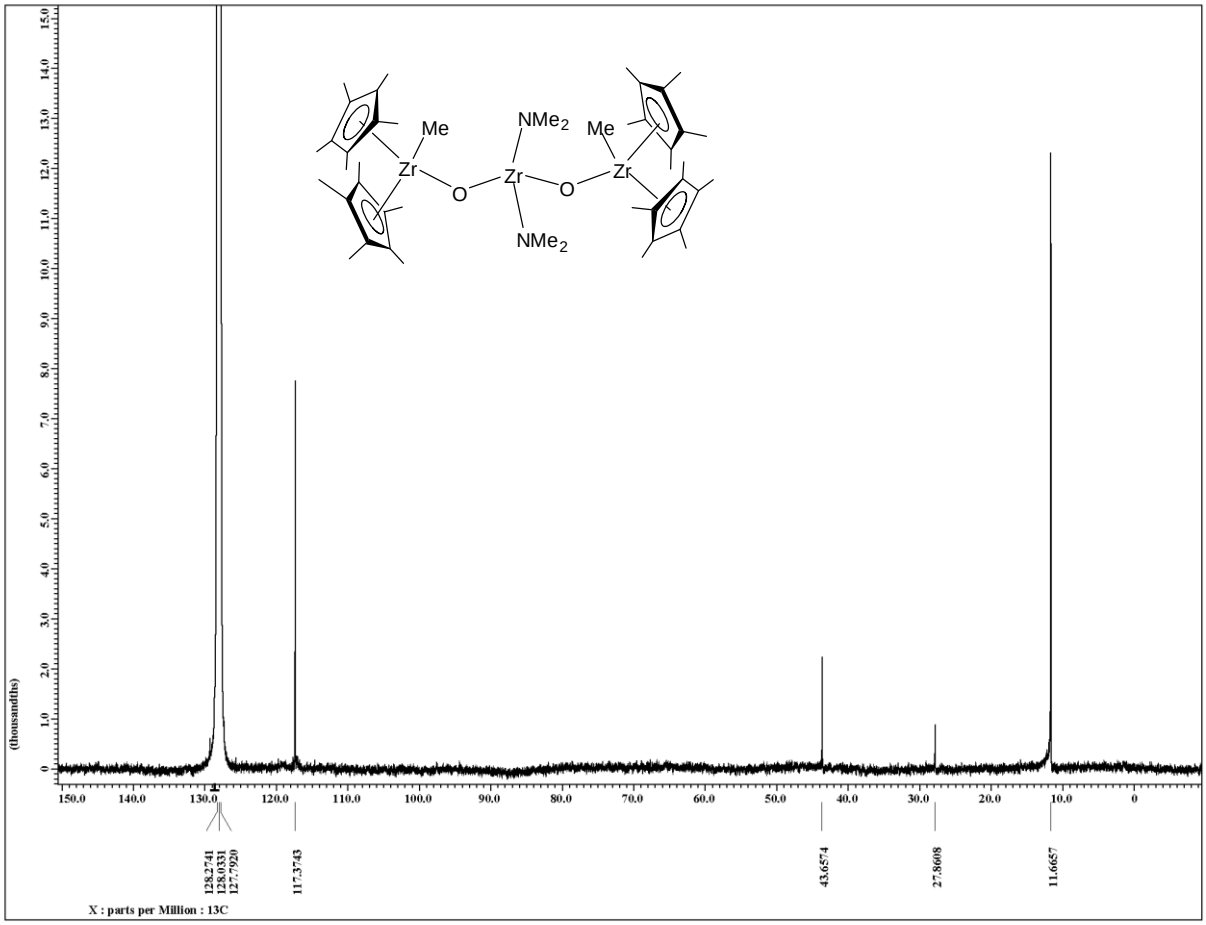


Fig. S2 ^{13}C NMR spectrum of complex **2** in C_6D_6.

^{1}H NMR of [PhNMe$_2$H][B(C$_6$F$_5$)$_4$].

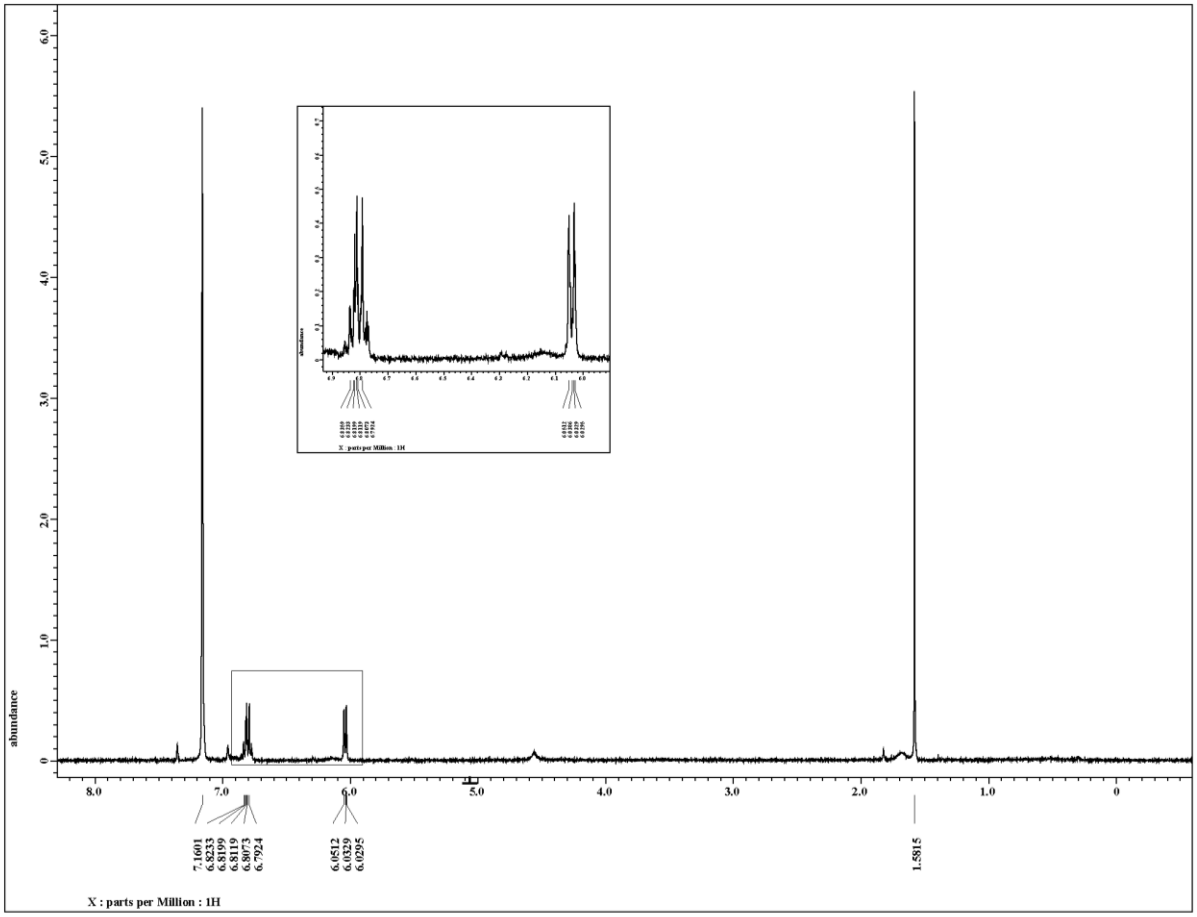


Fig. S3 ^{1}H NMR spectrum of [PhNMe$_2$H][B(C$_6$F$_5$)$_4$] in C$_6$D$_6$.

^{1}H NMR of [Cp*$_2$(Me)Zr(μ-O)Zr(NMe$_2$)$_2$(μ-O)Zr(Me)Cp*$_2$] (2) + 1 equivalent of [PhNMe$_2$H][B(C$_6$F$_5$)$_4$].

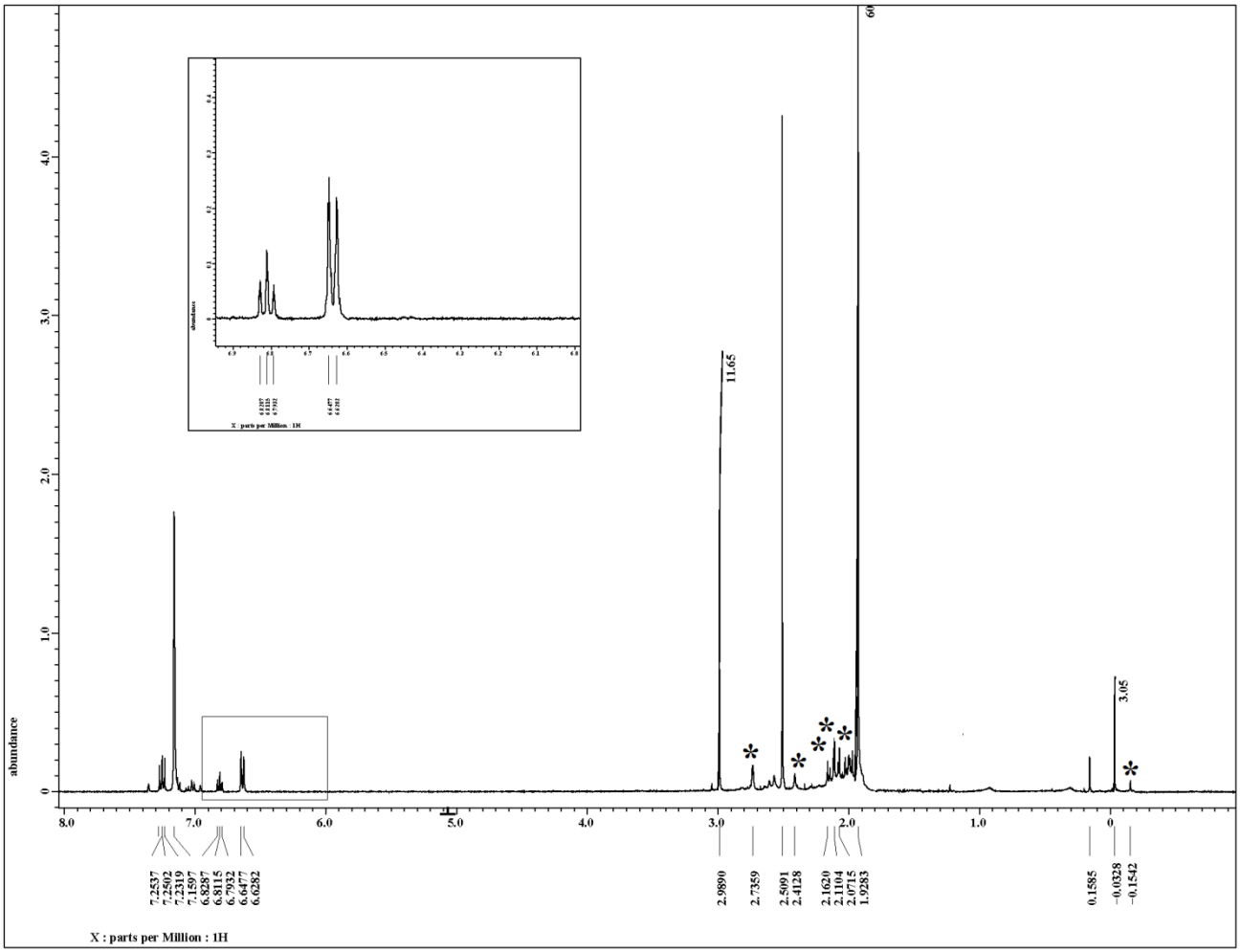


Fig. S4 ^{1}H NMR spectrum of complex **2** and one equivalent of the activator [PhNMe$_2$H] [B(C$_6$F$_5$)$_4$] in C$_6$D$_6$. * are the unidentified products of the reaction mixture.

