Electronic Supplementary Information for

Mechanistic studies of CO_2 reduction to methanol mediated by an *N*-heterocyclic germylene hydride

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Content

1. Selected NMR spectra

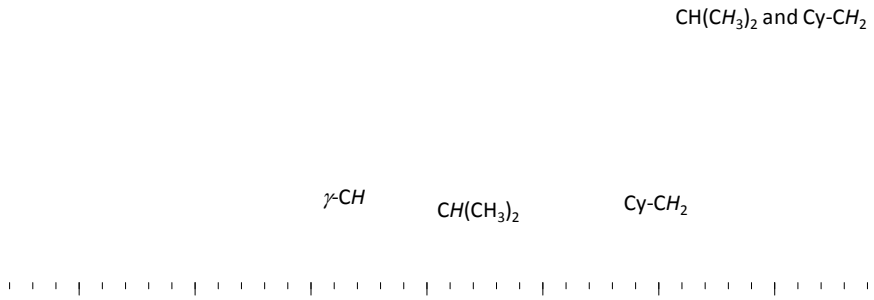

Fig. 1s. ^{1}H NMR spectrum of compound **1** in C_6D_6.

Fig.2s. $^{13}C\{^{1}H\}$ NMR spectrum of compound **1** in C_6D_6.

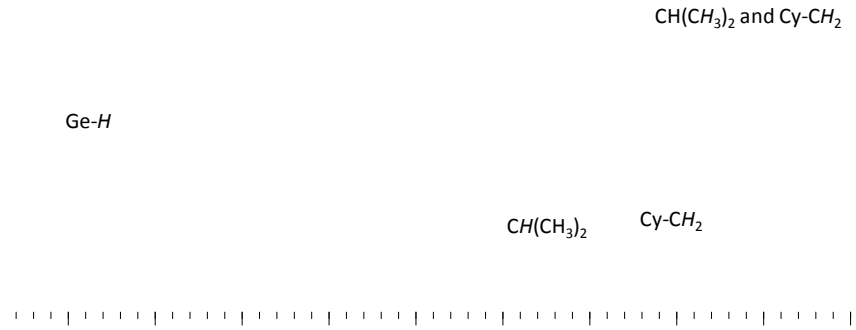

Fig. 3s. ^{1}H NMR spectrum of compound **2** in C_6D_6.

Fig.4s. $^{13}C\{^{1}H\}$ NMR spectrum of compound **2** in C_6D_6.

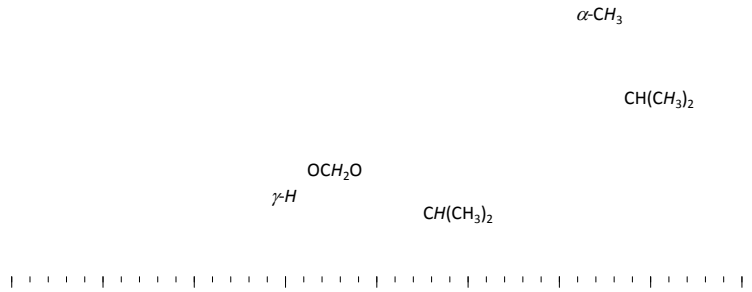

Fig. 5s. ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

Fig.6s. $^{13}C\{^{1}H\}$ NMR spectrum of compound **3** in $CDCl_3$.

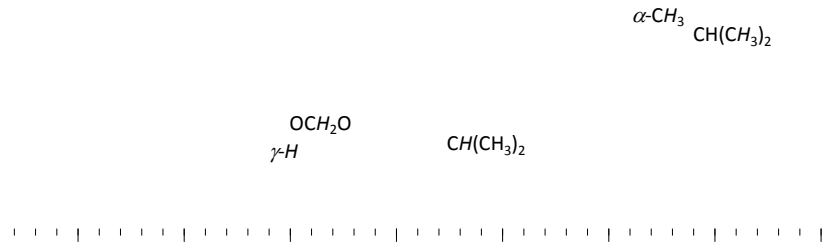

Fig. 7s. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

Fig.8s. $^{13}C\{^{1}H\}$ NMR spectrum of compound **4** in $CDCl_3$.

