Supporting Information

Reactivity of N-Heterocyclic Germylene Toward Ammonia and Water

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Single-Crystal X-ray Structure Determinations: Crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data of compounds **1**, **2**, **3**, **4,** and **8** were collected on an Oxford Diffraction Xcalibur S Sapphire at 150 K (Mo-K_α radiation, λ = 0.71073 Å). The structures were solved by direct methods and refined on F^2 with the SHELX-97[1] software package. The positions of the H atoms were calculated and considered isotropically according to a riding model.

Crystallographic data for compound 8:

Empirical formula	C37 H48 N2	
Formula weight	520.77	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.8485(5) Å	α= 65.748(4)°.
	b = 12.7284(7) Å	β= 86.290(3)°.
	c = 13.2348(4) Å	γ = 71.699(5)°.
Volume	1577.59(12) $Å^3$	
Z	2	
Density (calculated)	1.096 Mg/m^3	
Absorption coefficient	0.063 mm^{-1}	
F(000)	568	
Crystal size	0.29 x 0.22 x 0.18 mm^3	
Theta range for data collection	2.98 to 25.00°.	
Index ranges	-11<=h<=12, -15<=k<=15, -15<=l<=15	
Reflections collected	13428	
Independent reflections	5541 [R(int) = 0.0203]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	None	
Max. and min. transmission	0.9888 and 0.9820	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5541 / 0 / 364	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0439, wR2 = 0.0900	
R indices (all data)	R1 = 0.0633, wR2 = 0.0963	
Largest diff. peak and hole	0.188 and -0.193 $e.Å^{-3}$	

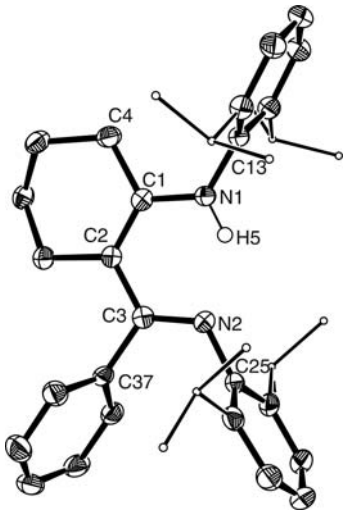

Figure 1. Molecular structure of compound **8.** Thermal ellipsoids are drawn at 50% probability level. Hydrogen atoms are omitted for clarity.

Table 1. Selected interatomic distances and angles of compound **8**

Interatomic distances (Å)		Angles(°)	
N(1)-C(1)	1.3600(17)	C(1)-N(1)-C(13)	123.90(11)
N(1)-C(13)	1.4349(18)	N(1)-C(1)-C(2)	122.21(12)
C(1)-C(2)	1.3769(19)	N(1)-C(1)-C(4)	115.66(12)
C(1)-C(4)	1.5136(18)	C(2)-C(1)-C(4)	122.12(12)
N(2)-C(3)	1.3046(16)	C(3)-N(2)-C(25)	121.10(11)
N(2)-C(25)	1.4297(17)	C(1)-C(2)-C(3)	122.30(12)
C(2)-C(3)	1.4515(18)	C(1)-C(2)-C(7)	120.38(12)
C(3)-C(37)	1.5079(19)	C(3)-C(2)-C(7)	117.25(12)
		N(2)-C(3)-C(2)	122.12(12)
		N(2)-C(3)-C(37)	120.59(12)
		C(2)-C(3)-C(37)	117.29(11)
		C(1)-C(4)-C(5)	114.14(12)

Crystallographic data for compound 1:

Empirical formula	C37 H46 Cl Ge N2	
Formula weight	626.80	
Temperature	150(2) K	
Wavelength	0.7107 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 11.7621(2) Å	α= 90°.
	b = 17.5495(4) Å	β= 107.053(2)°.
	c = 16.6051(3) Å	γ = 90°.
Volume	3276.91(11) Å^3	

Z	4
Density (calculated)	1.270 Mg/m^3
Absorption coefficient	1.044 mm^{-1}
F(000)	1324
Crystal size	0.40 x 0.32 x 0.22 mm^3
Theta range for data collection	3.42 to 25.00°.
Index ranges	-13<=h<=13, -19<=k<=20, -19<=l<=18
Reflections collected	16923
Independent reflections	5742 [R(int) = 0.0250]
Completeness to theta = 25.00°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.82078
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5742 / 0 / 378
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0328, wR2 = 0.0709
R indices (all data)	R1 = 0.0496, wR2 = 0.0742
Largest diff. peak and hole	0.736 and -0.362 $e.Å^{-3}$