^{1}H NMR of [Cp*$_2$(Me)Zr(μ-O)Zr(NMe$_2$)$_2$(μ-O)Zr(Me)Cp*$_2$] (2) + 2 equivalent of [PhNMe$_2$H][B(C$_6$F$_5$)$_4$].

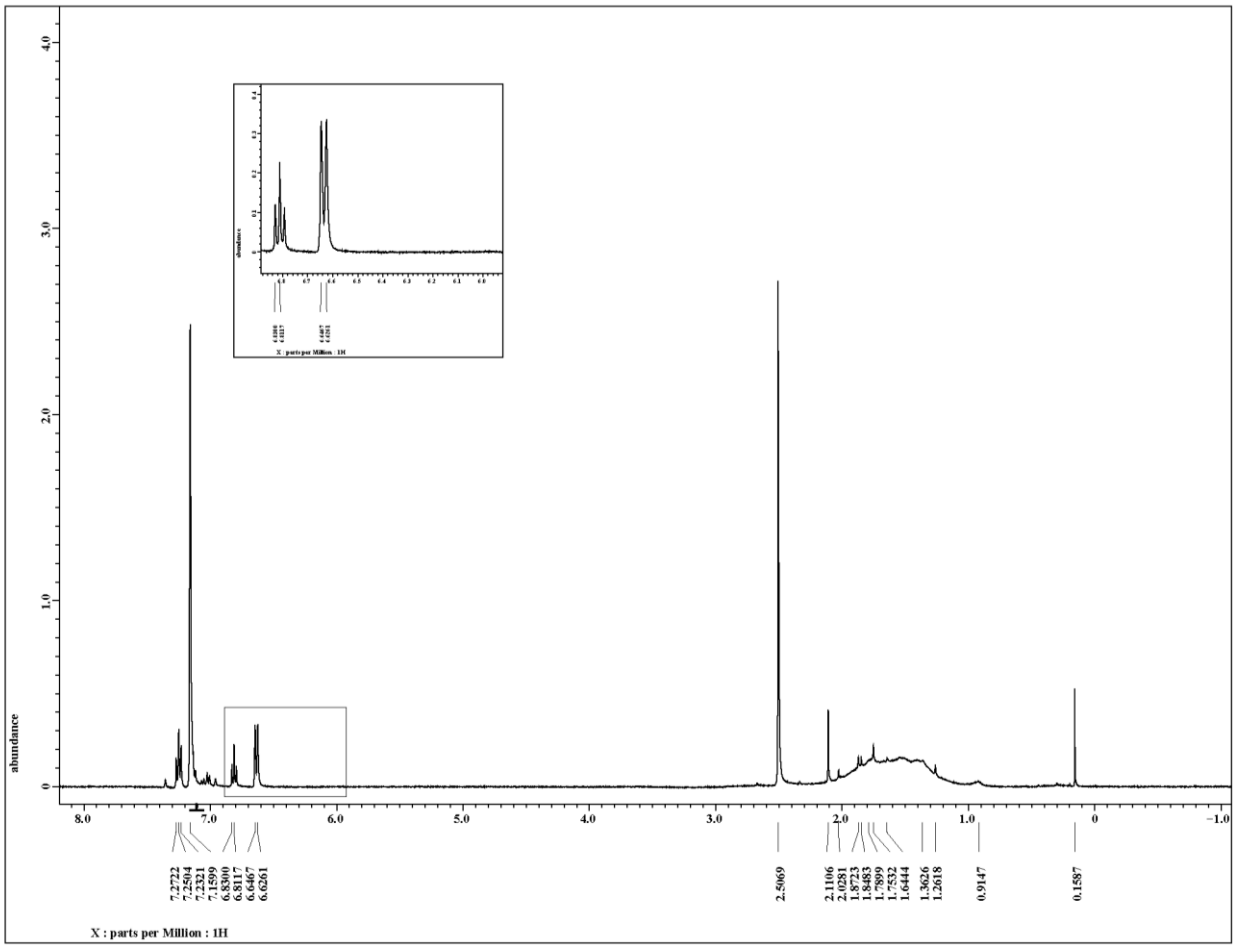
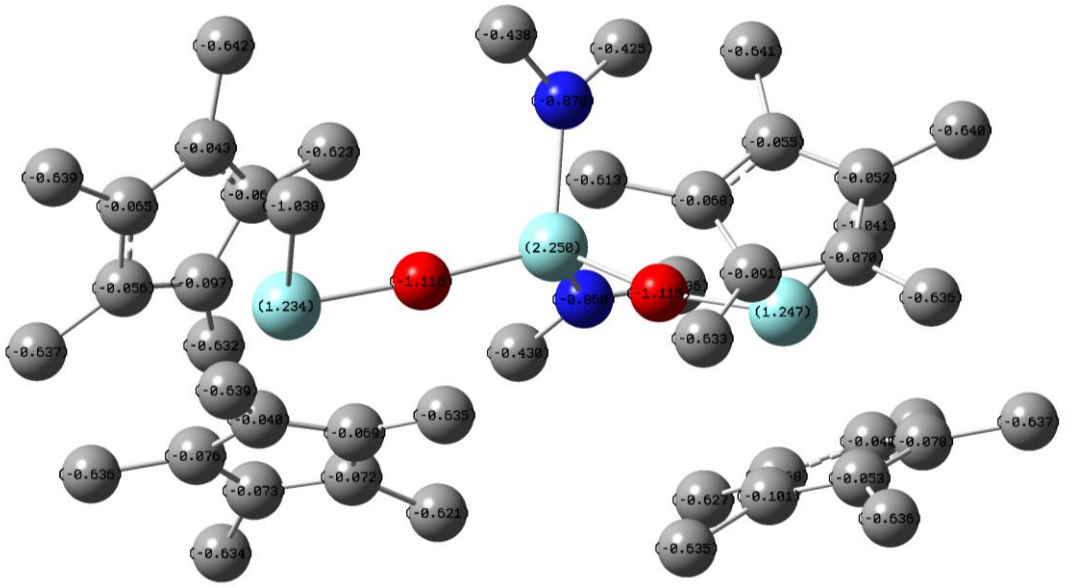


Fig. S5 ^{1}H NMR spectrum of complex **2** and two equivalent of the activator [PhNMe$_2$H][B(C$_6$F$_5$)$_4$] in C$_6$D$_6$.

Computational results.

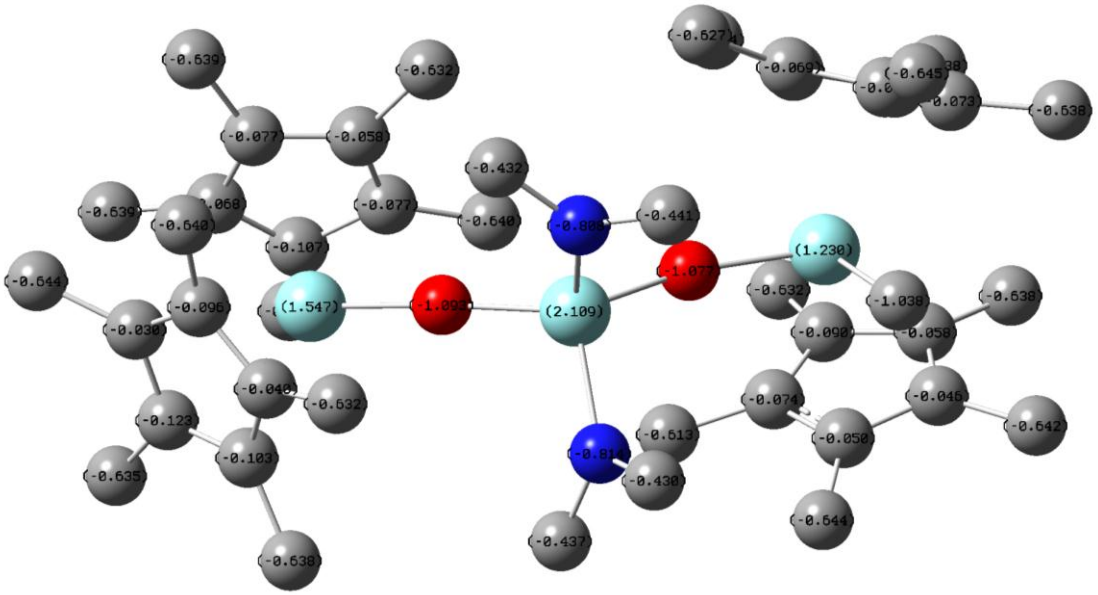
NBO analysis of the optimized structures showing corresponding charges on the different atoms.

(a)



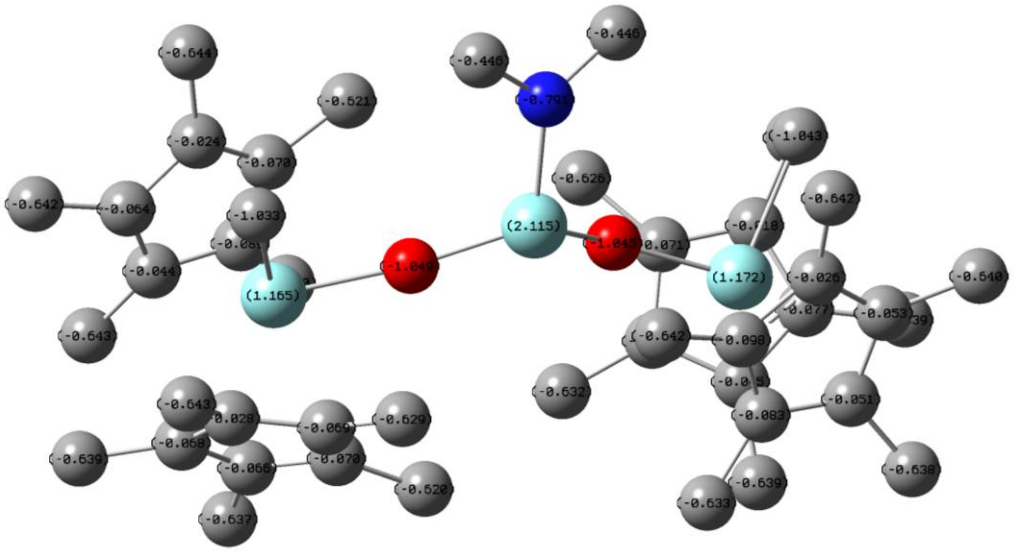
(**2**)

(b)