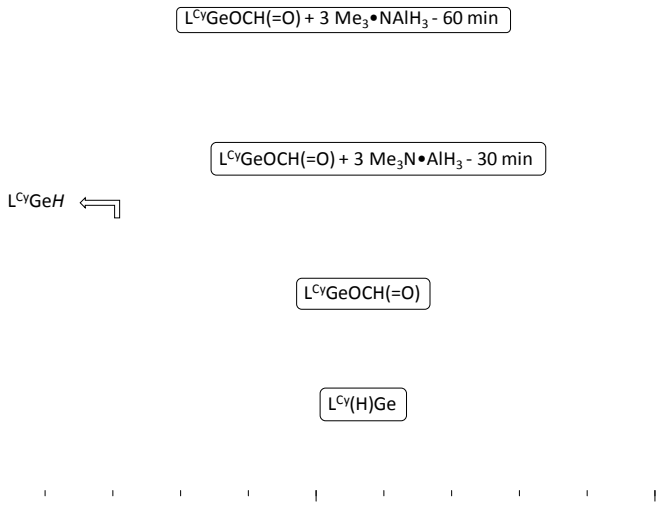

Fig. 9s. ^{1}H NMR investigation of the reaction of $L^{Cy}GeOCH(=O)$ with 3 eq. $Me_3N•AlH_3$ in C_6D_6.

2. Crystal data and refinement for complexes 1-4.

Table 1s. Crystal Data and Structure Refinement for **1-4** [a]

	1	**2**	**3**	**4**
formula	$C_{37}H_{48}GeN_2$	$C_{38}H_{48}GeN_2O_2$	$C_{59}H_{84}AlGeN_4O_2$	$C_{60}H_{86}Al_2N_4O_4$
formula weight	593.36	637.37	980.87	981.29
crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
space group	*P*1	*P*2(1)/*c*	*C*2/*c*	*C*2/*c*
a/Å	9.0288(5)	11.8770(11)	24.8625(3)	24.8530(10)
b/Å	9.0787(4)	18.4080(17)	15.1844(2)	15.1491(6)
c/Å	11.5349(6)	16.0265(15)	14.7693(2)	14.8791(6)
α/deg	71.459(4)			
β/deg	80.307(4)	105.434(9)	94.2710(10)	93.999(4)
γ/deg	65.603(5)			
V/Å^3	815.64(7)	3377.5(5)	5560.25(12)	5588.4(4)
Z	1	4	4	4
ρ_{calcd}/g·cm^{-3}	1.208	1.253	1.172	1.166
μ/mm^{-1}	0.965	0.942	1.228	0.844
F(000)	316	1352	2108	2128
crystal size/mm^3	0.20 x 0.19 x 0.06	0.35 x 0.22 x 0.10	0.12 x 0.08 x 0.08	0.17 x 0.14 x 0.08
θ range/deg	3.56-24.99	3.44-25.00	3.41-73.62	3.42-67.50
index ranges	-10<=h<=10 -10<=k<=7 -13<=l<=11	-14<=h<=13 -21<=k<=21 -14<=l<=19	-30<=h<=28 -11<=k<=18 -18<=l<=18	-29<=h<=24 -18<=k<=17 -14<=l<=17
collected data	6052	14941	10763	17256
unique data	3868 (R_{int} = 0.0137)	5913 (R_{int} = 0.0383)	5448 (R_{int} = 0.0138)	5037 (R_{int} = 0.0509)
completeness to *θ*	99.7 %	99.8%	97.1 %	100.0 %
data/restraints/parameters	3868 / 3 / 369	5913 / 73 / 414	5448 / 1 / 340	5037 / 0 / 327
GOF on F^2	1.049	1.030	1.022	1.052
final *R* indices [$I>2\sigma(I)$]	R_1 = 0.0224 wR_2 = 0.0582	R_1 = 0.0418 wR_2 = 0.0909	R_1 = 0.0437 wR_2 = 0.1225	R_1 = 0.0529 wR_2 = 0.1409
R indices (all data)	R_1 = 0.0224 wR_2 = 0.0583	R_1 = 0.0570 wR_2 = 0.0969	R_1 = 0.0474 wR_2 = 0.1291	R_1 = 0.0582 wR_2 = 0.1485
Largest diff peak/hole (e·Å^{-3})	0.306/-0.179	0.633/-0.307	0.469/-0.405	0.619/-0.316

[a] All data were collected at 150(2) K. $R_1 = \sum(||F_o| - |F_c||)/\sum|F_o|$, $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2/\sum[w(F_o^2)^2]\}^{2}\}^{1/2}$, GOF = $\{\sum[w(F_o^2 - F_c^2)^2]/(N_o - N_p)\}^{1/2}$.

