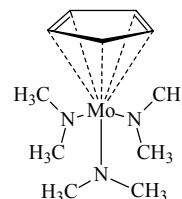


901 **C₁₁H₂₃MoN₃**
ED, DFT calculations

(η^5 -2,4-Cyclopentadien-1-yl)tris(*N*-methylmethan-aminato)molybdenum **C_s assumed**
Cyclopentadienyltris(dimethylamino)molybdenum

r_a	\AA^a	θ_a	deg b
Mo–N(1)	1.971(4) c	N(1)–Mo–N(2,3)	97(2)
Mo–N(2,3)	2.001(4) c	N(2)–Mo–N(3)	104(2)
Mo–C(1)	2.341(30)	Mo–N(1)–C(6)	115(3)
Mo–C(2,5)	2.387(9)	Mo–N(1)–C(7)	135(3)
Mo–C(3,4)	2.460(29)	C–N–C	110.2 d e
C–C (ring)	1.434(8) c	Mo–N(2)–C(8)	125(4)
N–C	1.476(7) c	Mo–N(2)–C(9)	117(4)
C–H (methyl)	1.104(4) c e	Mo–N(3)–C(10)	117(4)
C–H (ring)	1.094(4) c e	Mo–N(3)–C(11)	125(4)
		N(1)–Mo–N(2)–C(8)	41(9)
		N(1)–Mo–N(2)–C(9)	–105(6)



The results of ED, NMR and photoelectron spectra and DFT calculations were all consistent with a ground-state structure in which one dimethylamino group has the methyl groups in the axial position with respect to the Mo–ring vector and the other two dimethylamino groups have the methyl groups in the equatorial positions. It was assumed in the ED analysis that the cyclopentadienyl ring has local D_{5h} symmetry and each NCH_3 fragment has local C_{3v} symmetry, the methyl group orientations were assumed such that one of the dihedral angles $\tau(C-N-C-H)$ was 180° .

The nozzle was at *ca.* 80 °C.

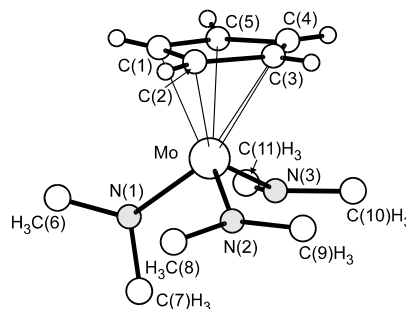
a) Three times the estimated standard errors.

b) Six times the estimated standard errors.

c) Differences $[Mo-N(1)] - [Mo-N(2,3)]$ and $[C-H(methyl)] - [C-H(ring)]$ were assumed at the values from BLYP/LanL2DZ calculations.

d) Assumed at the value from DFT calculations.

e) All C–N–C angles were assumed equal.



Green, J.C., Parkin, R.P.G., Yan, X., Haaland, A., Scherer, W., Tafipolsky, M.A.: J. Chem. Soc., Dalton Trans. (1997) 3219.