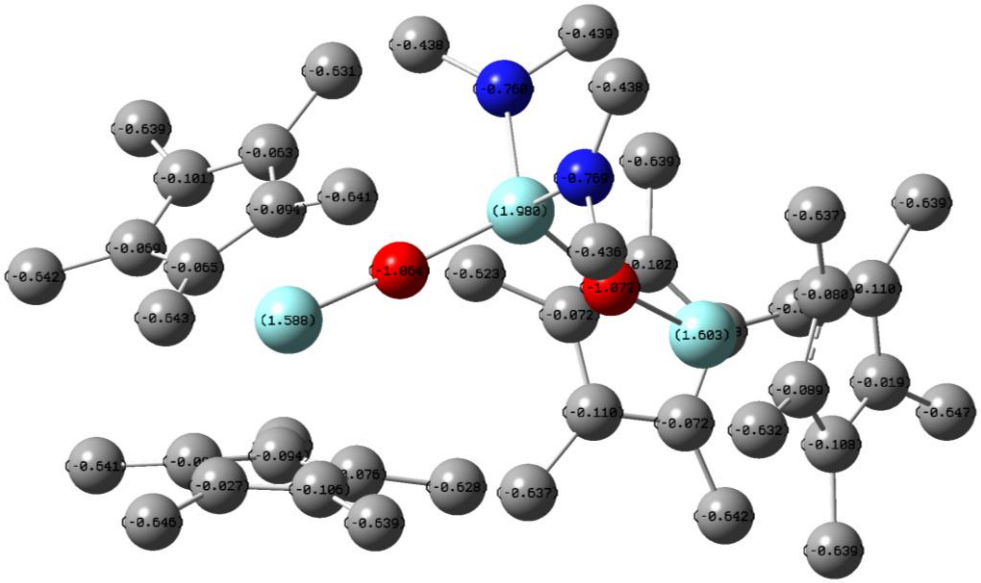
(**2a**)

(c)



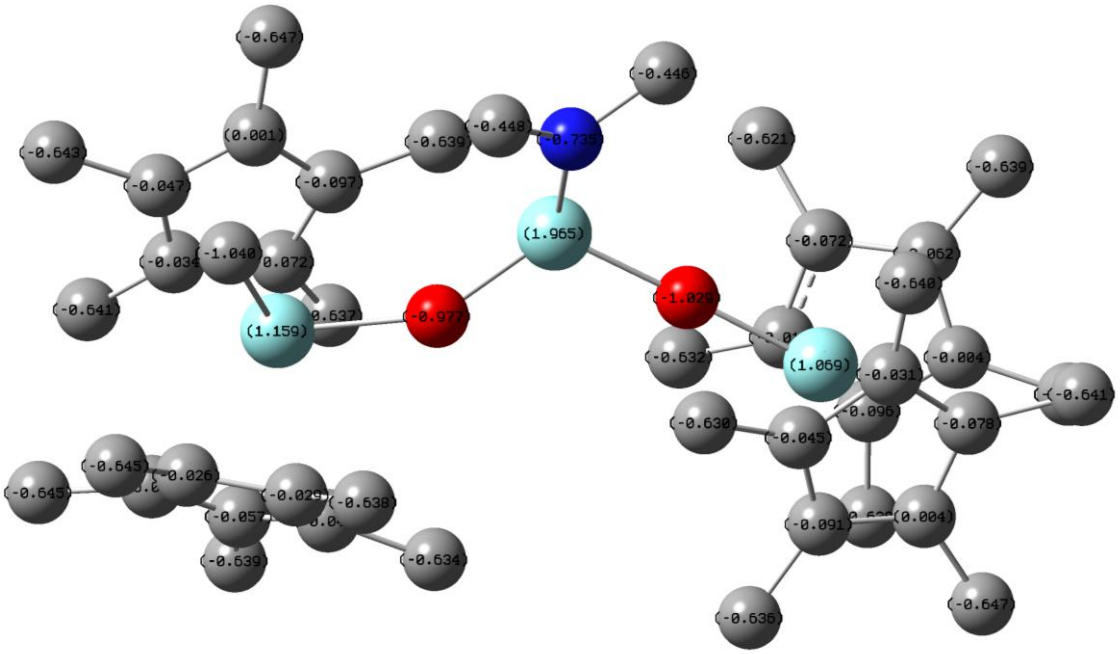
(**2b**)

(d)



(**2c**)

(e)



(**2d**)

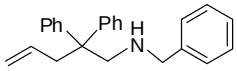
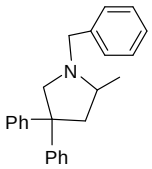
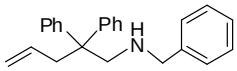
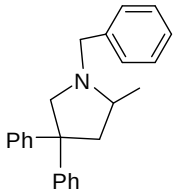
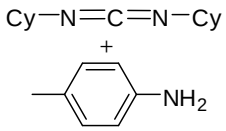
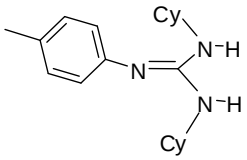
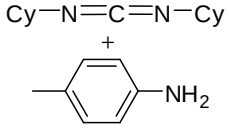
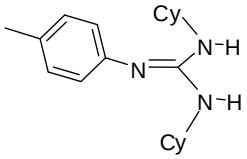
Fig. S6 Electronic charge on the different atoms of the optimized structure: (a) complex **2**; (b) cation at one of the terminal zirconium center (**2a**); (c) cation at the terminal zirconium center (**2b**); (d) cations at both the terminal zirconium centers (**2c**); (e) cations at one of the terminal zirconium center and one of the central zirconium center (**2d**). Counterions and hydrogens are not shown for the sake of clarity.

Control Experiments:

We carried out a set of control experiments to see the cooperative effect. We utilized following compounds to carry out these control experiments: $Cp^*_2Zr(Me)OH$, $Zr(NMe_2)_4$. We have particularly chosen $Cp^*_2Zr(Me)OH$ and $Zr(NMe_2)_4$ for our control experiments since they are assembled in the trimetallic zirconium catalyst $[Cp^*_2(Me)Zr(\mu\text{-}O)Zr(NMe_2)_2(\mu\text{-}O)Zr(Me)Cp^*_2]$ (**2**) . The catalytic results of control experiment indicates that $[Cp^*_2(Me)Zr(\mu\text{-}O)Zr(NMe_2)_2(\mu\text{-}O)Zr(Me)Cp^*_2]$ (**2**) is comparatively less active catalyst for hydroamination of secondary aminoalkene substrate than $Cp^*_2Zr(Me)OH$ under identical reaction condition (see entries 1 and

2, Table S1). Similarly, [Cp*$_2$(Me)Zr(μ-O)Zr(NMe$_2$)$_2$(μ-O)Zr(Me)Cp*$_2$] (2) also shows less activity than the Zr(NMe$_2$)$_4$ for intermolecular hydroamination reaction under identical reaction condition (see entries 3 and 4, Table S1).

Table S1. Control experiments carried out for the hydroamination catalysis reaction.[a]

Entry	Cat. (mol%)	Sub.	Product	Temp (°C)	Time	Conv. (%)
1	Cp*$_2$Zr(Me)OH (10)			110 °C	10 h	65[b]
2	[Cp*$_2$(Me)Zr(μ-O)Zr(NMe$_2$)$_2$(μ-O)Zr(Me)Cp*$_2$] **(2)**(10)			110 °C	10 h	35[b]
3	Zr(NMe$_2$)$_4$(10)			110°C	8 h	99
4	[Cp*$_2$(Me)Zr(μ-O)Zr(NMe$_2$)$_2$(μ-O)Zr(Me)Cp*$_2$] (**2**) (10)			110 °C	12 h	91

[a]The solvent used was C_6D_6 and the conversion was reported based on ^{1}H NMR spectroscopy of the reaction medium. [b] In this case 10 mol% of the activator [PhNMe$_2$H][B(C$_6$F$_5$)$_4$] was used into the catalyst solution.

Kinetic Study for the Hydroamination of Carbodiimides (4) and *p*-toluidine (5) Using Catalyst 2:

We carried out detailed kinetic studies of the hydroamination process of carbodiimides catalyzed by **2** using the *N*,*N*'-dicyclohexylcarbodiimide (**4**) and *p*-toluidine (**5**) in C_6D_6. Kinetic studies for the formation of *N*,*N*',*N*''-trisubstituted guanidine (**6**) were carried out with catalyst **2** and equi-molar amounts of **4** and **5** *via* ^{1}H NMR spectroscopy. The evolution of the specific

resonances of **6** was monitored by ^{1}H NMR spectroscopy relative to an internal standard (hexamethyl benzene) over the course of the first 7 h. Previous study by Marks and co-workers has shown that the rate equation of the lanthanide-catalyzed intermolecular hydroamination of alkyne and amine derivatives can be summarized as shown in eq 1. [S1]

$$\text{rate} = k[\text{amine}]^{0}[\text{alkyne}]^{1}[\text{catalyst}]^{1} \quad (1)$$

In the present case, we first determined the order of the reaction with respect to amine concentration by keeping the concentration of other components virtually unaltered. Initially, we began our study with 8.12 mM catalyst (**2**) concentration, and the carbodiimide to amine molar ratio was maintained at more than 10:1. The excess carbodiimide concentration maintains approximately zero-order condition. The amine to catalyst ratio was maintained at 10:1 during this study. In this experiment we observed that a plot of $\ln(C/C_0)$ versus time provides a linear plot with negative slope. This confirms the first order rate dependence of the reaction with respect to amine concentration (Fig. 7a).[S2]

Next, we determined the order of the reaction with respect to the concentration of carbodiimide. During this study we maintained the relative carbodiimide to amine ratio over 1:10. The catalyst: carbodiimide ratio was maintained to 1:10. This study provided evidence of a first-order dependence of the reaction rate on carbodiimide concentration as well. Fig. 7b reveals that with increasing concentration of carbodiimide the rate of reaction increases in a linear fashion.