Table 2s. Bond lengths (Å) and angles (°) in compound **1**.

Ge(1)-N(1)	1.8250(19)
Ge(1)-N(2)	1.867(2)
N(1)-C(26)	1.445(3)
N(1)-C(19)	1.482(3)
N(2)-C(13)	1.419(3)
N(2)-C(1)	1.456(3)
C(19)-C(14)	1.513(3)

C(19)-C(20)	1.534(3)
C(14)-C(13)	1.346(3)
C(14)-C(15)	1.521(3)
C(13)-C(18)	1.510(3)
C(18)-C(17)	1.525(4)
C(2)-C(3)	1.392(4)
C(2)-C(1)	1.404(3)
C(2)-C(10)	1.530(3)
C(20)-C(21)	1.385(3)
C(20)-C(25)	1.394(3)
C(27)-C(28)	1.397(4)
C(27)-C(26)	1.402(4)
C(27)-C(35)	1.525(4)
C(17)-C(16)	1.504(4)
C(31)-C(30)	1.396(4)
C(31)-C(26)	1.416(3)
C(31)-C(32)	1.523(4)
C(30)-C(29)	1.378(4)
C(1)-C(6)	1.406(4)
C(28)-C(29)	1.377(4)
C(15)-C(16)	1.529(4)
C(6)-C(5)	1.402(4)
C(6)-C(7)	1.522(4)
C(32)-C(34)	1.531(4)
C(32)-C(33)	1.535(4)
C(21)-C(22)	1.393(4)
C(10)-C(12)	1.526(4)
C(10)-C(11)	1.527(4)
C(7)-C(8)	1.525(4)
C(7)-C(9)	1.545(4)

C(4)-C(5)	1.381(4)
C(4)-C(3)	1.386(4)
C(22)-C(23)	1.385(4)
C(35)-C(37)	1.530(5)
C(35)-C(36)	1.533(4)
C(25)-C(24)	1.400(4)
C(24)-C(23)	1.375(5)
N(1)-Ge(1)-N(2)	95.89(9)
C(26)-N(1)-C(19)	114.16(18)
C(26)-N(1)-Ge(1)	118.37(16)
C(19)-N(1)-Ge(1)	127.42(15)
C(13)-N(2)-C(1)	119.9(2)
C(13)-N(2)-Ge(1)	125.49(16)
C(1)-N(2)-Ge(1)	112.21(15)
N(1)-C(19)-C(14)	113.99(19)
N(1)-C(19)-C(20)	110.46(19)
C(14)-C(19)-C(20)	112.7(2)
C(13)-C(14)-C(19)	125.8(2)
C(13)-C(14)-C(15)	121.7(2)
C(19)-C(14)-C(15)	112.5(2)
C(14)-C(13)-N(2)	123.0(2)
C(14)-C(13)-C(18)	121.7(2)
N(2)-C(13)-C(18)	115.2(2)
C(13)-C(18)-C(17)	114.1(2)
C(3)-C(2)-C(1)	118.8(2)
C(3)-C(2)-C(10)	120.5(2)
C(1)-C(2)-C(10)	120.7(2)
C(21)-C(20)-C(25)	119.0(2)
C(21)-C(20)-C(19)	121.7(2)
C(25)-C(20)-C(19)	119.2(2)