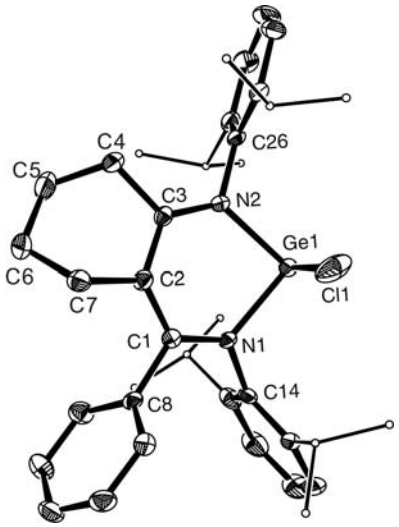

Figure 2. Molecular structure of compound **1.** Thermal ellipsoids are drawn at 50% probability level. Hydrogen atoms are omitted for clarity.

Table 2. Selected interatomic distances and angles of compound **1**

Interatomic distances (Å)		Angles(°)	
Ge(1)-N(1)	1.9760(16)	N(1)-Ge(1)-N(2)	91.23(7)
Ge(1)-N(2)	1.9804(17)	N(1)-Ge(1)-Cl(1)	95.60(5)
Ge(1)-Cl(1)	2.2956(7)	N(2)-Ge(1)-Cl(1)	93.92(5)
N(1)-C(1)	1.342(3)	C(1)-N(1)-C(14)	122.33(16)
N(1)-C(14)	1.458(3)	C(1)-N(1)-Ge(1)	125.68(13)

C(1)-C(2)	1.397(3)	C(14)-N(1)-Ge(1)	111.93(12)
C(1)-C(8)	1.502(3)	N(1)-C(1)-C(2)	123.52(17)
N(2)-C(3)	1.333(3)	N(1)-C(1)-C(8)	119.57(17)
N(2)-C(26)	1.463(2)	C(2)-C(1)-C(8)	116.82(18)
C(2)-C(3)	1.415(3)	C(3)-N(2)-C(26)	120.27(17)
C(2)-C(7)	1.522(3)	C(3)-N(2)-Ge(1)	125.15(13)
C(3)-C(4)	1.509(3)	C(26)-N(2)-Ge(1)	114.45(13)
C(4)-C(5)	1.522(3)	C(1)-C(2)-C(3)	125.03(19)
		C(1)-C(2)-C(7)	121.18(17)
		C(3)-C(2)-C(7)	113.53(17)
		N(2)-C(3)-C(2)	124.40(18)
		N(2)-C(3)-C(4)	120.70(17)
		C(2)-C(3)-C(4)	114.82(18)
		C(3)-C(4)-C(5)	110.84(18)
		C(4)-C(5)-C(6)	111.6(2)

Crystallographic data for compound 2:

Empirical formula	C37 H46 Ge N2	
Formula weight	591.35	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.8388(6) Å	α= 66.971(4)°.
	b = 12.7885(7) Å	β= 85.749(3)°.
	c = 13.2778(4) Å	γ = 71.833(5)°.
Volume	1606.95(13) $Å^3$	
Z	2	
Density (calculated)	1.222 Mg/m^3	
Absorption coefficient	0.980 mm^{-1}	
F(000)	628	
Crystal size	0.29 x 0.15 x 0.07 mm^3	
Theta range for data collection	3.07 to 25.00°.	
Index ranges	-12<=h<=12, -15<=k<=15, -15<=l<=15	
Reflections collected	13501	
Independent reflections	5636 [R(int) = 0.0366]	
Completeness to theta = 25.00°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.92510	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5636 / 0 / 369
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0489, wR2 = 0.1180
R indices (all data)	R1 = 0.0691, wR2 = 0.1242
Largest diff. peak and hole	0.539 and -0.501 e.Å^{-3}