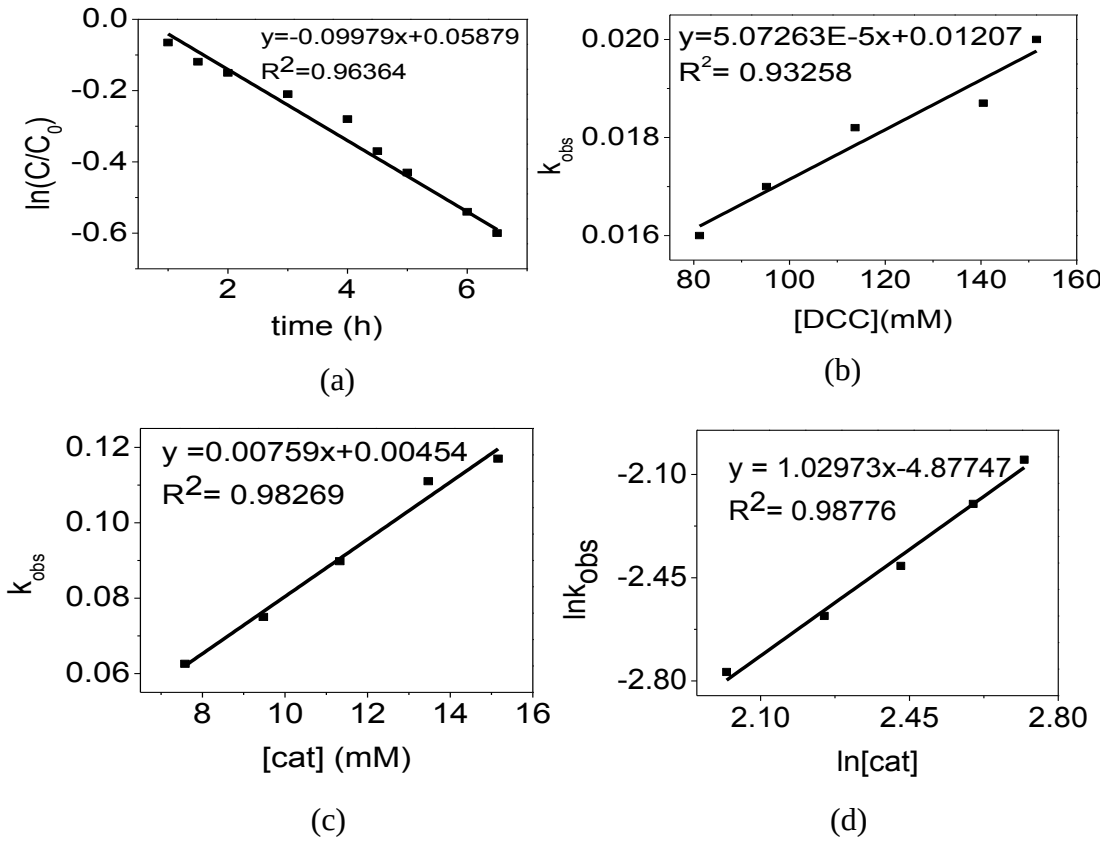


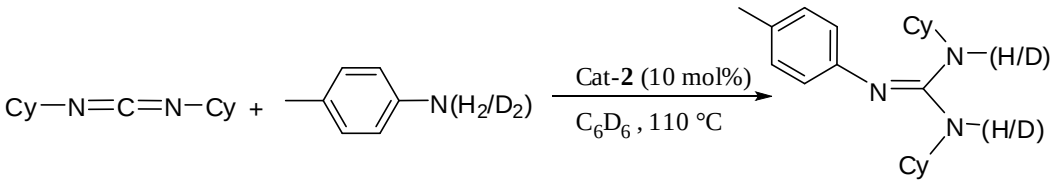
Fig. 7 Kinetic studies on the hydroamination of the carbodiimide for the formation of the guanidine (**6**) monitored by ^{1}H NMR spectroscopy in C_6D_6 at 110 °C: (a) plot of ln(C/C_0) versus time; (b) plot of k_{obs} and carbodiimide concentration for the formation of **6**, (c) plot of reaction rate versus concentration of the catalyst and (d) van't Hoff plot for the formation of **6**.

The similar observation was also noted by Marks and co-workers as well as by Hill and co-workers previously in the case of intermolecular hydroamination reaction.[S1,S2] The dependence of the rate of reaction with respect to catalyst concentration was studied by gradually changing the concentration of catalyst (from 7.6 mM to 15.4 mM) and holding the amine (151.6 mM) and carbodiimide (151.6 mM) concentrations fixed. A plot of reaction rate versus catalyst concentration reveals a linear increase of the reaction rate with catalyst concentration (Fig. 7c). This first order rate of the reaction with respect to the catalyst concentration was further confirmed from van't Hoff plot.[S3] A plot of lnk_{obs} versus ln[catalyst] provided a linear graph (Fig. 7d) and the value of the slope was determined to be 1.03 (slope = order of the reaction).[S3]

Thus, from the present study the overall rate law for the intermolecular hydroamination reaction of carbodiimides and amine catalyzed by **2** can be summarized as shown in eq 2.

$$\text{rate} = k[\text{amine}]^1[\text{carbodiimide}]^1[\text{catalyst}]^1 \qquad (2)$$

Kinetic Isotope Effect. We studied kinetic isotope effect by deuterium substitution of the NH_2 group present in *p*-toluidine to understand the role of NH_2 group in the catalytic process.



4 **5**/**5**-d_2 **6**/**6**-d_2

Scheme S1 Catalytic reaction of dicyclohexyl carbodiimide (**4**) and *p*-toluidine (**5**) and *p*-toluidine-d_2 (**5-*d*$_2$**) with **2** as catalyst at 110 °C keeping the concentration of carbodiimide as 151.56 mM, concentration of the amine as 151.56 mM and the concentration of catalyst as 15.2 mM.

Determination of the kinetic isotope effect (KIE) has proven to be a very useful mechanistic tool, which has already been applied in many organometallic systems.[S4] We carried out the H/D kinetic isotope effect (KIE) experiment using **5** and **5-*d*$_2$** using catalyst **2** in C_6D_6 (Scheme S1) under the identical reaction condition. The first order plots of the reaction of **5** and **5-*d*$_2$** under the reaction condition indicate k_{obs} = 0.117 h^{-1} and k_{obs} = 0.058 h^{-1}, respectively, which translates into a primary KIE of 2.02 (Fig. 8). These observations suggest that H/D derived from the -NH_2/-ND_2 moiety of **5**/**5-*d*$_2$** is involved in one of the key steps of the hydroamination of carbodiimides.

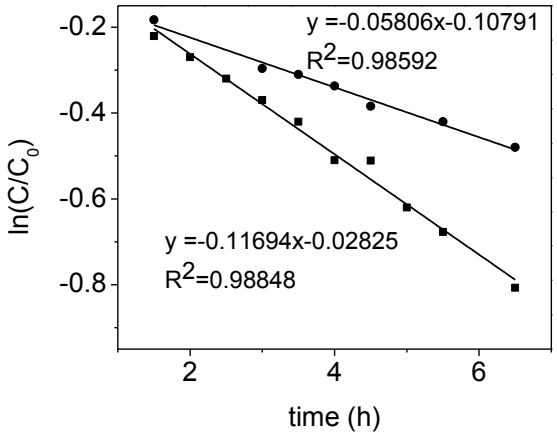


Fig. 8 H/D KIE for the formation of **6** and **6**-d_2 using catalyst **2** at 110 °C

X-ray Crystallographic Details of 2:

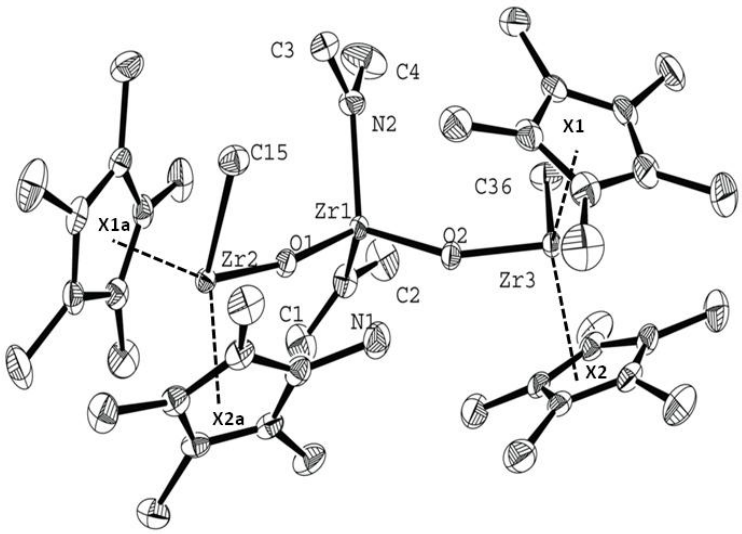


Fig. S9. Molecular structure of complex **2**. Thermal ellipsoids are drawn with 50% probability level. Hydrogen atoms have been omitted for clarity. x = centroid of Cp* ring.

Table S2. Crystal data and structure refinement for **2**

Empirical formula	$C_{46}\ H_{78}\ N_2\ O_2\ Zr_3$
Formula weight	967.79
Temperature	100(2) K
Wavelength	0.71073 Å

Crystal system, space group	monoclinic, $P2_1/n$
Unit cell dimensions	a = 14.8729(16) Å
	b = 18.838(2) Å
	c = 17.819(2) Å
	α = 90.00°
	β = 111.125(2)°
	γ = 90.00°
Volume	4657.1(9) $Å^3$
Z, Calculated density	4, 1.380 g/mm^3
Absorption coefficient	0.696 mm^{-1}
F(000)	2028
Crystal size	0.20 ×0.13 × 0.10 mm^3
Theta range for data collection	2.45-27.85 °
Limiting indices	-18<=h<=18, -24<=k<=22, -22<=l<=22
Reflections collected / unique	79448 / 10155
Refinement method	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.087
Final R indices [I>2σ(I)]	$R1$ = 0.0238, $wR2$ = 0.0617
R indices (all data)	$R1$ = 0.0309, $wR2$ = 0.0664
Largest diff. peak and hole	0.483 and -0.930 e. $Å^{-3}$

Table S3 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for **2**:

Atom	x	y	z	U(eq) [Ang^2]
Zr1	0.02669(1)	0.88933(1)	0.76696(1)	0.0158(1)
Zr2	-0.09889(1)	0.73339(1)	0.83741(1)	0.0152(1)
Zr3	0.28596(1)	0.88854(1)	0.77133(1)	0.0167(1)
O1	-0.03907(9)	0.80894(7)	0.79211(8)	0.0197(4)
O2	0.15653(9)	0.86319(7)	0.76926(8)	0.0197(4)
N1	-0.05582(12)	0.92805(10)	0.65541(10)	0.0264(5)
N2	0.03874(13)	0.96891(10)	0.84949(11)	0.0297(6)
C1	-0.13901(18)	0.89410(14)	0.59718(15)	0.0408(8)
C2	-0.0336(2)	0.99372(14)	0.62348(16)	0.0443(8)
C3	0.04565(19)	0.95226(16)	0.93056(15)	0.0462(9)
C4	0.0309(2)	1.04497(14)	0.83625(19)	0.0593(10)
C5	-0.20323(14)	0.81087(12)	0.89532(13)	0.0258(6)
C6	-0.22483(14)	0.83276(10)	0.81529(13)	0.0237(6)
C7	-0.21146(17)	0.90610(12)	0.78912(17)	0.0373(8)
C8	-0.27046(14)	0.77562(11)	0.76383(12)	0.0232(6)
C9	-0.27985(14)	0.71894(11)	0.81348(13)	0.0248(6)
C10	-0.34489(17)	0.65579(13)	0.78464(18)	0.0421(8)
C11	-0.23608(15)	0.74006(12)	0.89395(13)	0.0263(6)
C12	-0.2368(2)	0.69843(16)	0.96574(16)	0.0472(9)
C13	-0.31349(17)	0.77991(15)	0.67343(14)	0.0385(8)
C14	-0.16791(18)	0.85639(15)	0.96931(16)	0.0443(9)
C15	0.00110(15)	0.75064(11)	0.96802(12)	0.0259(6)
C16	-0.12341(15)	0.61939(10)	0.75197(12)	0.0224(6)
C17	-0.04318(15)	0.65590(10)	0.74578(12)	0.0226(6)
C18	0.03243(14)	0.65347(10)	0.82185(12)	0.0222(6)
C19	-0.00181(15)	0.61618(10)	0.87543(12)	0.0224(6)

Table S4 - Hydrogen Atom Positions and Isotropic Displacement Parameters for **2**:

Atom	x	y	z	U(iso) [Ang^2]
H1C	-0.19410	0.92460	0.58550	0.0610
H1D	-0.15130	0.85000	0.61870	0.0610
H1E	-0.12680	0.88520	0.54870	0.0610
H2C	-0.02400	0.98430	0.57400	0.0660
H2D	0.02410	1.01400	0.66160	0.0660
H2E	-0.08610	1.02640	0.61370	0.0660
H3A	0.10350	0.97270	0.96820	0.0690
H3B	0.04740	0.90170	0.93750	0.0690
H3C	-0.00930	0.97130	0.93990	0.0690
H4A	-0.02230	1.06290	0.84900	0.0890
H4B	0.02040	1.05490	0.78090	0.0890
H4C	0.08930	1.06750	0.87010	0.0890
H7A	-0.26690	0.93440	0.78460	0.0560
H7B	-0.20390	0.90400	0.73790	0.0560
H7C	-0.15500	0.92700	0.82810	0.0560
H10A	-0.31270	0.61400	0.81230	0.0630
H10B	-0.36040	0.64990	0.72780	0.0630
H10C	-0.40300	0.66310	0.79530	0.0630
H12A	-0.27550	0.72280	0.99060	0.0710
H12B	-0.17210	0.69380	1.00370	0.0710
H12C	-0.26330	0.65210	0.94870	0.0710
H13A	-0.34400	0.82520	0.65770	0.0580
H13B	-0.36040	0.74290	0.65320	0.0580
H13C	-0.26350	0.77440	0.65170	0.0580
H14A	-0.12650	0.89290	0.96230	0.0670
H14B	-0.13270	0.82770	1.01490	0.0670

H14C	-0.22190	0.87780	0.97800	0.0670
H15A	0.06620	0.73980	0.97340	0.0390
H15B	-0.01820	0.72010	1.00260	0.0390
H15C	-0.00280	0.79920	0.98280	0.0390
H16	-0.15370	0.66280	0.76170	0.0270
H21A	-0.11520	0.50060	0.88140	0.0450
H21B	-0.21330	0.53370	0.82560	0.0450
H21C	-0.16020	0.56450	0.91210	0.0450
H22A	0.01830	0.59700	0.99280	0.0460
H22B	0.11310	0.62130	0.98090	0.0460
H22C	0.07470	0.54360	0.95860	0.0460
H23A	0.16370	0.68660	0.89780	0.0450
H23B	0.12970	0.72650	0.81500	0.0450
H23C	0.16860	0.64860	0.82110	0.0450
H24A	-0.02420	0.65220	0.63820	0.0480
H24B	0.01050	0.72410	0.68370	0.0480
H24C	-0.09990	0.70950	0.63980	0.0480
H25A	-0.24020	0.64000	0.65030	0.0490
H25B	-0.25580	0.57380	0.69750	0.0490
H25C	-0.19060	0.56760	0.64560	0.0490
H27	0.36920	0.82370	0.74500	0.0310
H28A	0.44340	0.72800	0.67450	0.0610
H28B	0.43880	0.72980	0.76100	0.0610
H28C	0.50600	0.78290	0.73810	0.0610
H30A	0.16660	0.72280	0.67650	0.0680
H30B	0.27270	0.69580	0.71850	0.0680

Table S5 - (An)isotropic Displacement Parameters for **2**:

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Zr1	0.0147(1)	0.0158(1)	0.0174(1)	-0.0006(1)	0.0064(1)	0.0002(1)
Zr2	0.0156(1)	0.0161(1)	0.0141(1)	0.0008(1)	0.0056(1)	0.0006(1)
Zr3	0.0142(1)	0.0191(1)	0.0169(1)	-0.0004(1)	0.0057(1)	-0.0005(1)
O1	0.0193(7)	0.0203(7)	0.0210(7)	0.0002(5)	0.0092(5)	0.0001(5)
O2	0.0161(6)	0.0243(7)	0.0194(6)	0.0002(5)	0.0071(5)	0.0003(5)
N1	0.0227(9)	0.0298(9)	0.0250(9)	0.0076(7)	0.0064(7)	0.0059(7)
N2	0.0253(9)	0.0282(10)	0.0350(10)	-0.0133(8)	0.0100(8)	0.0000(8)
C1	0.0357(13)	0.0483(15)	0.0313(12)	0.0069(11)	0.0036(10)	-0.0033(11)
C2	0.0474(15)	0.0372(14)	0.0444(14)	0.0151(11)	0.0118(12)	0.0015(12)
C3	0.0443(15)	0.0612(17)	0.0426(14)	-0.0271(13)	0.0272(12)	0.0186(13)
C4	0.0624(19)	0.0313(14)	0.0627(19)	-0.0159(13)	-0.0034(15)	0.0163(13)
C5	0.0193(10)	0.0315(11)	0.0297(11)	-0.0074(9)	0.0126(8)	0.0011(8)
C6	0.0171(9)	0.0201(10)	0.0361(11)	0.0018(8)	0.0124(8)	0.0027(8)
C7	0.0305(12)	0.0239(11)	0.0623(16)	0.0095(11)	0.0227(12)	0.0065(9)
C8	0.0171(9)	0.0277(11)	0.0236(10)	0.0019(8)	0.0058(8)	0.0045(8)
C9	0.0178(9)	0.0229(10)	0.0356(11)	0.0009(8)	0.0120(8)	0.0000(8)
C10	0.0263(12)	0.0291(12)	0.0719(18)	-0.0050(12)	0.0190(12)	0.0078(10)
C11	0.0223(10)	0.0335(11)	0.0287(11)	0.0063(9)	0.0158(9)	0.0044(9)
C12	0.0494(16)	0.0609(18)	0.0432(14)	0.0181(13)	0.0310(13)	0.0049(14)
C13	0.0280(12)	0.0539(16)	0.0272(11)	0.0028(11)	0.0023(9)	0.0077(11)
C14	0.0354(13)	0.0566(17)	0.0441(14)	-0.0240(13)	0.0181(11)	0.0026(12)
C15	0.0270(11)	0.0280(11)	0.0193(9)	-0.0011(8)	0.0044(8)	0.0049(9)
C16	0.0306(11)	0.0146(9)	0.0229(10)	-0.0029(7)	0.0108(8)	0.0027(8)
C17	0.0311(11)	0.0180(9)	0.0218(9)	-0.0015(7)	0.0134(8)	0.0036(8)
C18	0.0247(10)	0.0180(9)	0.0263(10)	-0.0003(8)	0.0122(8)	0.0047(8)
C19	0.0282(11)	0.0176(9)	0.0224(10)	0.0024(7)	0.0102(8)	0.0058(8)
C20	0.0296(11)	0.0145(9)	0.0244(10)	0.0018(7)	0.0116(8)	0.0029(8)

C21	0.0355(12)	0.0212(10)	0.0370(12)	0.0067(9)	0.0169(10)	0.0016(9)
C22	0.0355(12)	0.0272(11)	0.0276(11)	0.0070(9)	0.0082(9)	0.0107(9)
C23	0.0266(11)	0.0267(11)	0.0398(12)	-0.0009(9)	0.0157(10)	0.0029(9)
C24	0.0483(14)	0.0273(11)	0.0266(11)	0.0012(9)	0.0218(10)	0.0032(10)
C25	0.0381(13)	0.0298(12)	0.0268(11)	-0.0066(9)	0.0082(10)	-0.0045(10)
C26	0.0241(10)	0.0309(11)	0.0249(10)	0.0000(8)	0.0151(8)	-0.0009(8)
C27	0.0286(11)	0.0312(11)	0.0227(10)	-0.0014(8)	0.0150(8)	0.0050(9)
C28	0.0429(14)	0.0380(14)	0.0471(15)	0.0029(11)	0.0227(12)	0.0157(11)
C29	0.0318(11)	0.0271(11)	0.0277(10)	-0.0095(8)	0.0199(9)	-0.0064(9)
C30	0.0620(17)	0.0345(13)	0.0558(16)	-0.0153(12)	0.0411(14)	-0.0178(12)
C31	0.0223(10)	0.0408(12)	0.0187(9)	-0.0089(9)	0.0100(8)	-0.0002(9)
C32	0.0256(12)	0.079(2)	0.0265(12)	-0.0163(12)	0.0056(10)	0.0005(12)
C33	0.0294(11)	0.0321(11)	0.0188(9)	0.0004(8)	0.0122(8)	0.0043(9)
C34	0.0619(17)	0.0457(15)	0.0296(12)	0.0132(11)	0.0242(12)	0.0173(13)
C35	0.0342(13)	0.0472(15)	0.0499(15)	0.0020(12)	0.0251(12)	-0.0087(11)
C36	0.0465(13)	0.0216(10)	0.0258(10)	0.0003(8)	0.0126(10)	-0.0007(10)
C37	0.0260(11)	0.0357(12)	0.0208(10)	0.0037(9)	0.0001(8)	0.0060(9)
C38	0.0517(16)	0.0403(14)	0.0404(14)	0.0106(11)	0.0075(12)	0.0151(12)
C39	0.0249(10)	0.0353(12)	0.0158(9)	0.0003(8)	0.0011(8)	-0.0021(9)
C40	0.0417(13)	0.0434(14)	0.0210(10)	0.0010(9)	0.0110(10)	-0.0080(11)
C41	0.0214(10)	0.0325(11)	0.0181(9)	-0.0053(8)	0.0012(8)	-0.0034(8)
C42	0.0338(12)	0.0400(13)	0.0294(11)	-0.0114(10)	0.0082(10)	-0.0010(10)
C43	0.0202(10)	0.0385(12)	0.0234(10)	-0.0054(9)	0.0008(8)	-0.0074(9)
C44	0.0337(13)	0.0509(16)	0.0410(14)	-0.0084(12)	0.0086(11)	-0.0216(12)
C45	0.0181(10)	0.0495(14)	0.0227(10)	-0.0033(9)	-0.0020(8)	0.0026(9)

Table S6 - Bond Distances (Angstrom) for **2**:

Zr1-O1	1.9407(14)	Zr2-H16	1.8600
Zr1-O2	1.9790(15)	Zr3-H27	1.9100
Zr1-N1	2.0569(17)	Zr3-H45	1.9300

Zr1-N2	2.0621(19)	N1-C1	1.446(3)
Zr2-O1	1.9966(14)	N1-C2	1.449(3)
Zr2-C5	2.600(2)	N2-C3	1.445(3)
Zr2-C6	2.576(2)	N2-C4	1.450(3)
Zr2-C8	2.540(2)	C5-C6	1.406(3)
Zr2-C9	2.583(2)	C5-C11	1.418(3)
Zr2-C11	2.584(2)	C5-C14	1.500(3)
Zr2-C15	2.289(2)	C6-C8	1.418(3)
Zr2-C16	2.5812(19)	C6-C7	1.494(3)
Zr2-C17	2.541(2)	C8-C9	1.425(3)
Zr2-C18	2.559(2)	C8-C13	1.506(3)
Zr2-C19	2.591(2)	C9-C10	1.502(3)
Zr2-C20	2.6092(19)	C9-C11	1.402(3)
Zr3-O2	1.9708(15)	C11-C12	1.504(4)
Zr3-C26	2.594(2)	C16-C20	1.424(3)
Zr3-C27	2.607(2)	C16-C25	1.513(3)
Zr3-C29	2.558(2)	C16-C17	1.416(3)
Zr3-C31	2.563(2)	C17-C24	1.505(3)
Zr3-C33	2.585(2)	C17-C18	1.416(3)
Zr3-C36	2.309(2)	C18-C19	1.419(3)
Zr3-C37	2.561(2)	C18-C23	1.499(3)
Zr3-C39	2.585(2)	C19-C20	1.413(3)
Zr3-C41	2.589(2)	C19-C22	1.503(3)
Zr3-C43	2.591(2)	C20-C21	1.503(3)
Zr3-C45	2.611(2)	C26-C33	1.412(3)
C26-C27	1.413(3)	C4-H4A	0.9600
C26-C35	1.504(4)	C4-H4B	0.9600
C27-C28	1.503(4)	C4-H4C	0.9600
C27-C29	1.414(3)	C7-H7A	0.9600
C29-C31	1.408(3)	C7-H7B	0.9600