C(28)-C(27)-C(26)	118.0(2)
C(28)-C(27)-C(35)	118.0(2)
C(26)-C(27)-C(35)	124.0(2)
C(16)-C(17)-C(18)	109.8(2)
C(30)-C(31)-C(26)	118.1(2)
C(30)-C(31)-C(32)	119.5(2)
C(26)-C(31)-C(32)	122.3(2)
C(29)-C(30)-C(31)	121.3(2)
C(2)-C(1)-C(6)	120.9(2)
C(2)-C(1)-N(2)	119.2(2)
C(6)-C(1)-N(2)	119.8(2)
C(27)-C(26)-C(31)	121.0(2)
C(27)-C(26)-N(1)	121.6(2)
C(31)-C(26)-N(1)	117.4(2)
C(29)-C(28)-C(27)	121.8(3)
C(14)-C(15)-C(16)	113.3(2)
C(5)-C(6)-C(1)	118.4(3)
C(5)-C(6)-C(7)	118.7(2)
C(1)-C(6)-C(7)	122.9(2)
C(31)-C(32)-C(34)	111.9(2)
C(31)-C(32)-C(33)	109.8(2)
C(34)-C(32)-C(33)	110.9(3)
C(20)-C(21)-C(22)	120.7(2)
C(12)-C(10)-C(11)	110.1(2)
C(12)-C(10)-C(2)	111.3(2)
C(11)-C(10)-C(2)	112.8(2)
C(6)-C(7)-C(8)	112.7(2)
C(6)-C(7)-C(9)	111.8(2)
C(8)-C(7)-C(9)	109.2(2)
C(28)-C(29)-C(30)	119.7(3)

C(5)-C(4)-C(3)	120.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 3s. Bond lengths (Å) and angles (°) in compound **2**.

Ge(1)-O(1)	1.957(2)
Ge(1)-N(1)	1.976(2)
Ge(1)-N(2)	1.989(2)
C(2)-N(1)	1.338(3)
C(2)-C(3)	1.411(4)
C(2)-C(1)	1.507(4)
C(3)-C(4)	1.400(4)
C(3)-C(35)	1.527(4)
C(4)-N(2)	1.339(3)
C(4)-C(5)	1.505(4)
C(5)-C(6)	1.388(4)
C(5)-C(10)	1.388(4)
C(6)-C(7)	1.385(4)
C(7)-C(8)	1.385(5)
C(8)-C(9)	1.371(5)
C(9)-C(10)	1.395(4)
C(11)-C(12)	1.402(4)
C(11)-C(16)	1.414(4)
C(11)-N(2)	1.456(3)
C(12)-C(13)	1.393(4)
C(12)-C(20)	1.517(4)
C(13)-C(14)	1.383(4)
C(14)-C(15)	1.373(4)
C(15)-C(16)	1.389(4)
C(16)-C(17)	1.517(4)
C(17)-C(18)	1.522(4)

C(17)-C(19)	1.536(4)
C(20)-C(22)	1.524(5)
C(20)-C(21)	1.537(4)
C(23)-C(24)	1.405(4)
C(23)-C(28)	1.407(4)
C(23)-N(1)	1.459(3)
C(24)-C(25)	1.391(4)
C(24)-C(32)	1.521(4)
C(25)-C(26)	1.369(5)
C(26)-C(27)	1.377(5)
C(27)-C(28)	1.394(4)
C(28)-C(29)	1.518(4)
C(29)-C(31)	1.530(4)
C(29)-C(30)	1.538(4)
C(32)-C(34)	1.522(5)
C(32)-C(33)	1.525(5)
C(35)-C(36A)	1.349(19)
C(35)-C(36)	1.520(15)
C(1)-C(38A)	1.449(7)
C(1)-C(38)	1.499(9)
C(36A)-C(38)	1.51(2)
C(36)-C(38A)	1.844(19)
C(37)-O(2)	1.213(4)
C(37)-O(1)	1.288(4)

O(1)-Ge(1)-N(1)	89.38(8)
O(1)-Ge(1)-N(2)	90.40(8)
N(1)-Ge(1)-N(2)	90.18(8)
N(1)-C(2)-C(3)	123.8(2)
N(1)-C(2)-C(1)	119.0(2)

