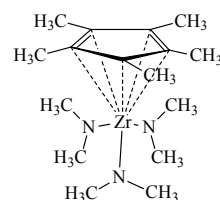


933
ED $\text{C}_{16}\text{H}_{33}\text{N}_3\text{Zr}$

Tris(*N*-methylmethanaminato)[(1,2,3,4,5- η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]zirconium
 Tris(dimethylamido)[(1,2,3,4,5- η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]zirconium

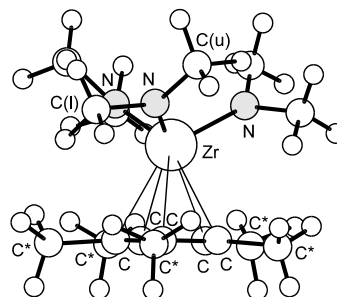
 C_1

r_a	\AA^a	θ_a	deg a
Zr–C	2.558(15)	Z...C–C* b c	179(2)
C–C	1.413(10)	C–C*–H	112.5 d
C–C*	1.54(2)	N–Zr–N	100.9(11)
C*–H	1.118(5)	Zr–N–C(u)	123.6(11) e
Zr...Z c	2.258(14)	Zr–N–C(l)	122.1(11) e
Zr–N	2.071(10)	C–N–C	114(2)
N–C	1.456(6)	N–C–H	111.0 e
C–H	1.118(5)	Z...Zr–N c	117.1(9)
		Z...Zr–N–C(u) c f	119(3)
		Z...Zr–N–C(l) c f	–61(3)
		C...Z...Zr–N c f	6.0 d



Local C_{5v} symmetry was assumed for the $\text{Zr}[\text{C}_5(\text{CH}_3)_5]$ fragment and C_3 for $\text{Zr}[\text{N}(\text{CH}_3)_2]_3$. The configurations around the N atoms were assumed to be planar. The $\text{N}(\text{CH}_3)_2$ groups were assumed to have C_{2v} symmetry. The nozzle temperature was 160(5) °C.

- a) Three times the estimated standard errors including a systematic error.
 b) The C* atom is bent away from the Ti atom.
 c) Z is the ring centroid.
 d) Assumed.
 e) Differences between the N–C–H angle and the Zr–N–C(u) and Zr–N–C(l) angles were assumed at the values for $\text{C}_5\text{H}_5\text{Zr}[\text{N}(\text{CH}_3)_2]_3$ molecule from B3LYP/LanDZ2 calculations.
 f) Torsional angle, zero degree for the *syn* position.



Haaland, A., Volden, H.V., Østby, K.-A., Mena, M., Yélamos, C., Palacios, F.: J. Mol. Struct. **567-568** (2001) 295.