C29-C30	1.510(3)	C7-H7C	0.9600
C31-C32	1.497(3)	C10-H10A	0.9600
C31-C33	1.414(3)	C10-H10B	0.9600
C33-C34	1.499(3)	C10-H10C	0.9600
C37-C38	1.506(3)	C12-H12A	0.9600
C37-C39	1.417(3)	C12-H12B	0.9600
C37-C45	1.421(3)	C12-H12C	0.9600
C39-C40	1.494(4)	C13-H13A	0.9600
C39-C41	1.416(3)	C13-H13B	0.9600
C41-C43	1.419(3)	C13-H13C	0.9600
C41-C42	1.495(3)	C14-H14A	0.9600

Table S7 - Bond Angles(Degrees)for **2**:

O1-Zr1-O2	111.74(6)	C6-Zr2-C9	52.73(7)
O1-Zr1-N1	108.97(7)	C6-Zr2-C11	52.52(7)
O1-Zr1-N2	108.91(7)	C6-Zr2-C15	102.86(7)
O2-Zr1-N1	110.25(7)	C6-Zr2-C16	125.03(7)
O2-Zr1-N2	109.44(7)	C6-Zr2-C17	134.96(7)
N1-Zr1-N2	107.43(7)	C6-Zr2-C18	162.22(7)
O1-Zr2-C5	100.20(6)	C6-Zr2-C19	164.84(7)
O1-Zr2-C6	79.95(6)	C6-Zr2-C20	137.21(7)
O1-Zr2-C8	94.54(6)	C8-Zr2-C9	32.29(7)
O1-Zr2-C9	126.73(6)	C8-Zr2-C11	53.02(7)
O1-Zr2-C11	130.74(6)	C8-Zr2-C15	130.10(7)
O1-Zr2-C15	95.11(7)	C8-Zr2-C16	93.10(7)
O1-Zr2-C16	110.08(6)	C8-Zr2-C17	110.35(7)
O1-Zr2-C17	81.59(6)	C8-Zr2-C18	142.40(6)
O1-Zr2-C18	84.65(6)	C8-Zr2-C19	139.76(7)
O1-Zr2-C19	115.19(6)	C8-Zr2-C20	108.24(7)

O1-Zr2-C20	133.66(6)	C9-Zr2-C11	31.49(7)
C5-Zr2-C6	31.52(7)	C9-Zr2-C15	116.06(8)
C5-Zr2-C8	52.89(7)	C9-Zr2-C16	84.13(7)
C5-Zr2-C9	52.35(7)	C9-Zr2-C17	113.26(7)
C5-Zr2-C11	31.75(7)	C9-Zr2-C18	135.29(7)
C5-Zr2-C15	77.22(7)	C9-Zr2-C19	113.74(7)
C5-Zr2-C16	136.36(7)	C9-Zr2-C20	84.69(7)
C5-Zr2-C17	163.15(7)	C11-Zr2-C15	84.93(8)

Table S8 - Torsion Angles (Degrees) (continued) for **2**:

C15-Zr2-C5-C6	143.76(14)
C15-Zr2-C5-C11	-101.22(13)
C15-Zr2-C5-C14	19.5(2)
C16-Zr2-C5-C6	-83.17(15)
C16-Zr2-C5-C11	31.86(17)
C16-Zr2-C5-C14	152.59(18)
C19-Zr2-C5-C6	-163.52(12)
C19-Zr2-C5-C11	-48.49(17)
C19-Zr2-C5-C14	72.2(2)
C20-Zr2-C5-C6	-123.63(13)
C20-Zr2-C5-C11	-8.60(16)
C20-Zr2-C5-C14	112.1(2)
O1-Zr2-C6-C5	-129.25(13)
O1-Zr2-C6-C7	-6.29(18)
O1-Zr2-C6-C8	115.63(13)
C5-Zr2-C6-C7	123.0(2)
C5-Zr2-C6-C8	-115.11(18)
C8-Zr2-C6-C5	115.11(18)
C8-Zr2-C6-C7	-121.9(2)

C9-Zr2-C6-C5	76.86(14)
C9-Zr2-C6-C7	-160.2(2)
C9-Zr2-C6-C8	-38.26(12)
C11-Zr2-C6-C5	36.93(12)
C11-Zr2-C6-C7	159.9(2)
C11-Zr2-C6-C8	-78.19(13)
C15-Zr2-C6-C5	-36.26(14)
C15-Zr2-C6-C7	86.71(19)
C15-Zr2-C6-C8	-151.37(12)

Atomic co-ordinates of the optimized structures:

2:

Zr	-0.04989	-1.48975	0.47034
Zr	-3.50702	0.38182	-0.31469
Zr	3.60426	0.02094	-0.05319
O	-1.75762	-0.51785	0.13350
O	1.68491	-0.47495	0.20276
N	-0.00153	-2.17964	2.42251
N	0.00198	-3.18555	-0.74417
C	-1.07546	-2.00414	3.42871
H	-1.49804	-2.98189	3.75710
H	-1.89616	-1.39780	3.00515
H	-0.69627	-1.48087	4.33706
C	1.14835	-2.93877	2.97249
H	1.52819	-2.47560	3.91139
H	1.98681	-2.95855	2.24980
H	0.86831	-3.99220	3.20581
C	-0.62669	-3.25116	-2.08702
H	0.11666	-3.47419	-2.88622
H	-1.11783	-2.29151	-2.33720
H	-1.40193	-4.05160	-2.13113
C	0.58428	-4.49546	-0.36356
H	-0.20004	-5.28646	-0.30485
H	1.07419	-4.43465	0.62512
H	1.34834	-4.83788	-1.09922
C	-4.87178	-1.74525	-1.21284
C	-4.45771	-2.03693	0.14136
C	-3.58627	-3.22218	0.56974
H	-4.15767	-4.14617	0.50077
H	-3.25622	-3.10936	1.59643
H	-2.70893	-3.32306	-0.06165

C	-5.16623	-1.13165	1.03414
C	-6.06098	-0.31772	0.22051
C	-7.27101	0.45874	0.75320
H	-7.64178	1.16863	0.02289
H	-7.04779	0.98901	1.67181
H	-8.07275	-0.24647	0.96693
C	-5.84799	-0.66628	-1.16696
C	-6.67611	-0.16108	-2.35575
H	-7.58213	-0.75542	-2.46290
H	-6.11439	-0.23610	-3.28102
H	-6.97086	0.87475	-2.21963
C	-5.23384	-1.26285	2.56347
H	-5.90299	-2.07640	2.83854
H	-5.61276	-0.35367	3.01718
H	-4.25926	-1.47692	2.99019
C	-4.57068	-2.61369	-2.43883
H	-3.57581	-3.04149	-2.38538
H	-4.65255	-2.04428	-3.35830
H	-5.28650	-3.43308	-2.48548
C	-3.05465	0.40656	-2.56043
H	-2.15360	1.02152	-2.74888
H	-3.87733	0.78463	-3.19941
H	-2.82830	-0.63386	-2.86653
C	-3.89029	2.43187	1.32464
C	-2.45871	2.29389	1.12349
C	-2.15864	2.63018	-0.25246
C	-3.40474	2.98392	-0.90910
C	-4.47367	2.87118	0.06428
C	-5.87899	3.44706	-0.15479
H	-5.81155	4.52782	-0.26514
H	-6.52790	3.23920	0.68763
H	-6.34298	3.05341	-1.05460
C	-3.56236	3.62339	-2.29339
H	-4.50385	3.33746	-2.75212
H	-2.75653	3.33363	-2.95848
H	-3.55035	4.70823	-2.19877
C	-0.75095	2.75615	-0.84327
H	-0.78530	2.76155	-1.92710
H	-0.11617	1.93503	-0.52351
H	-0.28923	3.68645	-0.51702
C	-1.42573	2.00448	2.21624
H	-1.04548	2.93598	2.63234
H	-0.58463	1.44876	1.81495
H	-1.86048	1.42850	3.02683
C	-4.56522	2.44755	2.70336
H	-4.18044	1.65998	3.34370
H	-5.63982	2.33128	2.62459
H	-4.36921	3.39941	3.19419
C	5.53267	0.95149	1.60768
C	4.89427	2.12500	1.05167
C	5.60793	3.34614	0.45889
H	5.74295	4.08732	1.24506
H	5.03384	3.81232	-0.33443

H	6.58799	3.08998	0.07456
C	3.50540	2.13361	1.49184
C	2.52896	3.30207	1.29358
H	1.50029	2.96796	1.37186
H	2.66373	3.76597	0.32155
H	2.69291	4.06586	2.05225
C	3.31662	1.00973	2.39372
C	2.08211	0.74987	3.26561
H	1.54178	1.67527	3.43664
H	2.38658	0.35593	4.23052
H	1.40082	0.03524	2.81100
C	4.55780	0.26994	2.44798
C	4.89238	-0.84094	3.45040
H	5.66652	-1.49764	3.06824
H	4.01890	-1.44019	3.68436
H	5.25485	-0.39638	4.37631
C	7.02363	0.59458	1.53775
H	7.53338	0.92623	2.44080
H	7.50376	1.07158	0.69021
H	7.16560	-0.47864	1.45059
C	4.37642	-2.07374	0.49643
H	3.95021	-2.36124	1.47758
H	5.48078	-2.13775	0.57288
H	4.03455	-2.80867	-0.25662
C	3.68407	1.26522	-2.37205
C	3.25540	2.71631	-2.63953
H	3.19058	2.89488	-3.71153
H	3.96864	3.42200	-2.22909
H	2.28123	2.92727	-2.20879
C	2.82740	0.10652	-2.56523
C	1.35448	0.12613	-2.98018
H	0.78729	-0.63170	-2.44863
H	1.26398	-0.07856	-4.04557
H	0.90470	1.09268	-2.78441
C	3.64282	-1.08210	-2.47207
C	3.14444	-2.50008	-2.77161
H	3.92023	-3.23355	-2.58280
H	2.85541	-2.57631	-3.81820
H	2.28005	-2.74832	-2.16389
C	5.01611	-0.66881	-2.23598
C	6.25753	-1.56899	-2.25917
H	6.65910	-1.62405	-3.26993
H	6.01916	-2.57618	-1.93505
H	7.03592	-1.17746	-1.61126
C	5.04905	0.77856	-2.20672
C	6.33877	1.59742	-2.34459
H	7.08442	1.31293	-1.60877
H	6.14791	2.65976	-2.25175
H	6.76660	1.42164	-3.33008