C(3)-C(2)-C(1)	117.2(3)
C(4)-C(3)-C(2)	123.9(3)
C(4)-C(3)-C(35)	118.4(2)
C(2)-C(3)-C(35)	117.3(2)
N(2)-C(4)-C(3)	125.1(2)
N(2)-C(4)-C(5)	118.6(2)
C(3)-C(4)-C(5)	116.3(2)
C(6)-C(5)-C(10)	118.9(3)
C(6)-C(5)-C(4)	120.8(2)
C(10)-C(5)-C(4)	120.1(3)
C(7)-C(6)-C(5)	120.6(3)
C(6)-C(7)-C(8)	120.1(3)
C(9)-C(8)-C(7)	119.9(3)
C(8)-C(9)-C(10)	120.3(3)
C(5)-C(10)-C(9)	120.2(3)
C(12)-C(11)-C(16)	120.6(2)
C(12)-C(11)-N(2)	119.7(2)
C(16)-C(11)-N(2)	119.4(2)
C(13)-C(12)-C(11)	118.9(3)
C(13)-C(12)-C(20)	117.2(3)
C(11)-C(12)-C(20)	123.9(2)
C(14)-C(13)-C(12)	120.8(3)
C(15)-C(14)-C(13)	119.6(3)
C(14)-C(15)-C(16)	122.2(3)
C(15)-C(16)-C(11)	117.8(3)
C(15)-C(16)-C(17)	118.4(2)
C(11)-C(16)-C(17)	123.7(2)
C(16)-C(17)-C(18)	109.9(2)
C(16)-C(17)-C(19)	112.7(2)
C(18)-C(17)-C(19)	109.8(2)

C(12)-C(20)-C(22)	110.1(2)
C(12)-C(20)-C(21)	111.3(3)
C(22)-C(20)-C(21)	110.1(3)
C(24)-C(23)-C(28)	121.2(3)
C(24)-C(23)-N(1)	118.5(3)
C(28)-C(23)-N(1)	120.2(3)
C(25)-C(24)-C(23)	118.0(3)
C(25)-C(24)-C(32)	120.3(3)
C(23)-C(24)-C(32)	121.6(3)
C(26)-C(25)-C(24)	121.7(3)
C(25)-C(26)-C(27)	119.7(3)
C(26)-C(27)-C(28)	121.8(3)
C(27)-C(28)-C(23)	117.6(3)
C(27)-C(28)-C(29)	118.3(3)
C(23)-C(28)-C(29)	124.1(2)
C(28)-C(29)-C(31)	109.9(3)
C(28)-C(29)-C(30)	111.7(2)
C(31)-C(29)-C(30)	110.0(3)
C(24)-C(32)-C(34)	113.8(3)
C(24)-C(32)-C(33)	111.2(3)
C(34)-C(32)-C(33)	109.6(3)
C(36A)-C(35)-C(36)	14.7(15)
C(36A)-C(35)-C(3)	117.7(9)
C(36)-C(35)-C(3)	114.2(7)
C(38A)-C(1)-C(38)	51.9(5)
C(38A)-C(1)-C(2)	118.3(3)
C(38)-C(1)-C(2)	111.4(4)
C(35)-C(36A)-C(38)	123.3(15)
C(35)-C(36)-C(38A)	88.5(7)
C(1)-C(38)-C(36A)	107.2(9)

C(1)-C(38A)-C(36)	99.7(8)
O(2)-C(37)-O(1)	127.2(3)
C(2)-N(1)-C(23)	120.9(2)
C(2)-N(1)-Ge(1)	125.42(17)
C(23)-N(1)-Ge(1)	113.52(17)
C(4)-N(2)-C(11)	121.1(2)
C(4)-N(2)-Ge(1)	124.62(17)
C(11)-N(2)-Ge(1)	114.30(16)
C(37)-O(1)-Ge(1)	119.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 4s. Bond lengths (Å) and angles (°) in compound **3**.

Al(1)-Ge(1)#1	0.6683(11)
Al(1)-O(1)#1	1.371(5)
Al(1)-O(2A)	1.833(3)
Al(1)-N(1)#1	1.9037(17)
Al(1)-N(2)#1	1.9191(17)
Ge(1)-Al(1)#1	0.6683(11)
Ge(1)-O(2A)#1	1.231(2)
Ge(1)-O(1)	1.826(5)
Ge(1)-N(1)	2.0191(14)
Ge(1)-N(2)	2.0324(14)
Ge(1)-C(50)#1	2.358(3)
N(1)-C(2)	1.331(2)
N(1)-C(6)	1.452(2)
N(1)-Al(1)#1	1.9037(17)
N(2)-C(4)	1.329(2)
N(2)-C(18)	1.4479(19)
N(2)-Al(1)#1	1.9191(17)

