Electronic Supplementary Information for Dalton Transactions

Dimethylalkoxygallane incorporating a donor-functionalised alkoxide: the monomeric gas-phase structure

Caroline E. Knapp, Claire J. Carmalt, Paul F. McMillan, Derek A. Wann, Heather E. Robertson and David W. H. Rankin

Electronic Supplementary Information

Table S1 Nozzle-to-film distances / mm, weighting functions / nm^{-1}, scale factors, correlation parameters and electron wavelengths / pm used in the electron diffraction study of $Me_2GaOCH_2CH_2NMe_2$.

Nozzle-to-film distance[a]	Δs	s_{min}	sw_1	sw_2	s_{max}	Scale factor[b]	Correlation parameter	Electron wavelength
93.39	0.4	10.0	12.0	27.6	30.0	0.900(38)	0.334	6.18
254.54	0.2	2.0	4.0	12.0	13.0	1.282(37)	0.344	6.18

[a] Determined by reference to the scattering pattern of benzene. [b] Values in parentheses are the estimated standard deviations.

Table S2 GED coordinates (in Å) for $Me_2GaOCH_2CH_2NMe_2$.

Atom	*x*	*y*	*z*
C(1)	1.7386	1.9461	3.0477
C(2)	1.2864	4.0551	0.1823
C(3)	–1.7980	3.2018	0.5985
Ga(4)	1.1479	2.3115	1.1653
O(5)	1.1653	0.8031	0.0000
C(6)	0.0000	0.0000	0.0000
C(7)	–1.2717	0.8765	0.0000
H(8)	2.8089	2.0875	3.1493
H(9)	1.2424	2.6141	3.7431
H(10)	1.5042	0.9266	3.3334
H(11)	0.8419	3.9771	–0.8038
H(12)	0.7734	4.8431	0.7225
H(13)	2.3237	4.3478	0.0627
H(14)	–1.3314	3.5688	–0.3090
H(15)	–2.8515	3.0433	0.3960
H(16)	–1.7122	3.9716	1.3573
H(17)	0.0000	–0.6471	–0.8702
H(18)	0.0000	–0.6471	0.8702
H(19)	–2.1480	0.2748	0.2150
H(20)	–1.4029	1.3559	–0.9638
N(21)	–1.1519	1.9401	1.0511
C(22)	–1.5070	1.3876	2.3885
H(23)	–0.8384	0.5709	2.6375
H(24)	–1.4176	2.1628	3.1415
H(25)	–2.5256	1.0156	2.3929

Table S3 Calculated coordinates [MP2(full)/6-311+G*] for $Me_2GaOCH_2CH_2NMe_2$.

Atom	*x*	*y*	*z*
C(1)	–1.5511	–0.0374	1.8724
C(2)	–1.7348	–0.9389	–1.4900
C(3)	1.4189	–1.8337	–0.5950
Ga(4)	–0.9184	0.0576	0.0037
O(5)	–0.2770	1.7407	–0.5274
C(6)	1.0969	1.8797	–0.3170
C(7)	1.8055	0.5712	–0.6672
H(8)	–2.6077	0.2448	1.9171
H(9)	–1.4773	–1.0455	2.2931
H(10)	–1.0091	0.6461	2.5314
H(11)	–1.1740	–0.8099	–2.4201
H(12)	–1.8247	–2.0110	–1.2886
H(13)	–2.7466	–0.5643	–1.6757
H(14)	1.0163	–1.8076	–1.6072
H(15)	2.4954	–2.0436	–0.6373
H(16)	0.9236	–2.6340	–0.0412
H(17)	1.4999	2.6720	–0.9623
H(18)	1.3297	2.1710	0.7221
H(19)	2.8860	0.5929	–0.4587
H(20)	1.6581	0.3813	–1.7343
N(21)	1.1632	–0.5461	0.0708
C(22)	1.6658	–0.6084	1.4553
H(23)	1.5002	0.3441	1.9563
H(24)	1.1280	–1.3825	2.0037
H(25)	2.7394	–0.8372	1.4614

Energy = –2290.99283 Hartrees (not corrected for ZPE).