2a:

Zr	-0.10953	-1.50657	0.39329
Zr	-3.56849	0.38577	-0.31410
Zr	3.53338	0.04963	-0.05528
O	-1.84577	-0.52337	0.07862
O	1.59722	-0.47459	0.17889
N	-0.06710	-2.29337	2.30238
N	-0.03427	-3.15178	-0.89654
C	-1.14887	-2.17670	3.31035
H	-1.55718	-3.17420	3.58863
H	-1.97753	-1.56027	2.91599
H	-0.77841	-1.69483	4.24288
C	1.09289	-3.06175	2.82170
H	1.45763	-2.63972	3.78369
H	1.93701	-3.03510	2.10633
H	0.82349	-4.12687	3.00079
C	-0.63522	-3.15987	-2.25444
H	0.12593	-3.34678	-3.04362
H	-1.12606	-2.19243	-2.47657
H	-1.40246	-3.96193	-2.34725
C	0.56336	-4.46983	-0.56617
H	-0.21166	-5.26962	-0.55304
H	1.04165	-4.44806	0.42898
H	1.33743	-4.76686	-1.30830
C	-4.73958	-1.58374	-1.38319
C	-4.47716	-1.99273	-0.01923
C	-3.64215	-3.20316	0.40590
H	-4.20816	-4.11562	0.22741
H	-3.40361	-3.15598	1.46265
H	-2.71433	-3.26698	-0.15454
C	-5.25777	-1.13751	0.86943
C	-6.06913	-0.25446	0.03184
C	-7.31689	0.49970	0.49927
H	-7.60559	1.26980	-0.20675
H	-7.18286	0.94893	1.47646
H	-8.13744	-0.21252	0.57141
C	-5.70719	-0.48690	-1.35092
C	-6.39781	0.12945	-2.57576
H	-7.28877	-0.44376	-2.82531
H	-5.74221	0.12219	-3.44126
H	-6.70201	1.15363	-2.38361
C	-5.43991	-1.35297	2.37812
H	-6.13347	-2.17515	2.54498
H	-5.84894	-0.46774	2.85256
H	-4.50131	-1.60319	2.86206
C	-4.29830	-2.34071	-2.64161
H	-3.31995	-2.79025	-2.50983
H	-4.26774	-1.68846	-3.50901
H	-5.01060	-3.13809	-2.84529
C	-4.04566	2.34600	1.28386
C	-2.59764	2.23810	1.16598
C	-2.23044	2.55415	-0.20128

C	-3.45136	2.85652	-0.93889
C	-4.56985	2.74730	-0.01951
C	-5.97014	3.29102	-0.32554
H	-5.90807	4.36993	-0.45502
H	-6.65794	3.09080	0.48727
H	-6.37791	2.87122	-1.24056
C	-3.54407	3.43998	-2.35526
H	-4.45428	3.12014	-2.85440
H	-2.69429	3.14575	-2.96349
H	-3.55750	4.52669	-2.29725
C	-0.79653	2.68141	-0.72684
H	-0.77754	2.66565	-1.81174
H	-0.16968	1.87533	-0.35681
H	-0.36478	3.62396	-0.39644
C	-1.61649	1.96875	2.30870
H	-1.27419	2.91200	2.73076
H	-0.74824	1.42414	1.95255
H	-2.08436	1.39413	3.10163
C	-4.79624	2.37104	2.62071
H	-4.42688	1.60745	3.29812
H	-5.86207	2.22995	2.48443
H	-4.64403	3.33971	3.09359
C	5.45827	0.86636	1.61936
C	4.82102	2.07605	1.14101
C	5.53608	3.32578	0.61403
H	5.68387	4.01672	1.44243
H	4.95688	3.84222	-0.14365
H	6.51043	3.08686	0.20503
C	3.43764	2.06587	1.59499
C	2.46464	3.24764	1.47218
H	1.43523	2.91381	1.54105
H	2.59341	3.76622	0.52721
H	2.63788	3.96644	2.27158
C	3.25315	0.89258	2.43376
C	2.02955	0.59391	3.30905
H	1.50031	1.51262	3.54072
H	2.34514	0.14490	4.24585
H	1.33509	-0.08957	2.82753
C	4.49099	0.14327	2.43168
C	4.83358	-1.02079	3.36851
H	5.60036	-1.65833	2.94170
H	3.96104	-1.62883	3.58231
H	5.20994	-0.62628	4.31128
C	6.94616	0.50779	1.51303
H	7.46479	0.78536	2.42901
H	7.41979	1.03142	0.68975
H	7.08200	-0.55927	1.36319
C	4.30952	-2.06683	0.37483
H	3.88911	-2.40983	1.34069
H	5.41331	-2.13175	0.44452
H	3.96952	-2.76082	-0.41707
C	3.60236	1.41985	-2.29745
C	3.16921	2.88203	-2.48548

H	3.10415	3.11863	-3.54620
H	3.88078	3.56605	-2.03744
H	2.19492	3.06767	-2.04355
C	2.75189	0.26928	-2.55404
C	1.27917	0.30642	-2.96955
H	0.71466	-0.48223	-2.48048
H	1.18883	0.16009	-4.04469
H	0.82740	1.26047	-2.72207
C	3.57319	-0.92071	-2.52778
C	3.08547	-2.32200	-2.91197
H	3.86640	-3.05942	-2.76479
H	2.80013	-2.33853	-3.96225
H	2.22224	-2.61295	-2.32222
C	4.94292	-0.51492	-2.26683
C	6.18860	-1.40554	-2.34132
H	6.58834	-1.39952	-3.35416
H	5.95612	-2.43096	-2.07519
H	6.96509	-1.04649	-1.67277
C	4.96853	0.92974	-2.15812
C	6.25424	1.76005	-2.25170
H	7.00121	1.43804	-1.53299
H	6.05944	2.81510	-2.10169
H	6.68049	1.63809	-3.24586

2b:

Zr	-0.11345	1.24415	0.71874
Zr	-3.64550	-0.16673	0.17088
Zr	3.62885	0.09324	-0.06928
O	-1.65725	0.09422	0.66066
O	1.62768	0.55634	0.26069
N	-0.07616	2.39087	2.40484
C	-1.20568	2.50015	3.37506
H	-0.89894	2.12235	4.37259
H	-2.07401	1.90711	3.03655
H	-1.52241	3.55720	3.49351
C	1.12247	3.15357	2.86131
H	0.88433	4.23413	2.94840
H	1.95958	3.04064	2.14811
H	1.46532	2.79849	3.85528
C	-4.05414	2.46770	-0.33942
C	-2.97035	2.01632	-1.18612
C	-1.56001	2.62516	-1.22359
H	-1.48015	3.41634	-1.97076
H	-0.80697	1.88191	-1.51214
H	-1.30356	3.10211	-0.27085
C	-3.48634	1.04759	-2.14094
C	-4.91605	0.92695	-1.89624
C	-5.95803	0.34399	-2.85887
H	-6.73783	-0.19701	-2.33464
H	-5.50280	-0.31563	-3.58740
H	-6.43021	1.16323	-3.39820
C	-5.25537	1.77161	-0.76285

C	-6.68271	2.04707	-0.27387
H	-7.18409	2.72972	-0.95789
H	-6.67583	2.49844	0.71237
H	-7.26563	1.13214	-0.22806
C	-2.71751	0.51992	-3.36054
H	-2.60933	1.30859	-4.10304
H	-3.24485	-0.30463	-3.82630
H	-1.72314	0.17636	-3.08945
C	-3.99686	3.65613	0.62694
H	-3.03719	3.72132	1.13071
H	-4.77319	3.58909	1.38099
H	-4.14874	4.57995	0.07098
C	-4.48624	0.55962	2.16220
H	-4.00227	-0.00797	2.98240
H	-5.58137	0.41327	2.25033
H	-4.28273	1.63585	2.31518
C	-4.24813	-2.46857	-0.96964
C	-2.95524	-2.59103	-0.32120
C	-3.16233	-2.50461	1.11590
C	-4.58010	-2.32649	1.35759
C	-5.25095	-2.26967	0.06946
C	-6.77615	-2.29032	-0.10037
H	-7.16436	-3.26323	0.19534
H	-7.06243	-2.11674	-1.13089
H	-7.25278	-1.53874	0.52277
C	-5.29448	-2.47811	2.70357
H	-6.18429	-1.85919	2.75392
H	-4.64344	-2.21699	3.53075
H	-5.59780	-3.51681	2.82554
C	-2.08323	-2.73616	2.17820
H	-2.33367	-2.23309	3.10710
H	-1.12541	-2.36456	1.83334
H	-1.98020	-3.80003	2.38577
C	-1.62321	-2.93751	-1.00093
H	-1.33694	-3.96012	-0.76311
H	-0.82709	-2.28035	-0.66286
H	-1.70558	-2.85280	-2.07959
C	-4.52752	-2.84633	-2.42957
H	-3.78080	-2.44246	-3.10502
H	-5.50500	-2.50648	-2.74796
H	-4.50602	-3.93099	-2.52010
C	4.76054	1.28613	-2.14154
C	5.12722	-0.11383	-2.24119
C	6.57814	-0.59879	-2.37358
H	7.05553	-0.07770	-3.20049
H	6.61786	-1.66176	-2.58157
H	7.15906	-0.39843	-1.47778
C	3.91161	-0.88174	-2.48506
C	3.82371	-2.33061	-2.98384
H	2.98040	-2.85808	-2.54895
H	4.72818	-2.88239	-2.76013
H	3.69251	-2.32871	-4.06444
C	2.80240	0.05477	-2.53477

C	1.37266	-0.31895	-2.94265
H	1.27363	-0.29969	-4.02673
H	0.65116	0.37922	-2.53025
H	1.11644	-1.31673	-2.60041
C	3.32325	1.39161	-2.31992
C	2.54435	2.70878	-2.45401
H	2.62787	3.32290	-1.56098
H	1.49383	2.51587	-2.64551
H	2.93270	3.28614	-3.29000
C	5.76385	2.44410	-2.13626
H	6.21098	2.53529	-3.12482
H	6.56263	2.27497	-1.42037
H	5.27791	3.38354	-1.89615
C	4.39752	2.08166	0.76702
H	4.15948	2.93219	0.10025
H	5.48897	2.09739	0.95764
H	3.89471	2.24944	1.74116
C	4.80801	-2.12754	0.73961
C	5.53088	-3.24777	-0.01721
H	5.93966	-3.94909	0.70835
H	6.35263	-2.87373	-0.61688
H	4.84953	-3.79461	-0.65803
C	3.40950	-2.17027	1.14410
C	2.41110	-3.27028	0.75322
H	1.39189	-2.96012	0.95391
H	2.60662	-4.17398	1.32776
H	2.48948	-3.52245	-0.29944
C	3.21645	-1.16023	2.17504
C	1.97457	-0.97537	3.05423
H	1.73169	0.07612	3.18571
H	2.15218	-1.39945	4.04087
H	1.11576	-1.47856	2.62632
C	4.47807	-0.47998	2.38006
C	4.80223	0.46683	3.53952
H	5.11177	-0.12048	4.40280
H	3.93624	1.05458	3.82644
H	5.61119	1.14278	3.28287
C	5.45796	-1.06052	1.47996
C	6.96153	-0.75024	1.50924
H	7.17004	0.27126	1.20135
H	7.50594	-1.42468	0.85723
H	7.34243	-0.87702	2.51994