C(1)-C(2)	1.512(2)
C(2)-C(3)	1.399(2)
C(3)-C(4)	1.399(2)
C(4)-C(5)	1.511(2)
C(6)-C(11)	1.405(2)
C(6)-C(7)	1.407(2)
C(7)-C(8)	1.390(2)
C(7)-C(15)	1.523(3)
C(8)-C(9)	1.383(3)
C(9)-C(10)	1.380(3)
C(10)-C(11)	1.399(2)
C(11)-C(12)	1.518(2)
C(12)-C(13)	1.524(3)
C(12)-C(14)	1.535(2)
C(15)-C(17)	1.518(3)
C(15)-C(16)	1.525(3)
C(18)-C(19)	1.402(2)
C(18)-C(23)	1.405(2)
C(19)-C(20)	1.398(2)
C(19)-C(27)	1.517(2)
C(20)-C(21)	1.382(3)
C(21)-C(22)	1.379(3)
C(22)-C(23)	1.392(2)
C(23)-C(24)	1.519(3)
C(24)-C(26)	1.512(3)
C(24)-C(25)	1.533(3)
C(27)-C(29)	1.519(3)
C(27)-C(28)	1.526(3)
C(50)-O(2A)	1.391(4)
C(50)-O(1)	1.398(5)

C(50)-Ge(1)#1	2.358(3)
O(1)-Al(1)#1	1.371(5)
O(2A)-Ge(1)#1	1.231(2)

Ge(1)#1-Al(1)-O(1)#1	123.4(2)
Ge(1)#1-Al(1)-O(2A)	20.67(12)
O(1)#1-Al(1)-O(2A)	103.03(18)
Ge(1)#1-Al(1)-N(1)#1	90.14(14)
O(1)#1-Al(1)-N(1)#1	121.9(2)
O(2A)-Al(1)-N(1)#1	105.64(11)
Ge(1)#1-Al(1)-N(2)#1	90.03(14)
O(1)#1-Al(1)-N(2)#1	125.7(2)
O(2A)-Al(1)-N(2)#1	101.60(10)
N(1)#1-Al(1)-N(2)#1	96.11(8)
Al(1)#1-Ge(1)-O(2A)#1	148.29(19)
Al(1)#1-Ge(1)-O(1)	38.77(16)
O(2A)#1-Ge(1)-O(1)	109.80(16)
Al(1)#1-Ge(1)-N(1)	70.53(13)
O(2A)#1-Ge(1)-N(1)	131.22(13)
O(1)-Ge(1)-N(1)	96.62(14)
Al(1)#1-Ge(1)-N(2)	70.78(13)
O(2A)#1-Ge(1)-N(2)	124.22(12)
O(1)-Ge(1)-N(2)	99.05(14)
N(1)-Ge(1)-N(2)	89.14(6)
Al(1)#1-Ge(1)-C(50)#1	132.65(15)
O(2A)#1-Ge(1)-C(50)#1	27.67(14)
O(1)-Ge(1)-C(50)#1	96.78(14)
N(1)-Ge(1)-C(50)#1	111.98(9)
N(2)-Ge(1)-C(50)#1	151.86(9)
C(2)-N(1)-C(6)	118.36(13)

C(2)-N(1)-Al(1)#1	115.98(12)
C(6)-N(1)-Al(1)#1	123.72(11)
C(2)-N(1)-Ge(1)	127.58(11)
C(6)-N(1)-Ge(1)	114.00(10)
Al(1)#1-N(1)-Ge(1)	19.33(4)
C(4)-N(2)-C(18)	118.86(13)
C(4)-N(2)-Al(1)#1	116.35(11)
C(18)-N(2)-Al(1)#1	123.79(10)
C(4)-N(2)-Ge(1)	127.61(11)
C(18)-N(2)-Ge(1)	113.17(9)
Al(1)#1-N(2)-Ge(1)	19.20(4)
N(1)-C(2)-C(3)	123.20(15)
N(1)-C(2)-C(1)	120.35(15)
C(3)-C(2)-C(1)	116.43(15)
C(4)-C(3)-C(2)	127.38(15)
N(2)-C(4)-C(3)	122.85(14)
N(2)-C(4)-C(5)	120.06(14)
C(3)-C(4)-C(5)	117.02(14)
C(11)-C(6)-C(7)	121.45(15)
C(11)-C(6)-N(1)	119.81(14)
C(7)-C(6)-N(1)	118.74(14)
C(8)-C(7)-C(6)	117.88(16)
C(8)-C(7)-C(15)	120.47(16)
C(6)-C(7)-C(15)	121.64(15)
C(9)-C(8)-C(7)	121.66(17)
C(10)-C(9)-C(8)	119.48(16)
C(9)-C(10)-C(11)	121.53(17)
C(10)-C(11)-C(6)	117.74(16)
C(10)-C(11)-C(12)	119.16(15)
C(6)-C(11)-C(12)	123.08(14)

C(11)-C(12)-C(13)	109.99(15)
C(11)-C(12)-C(14)	112.27(16)
C(13)-C(12)-C(14)	109.82(16)
C(17)-C(15)-C(7)	111.84(18)
C(17)-C(15)-C(16)	110.60(17)
C(7)-C(15)-C(16)	112.48(16)
C(19)-C(18)-C(23)	121.67(15)
C(19)-C(18)-N(2)	119.88(14)
C(23)-C(18)-N(2)	118.44(14)
C(20)-C(19)-C(18)	118.08(16)
C(20)-C(19)-C(27)	119.13(16)
C(18)-C(19)-C(27)	122.78(15)
C(21)-C(20)-C(19)	120.94(18)
C(22)-C(21)-C(20)	119.97(17)
C(21)-C(22)-C(23)	121.56(17)
C(22)-C(23)-C(18)	117.75(17)
C(22)-C(23)-C(24)	120.11(16)
C(18)-C(23)-C(24)	122.14(15)
C(26)-C(24)-C(23)	111.89(17)
C(26)-C(24)-C(25)	111.01(17)
C(23)-C(24)-C(25)	111.70(17)
C(19)-C(27)-C(29)	110.27(16)
C(19)-C(27)-C(28)	112.32(16)
C(29)-C(27)-C(28)	109.31(19)
O(2A)-C(50)-O(1)	113.1(3)
O(2A)-C(50)-Ge(1)#1	24.27(12)
O(1)-C(50)-Ge(1)#1	124.5(3)
Al(1)#1-O(1)-C(50)	131.6(4)
Al(1)#1-O(1)-Ge(1)	17.78(9)
C(50)-O(1)-Ge(1)	116.1(3)

Ge(1)#1-O(2A)-C(50)	128.1(2)
Ge(1)#1-O(2A)-Al(1)	11.05(7)
C(50)-O(2A)-Al(1)	123.9(2)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+1/2,-z+2

Table 5s. Bond lengths (Å) and angles (°) in compound **4**.

Al(1)-O(1)	1.7123(11)
Al(1)-O(2)	1.7239(11)
Al(1)-N(2)	1.8963(13)
Al(1)-N(1)	1.8979(13)
N(1)-C(2)	1.340(2)
N(1)-C(6)	1.4507(19)
N(2)-C(4)	1.337(2)
N(2)-C(18)	1.451(2)
O(1)-C(30)#1	1.397(2)
O(2)-C(30)	1.3981(19)
C(1)-C(2)	1.511(2)
C(2)-C(3)	1.400(2)
C(3)-C(4)	1.397(2)
C(4)-C(5)	1.513(2)
C(6)-C(11)	1.399(2)
C(6)-C(7)	1.408(2)
C(7)-C(8)	1.400(2)
C(7)-C(15)	1.515(3)
C(8)-C(9)	1.379(3)
C(9)-C(10)	1.377(3)
C(10)-C(11)	1.398(2)
C(11)-C(12)	1.522(2)
C(12)-C(13)	1.534(3)
C(12)-C(14)	1.538(3)

C(15)-C(17)	1.513(3)
C(15)-C(16)	1.539(3)
C(18)-C(23)	1.403(2)
C(18)-C(19)	1.408(2)
C(19)-C(20)	1.393(3)
C(19)-C(27)	1.522(2)
C(20)-C(21)	1.382(3)
C(21)-C(22)	1.379(3)
C(22)-C(23)	1.400(2)
C(23)-C(24)	1.520(2)
C(24)-C(25)	1.526(3)
C(24)-C(26)	1.534(2)
C(27)-C(28)	1.522(3)
C(27)-C(29)	1.531(3)
C(30)-O(1)#1	1.397(2)