2c:

Zr	0.04418	1.45365	0.22659
Zr	3.59628	-0.37082	0.00153
Zr	-3.57421	-0.26595	-0.03493
O	1.77852	0.39530	0.24072
O	-1.72749	0.42476	-0.04161
N	-0.24840	2.58559	1.90213
N	0.28933	2.78148	-1.33177
C	0.47476	2.60069	3.19990

H	0.94283	3.58913	3.39020
H	1.26727	1.83030	3.21328
H	-0.21634	2.39105	4.04399
C	-1.38632	3.55211	1.88339
H	-2.09962	3.34946	2.70931
H	-1.94341	3.49257	0.92607
H	-1.02599	4.59617	1.99497
C	0.66007	2.25836	-2.67807
H	-0.10115	2.51878	-3.44356
H	0.76325	1.15390	-2.66235
H	1.62769	2.68269	-3.02092
C	0.19665	4.26715	-1.33155
H	1.16312	4.72232	-1.63732
H	-0.04654	4.64300	-0.32329
H	-0.57935	4.63007	-2.03880
C	4.91286	1.72409	-0.67515
C	4.37157	1.98948	0.64500
C	3.47115	3.17366	1.00053
H	4.05504	4.09163	0.96313
H	3.07084	3.07024	2.00204
H	2.64658	3.27208	0.30014
C	4.99480	1.06196	1.57665
C	5.97382	0.26314	0.83732
C	7.06947	-0.58738	1.48929
H	7.48097	-1.30983	0.79337
H	6.69966	-1.11339	2.36350
H	7.87734	0.06871	1.80958
C	5.92120	0.67385	-0.55579
C	6.95333	0.36412	-1.64622
H	7.62603	1.21522	-1.73754
H	6.48428	0.20567	-2.61291
H	7.54685	-0.50708	-1.39564
C	4.85461	1.08329	3.10691
H	5.58616	1.77032	3.52868
H	5.03427	0.10011	3.53117
H	3.86645	1.41604	3.40794
C	4.68762	2.58265	-1.92693
H	3.73667	3.10199	-1.87544
H	4.71230	1.98153	-2.83125
H	5.47787	3.32814	-1.99778
C	4.19416	-2.87072	0.33194
C	2.73717	-2.72444	0.36375
C	2.29237	-2.32495	-0.95456
C	3.47369	-2.18679	-1.80468
C	4.63762	-2.58230	-1.02112
C	6.00796	-2.93790	-1.60223
H	5.99428	-3.98898	-1.88727
H	6.80265	-2.79942	-0.87765
H	6.23097	-2.35415	-2.48829
C	3.46733	-1.94723	-3.32260
H	4.39488	-1.48801	-3.65009
H	2.64221	-1.30620	-3.61730
H	3.36006	-2.89772	-3.84227

C	0.83497	-2.22767	-1.41408
H	0.75226	-1.64639	-2.32684
H	0.21370	-1.76795	-0.65104
H	0.44661	-3.22518	-1.61279
C	1.84248	-3.12890	1.54208
H	1.54954	-4.17227	1.43833
H	0.94319	-2.52445	1.57472
H	2.36700	-3.02052	2.48635
C	5.02435	-3.54447	1.43299
H	4.76342	-3.16970	2.41847
H	6.08554	-3.39158	1.27266
H	4.83165	-4.61579	1.41940
C	-5.22005	-1.10509	1.83985
C	-4.67618	-2.28838	1.20074
C	-5.46779	-3.48284	0.65537
H	-5.56151	-4.23130	1.44047
H	-4.96385	-3.94508	-0.18783
H	-6.46619	-3.19261	0.34941
C	-3.23384	-2.30771	1.45038
C	-2.31040	-3.49150	1.12870
H	-1.27616	-3.17403	1.05888
H	-2.59174	-3.96807	0.19443
H	-2.38363	-4.23567	1.91991
C	-2.89797	-1.15433	2.26529
C	-1.54047	-0.88221	2.91596
H	-0.72713	-1.09980	2.23041
H	-1.41898	-1.51434	3.79409
H	-1.46130	0.15316	3.22980
C	-4.11451	-0.38488	2.46926
C	-4.28767	0.81680	3.40970
H	-5.07176	1.48051	3.05751
H	-3.36682	1.38310	3.49962
H	-4.56673	0.46373	4.40096
C	-6.69733	-0.80710	2.11809
H	-6.91387	-1.06224	3.15402
H	-7.34626	-1.39958	1.48401
H	-6.93216	0.24390	1.97876
C	-4.73459	-0.84596	-2.26054
C	-4.85721	-2.21845	-2.93819
H	-5.23617	-2.08925	-3.95051
H	-5.54667	-2.86066	-2.40061
H	-3.89471	-2.71733	-3.00198
C	-3.67643	0.13364	-2.53047
C	-2.49144	-0.08675	-3.47761
H	-1.65955	0.55616	-3.21306
H	-2.79131	0.14817	-4.49754
H	-2.15774	-1.11972	-3.45608
C	-4.04764	1.38132	-1.90416
C	-3.32808	2.72281	-2.07597
H	-3.62447	3.42465	-1.30334
H	-3.59106	3.15378	-3.04031
H	-2.25091	2.59913	-2.03943
C	-5.33353	1.18340	-1.22757

C	-6.19095	2.29819	-0.60919
H	-6.75123	2.80415	-1.39344
H	-5.57477	3.03722	-0.10616
H	-6.90132	1.89618	0.10575
C	-5.78378	-0.17006	-1.51625
C	-7.21414	-0.68414	-1.34243
H	-7.72690	-0.17619	-0.53382
H	-7.24361	-1.75357	-1.16637
H	-7.75927	-0.48284	-2.26358

2d:

Zr	-0.09022	1.08070	0.98542
Zr	-3.60000	-0.19387	0.09158
Zr	3.55922	-0.08670	-0.17383
O	-1.56530	-0.06055	0.67400
O	1.73126	0.52921	0.37264
N	-0.08249	1.70232	2.91441
C	-1.11830	1.44247	3.95751
H	-0.68226	0.87176	4.80200
H	-1.95533	0.85886	3.53939
H	-1.51682	2.39559	4.35917
C	1.06218	2.50645	3.44414
H	0.71259	3.50085	3.78639
H	1.83571	2.66496	2.66546
H	1.53984	1.99740	4.30489
C	-3.99767	2.47303	0.18127
C	-2.91015	2.22184	-0.74157
C	-1.50895	2.84358	-0.64306
H	-1.44283	3.79357	-1.17849
H	-0.74336	2.20167	-1.10726
H	-1.25111	3.09978	0.40058
C	-3.41329	1.48937	-1.89140
C	-4.84418	1.31995	-1.68768
C	-5.86251	0.97604	-2.78055
H	-6.77939	0.57966	-2.35907
H	-5.46804	0.26320	-3.49514
H	-6.11083	1.88809	-3.32098
C	-5.19371	1.89305	-0.39561
C	-6.62032	2.06889	0.13804
H	-7.05716	2.97745	-0.27299
H	-6.62596	2.14833	1.22015
H	-7.25083	1.23311	-0.14820
C	-2.64448	1.26217	-3.20058
H	-2.53627	2.20414	-3.73568
H	-3.17575	0.57241	-3.84648
H	-1.65021	0.86231	-3.02019
C	-3.93921	3.40920	1.39314
H	-3.03865	3.25814	1.98146
H	-4.79654	3.26024	2.03999
H	-3.95091	4.44306	1.05174
C	-4.44212	0.08231	2.18590
H	-4.03693	-0.70506	2.85134

H	-5.54695	0.01673	2.23012
H	-4.16060	1.07191	2.59508
C	-3.88101	-2.21206	-1.53850
C	-2.79290	-2.52307	-0.63392
C	-3.34021	-2.67780	0.70561
C	-4.77439	-2.47293	0.62950
C	-5.11032	-2.16235	-0.75111
C	-6.54573	-2.14799	-1.29353
H	-6.95763	-3.15384	-1.23714
H	-6.57341	-1.83271	-2.32991
H	-7.18769	-1.49298	-0.71135
C	-5.80299	-2.80024	1.71549
H	-6.68130	-2.16850	1.62875
H	-5.38677	-2.68121	2.70969
H	-6.11841	-3.83602	1.59977
C	-2.55407	-3.16522	1.92896
H	-3.08788	-2.94502	2.84741
H	-1.57711	-2.69445	1.97811
H	-2.40888	-4.24272	1.87255
C	-1.34363	-2.81730	-1.03726
H	-1.20007	-3.88994	-1.15585
H	-0.65396	-2.46625	-0.27609
H	-1.09420	-2.33907	-1.97930
C	-3.78836	-2.27593	-3.06798
H	-2.85216	-1.86409	-3.43062
H	-4.60716	-1.74692	-3.54134
H	-3.83966	-3.31714	-3.38194
C	5.49195	0.72082	-1.76862
C	4.40621	0.18911	-2.57689
C	4.53831	-0.88128	-3.66987
H	4.74736	-0.39812	-4.62278
H	3.62264	-1.45528	-3.77808
H	5.35300	-1.56354	-3.45223
C	3.24647	1.07175	-2.40183
C	1.96385	1.01100	-3.24116
H	1.12045	1.42943	-2.70211
H	1.72631	-0.01064	-3.52235
H	2.10016	1.58821	-4.15433
C	3.60536	2.10283	-1.45336
C	2.77045	3.33844	-1.09903
H	1.70826	3.12649	-1.17053
H	2.99708	4.14334	-1.79651
H	2.99236	3.69196	-0.09656
C	4.98238	1.86124	-1.01757
C	5.83171	2.82764	-0.17855
H	6.64660	2.30734	0.31442
H	5.23161	3.32738	0.57561
H	6.26125	3.58892	-0.82759
C	6.97048	0.35579	-1.91175
H	7.38858	0.95698	-2.71814
H	7.10596	-0.68843	-2.16957
H	7.52729	0.57628	-1.00792
C	3.55068	-2.54291	0.49663

C	2.74245	-3.65930	-0.18091
H	2.96783	-4.60898	0.30134
H	2.99876	-3.74763	-1.23233
H	1.67549	-3.48215	-0.09489
C	3.15012	-1.78726	1.67578
C	1.83662	-1.94640	2.44485
H	1.55740	-1.02122	2.94104
H	1.95284	-2.71379	3.20853
H	1.03087	-2.25027	1.78432
C	4.28515	-0.98257	2.09504
C	4.38433	-0.16595	3.39103
H	5.07461	0.66503	3.28042
H	4.75339	-0.80586	4.19080
H	3.41486	0.22046	3.68794
C	5.40468	-1.26596	1.19810
C	6.85700	-0.86907	1.48939
H	7.21572	-1.45577	2.33340
H	6.94362	0.18107	1.75226
H	7.49937	-1.07416	0.64107
C	4.95142	-2.24009	0.21501
C	5.83439	-3.06169	-0.73030
H	6.76472	-2.55136	-0.95073
H	5.32461	-3.28484	-1.66230
H	6.07556	-4.00651	-0.24568

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