O(1)-Al(1)-O(2)	114.22(6)
O(1)-Al(1)-N(2)	114.11(6)
O(2)-Al(1)-N(2)	107.98(6)
O(1)-Al(1)-N(1)	108.58(6)
O(2)-Al(1)-N(1)	113.27(6)
N(2)-Al(1)-N(1)	97.59(6)
C(2)-N(1)-C(6)	117.96(13)
C(2)-N(1)-Al(1)	121.03(11)
C(6)-N(1)-Al(1)	121.01(10)
C(4)-N(2)-C(18)	118.01(13)
C(4)-N(2)-Al(1)	120.87(11)
C(18)-N(2)-Al(1)	121.03(10)
C(30)#1-O(1)-Al(1)	124.12(10)
C(30)-O(2)-Al(1)	124.14(10)

N(1)-C(2)-C(3)	122.88(14)
N(1)-C(2)-C(1)	120.35(14)
C(3)-C(2)-C(1)	116.67(14)
C(4)-C(3)-C(2)	127.82(14)
N(2)-C(4)-C(3)	122.98(14)
N(2)-C(4)-C(5)	120.29(15)
C(3)-C(4)-C(5)	116.71(14)
C(11)-C(6)-C(7)	121.59(15)
C(11)-C(6)-N(1)	120.30(14)
C(7)-C(6)-N(1)	118.11(14)
C(8)-C(7)-C(6)	117.58(16)
C(8)-C(7)-C(15)	119.53(15)
C(6)-C(7)-C(15)	122.89(15)
C(9)-C(8)-C(7)	121.35(16)
C(10)-C(9)-C(8)	120.20(16)
C(9)-C(10)-C(11)	120.97(17)
C(10)-C(11)-C(6)	118.28(16)
C(10)-C(11)-C(12)	118.81(16)
C(6)-C(11)-C(12)	122.91(14)
C(11)-C(12)-C(13)	109.99(14)
C(11)-C(12)-C(14)	112.08(15)
C(13)-C(12)-C(14)	109.37(15)
C(17)-C(15)-C(7)	112.18(17)
C(17)-C(15)-C(16)	110.68(16)
C(7)-C(15)-C(16)	111.46(16)
C(23)-C(18)-C(19)	121.34(15)
C(23)-C(18)-N(2)	120.09(14)
C(19)-C(18)-N(2)	118.56(14)
C(20)-C(19)-C(18)	118.00(16)
C(20)-C(19)-C(27)	120.01(16)

C(18)-C(19)-C(27)	121.98(15)
C(21)-C(20)-C(19)	121.40(17)
C(22)-C(21)-C(20)	119.76(16)
C(21)-C(22)-C(23)	121.39(16)
C(22)-C(23)-C(18)	117.91(15)
C(22)-C(23)-C(24)	118.81(15)
C(18)-C(23)-C(24)	123.26(14)
C(23)-C(24)-C(25)	110.18(14)
C(23)-C(24)-C(26)	112.04(15)
C(25)-C(24)-C(26)	109.78(16)
C(19)-C(27)-C(28)	111.95(17)
C(19)-C(27)-C(29)	112.65(16)
C(28)-C(27)-C(29)	110.19(16)
O(1)#1-C(30)-O(2)	113.16(13)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+1/2,-z+1

3. Reference

Complete author list for ref. 1. in the main text: H. Arakawa, M. Aresta, J. N. Armor, M. A. Barteau, E. J. Beckman, A. T. Bell, J. E. Bercaw, C. Creutz, E. Dinjus, D. A. Dixon, K. Domen, D. L. DuBois, J. Eckert, E. Fujita, D. H. Gibson, W. A. Goddard, D. W. Goodman, J. Keller, G. J. Kubas, H. H. Kung, J. E. Lyons, L. E. Manzer, T. J. Marks, K. Morokuma, K. M. Nicholas, R. Periana, L. Que, J. Rostrup-Nielson, W. M. H. Sachtler, L. D. Schmidt, A. Sen, G. A. Somorjai, P. C. Stair, B. R. Stults and W. Tumas, *Chem. Rev.*, 2001, **101**, 953.