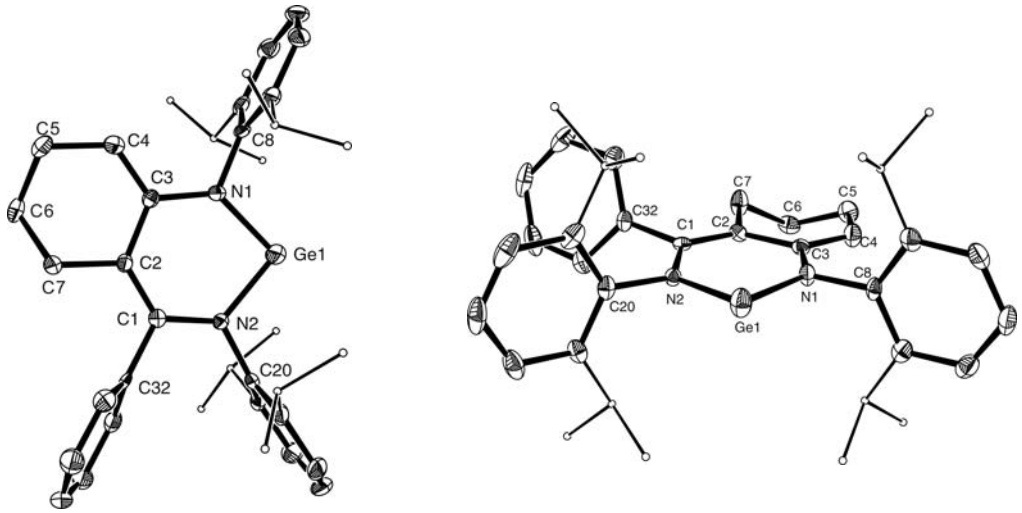

Figure 3. Molecular structure of compound **2.** Thermal ellipsoids are drawn at 50% probability level. Hydrogen atoms are omitted for clarity.

Table 3. Selected interatomic distances and angles of compound **2**

Interatomic distances (Å)		Angles(°)	
Ge(1)-N(1)	1.843(3)	N(1)-Ge(1)-N(2)	95.09(11)
Ge(1)-N(2)	1.861(3)	C(3)-N(1)-C(8)	117.6(2)
N(1)-C(3)	1.426(4)	C(3)-N(1)-Ge(1)	130.0(2)
N(1)-C(8)	1.442(4)	C(8)-N(1)-Ge(1)	112.32(19)
C(1)-C(2)	1.359(4)	C(2)-C(1)-N(2)	124.1(3)
C(1)-N(2)	1.408(4)	C(2)-C(1)-C(32)	120.0(3)
C(1)-C(32)	1.498(4)	N(2)-C(1)-C(32)	115.9(3)
N(2)-C(20)	1.454(4)	C(1)-N(2)-C(20)	121.4(2)
C(2)-C(3)	1.461(4)	C(1)-N(2)-Ge(1)	125.9(2)
C(2)-C(7)	1.525(4)	C(20)-N(2)-Ge(1)	112.00(18)
C(3)-C(4)	1.360(4)	C(1)-C(2)-C(3)	126.7(3)
C(4)-C(5)	1.501(4)	C(1)-C(2)-C(7)	119.3(3)
C(5)-C(6)	1.504(5)	C(3)-C(2)-C(7)	114.0(3)
		C(4)-C(3)-N(1)	119.6(3)
		C(4)-C(3)-C(2)	122.8(3)
		N(1)-C(3)-C(2)	117.6(3)

	C(3)-C(4)-C(5)	122.8(3)
	C(4)-C(5)-C(6)	110.8(3)

Crystallographic data for compound 3:

Empirical formula	C37 H49 Ge N3	
Formula weight	608.38	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 11.7714(4) Å	α= 90°.
	b = 17.4309(6) Å	β= 106.866(4)°.
	c = 16.6868(6) Å	γ = 90°.
Volume	3276.6(2) $Å^3$	
Z	4	
Density (calculated)	1.233 Mg/m^3	
Absorption coefficient	0.964 mm^{-1}	
F(000)	1296	
Crystal size	0.30 x 0.23 x 0.19 mm^3	
Theta range for data collection	3.42 to 25.00°.	
Index ranges	-8<=h<=13, -10<=k<=20, -19<=l<=16	
Reflections collected	12816	
Independent reflections	5749 [R(int) = 0.0325]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.95425	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5749 / 0 / 378	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0464, wR2 = 0.1084	
R indices (all data)	R1 = 0.0699, wR2 = 0.1133	
Largest diff. peak and hole	1.717 and -0.738 $e.Å^{-3}$	

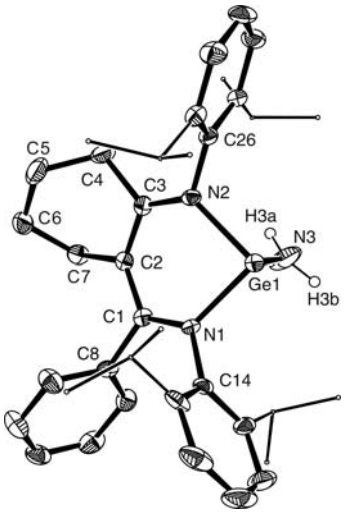

Figure 3. Molecular structure of compound **3.** Thermal ellipsoids are drawn at 50% probability level. Hydrogen atoms are omitted for clarity.

Table 3. Selected interatomic distances and angles of compound **3**

Interatomic distances (Å)		Angles(°)	
Ge(1)-N(3)	1.829(3)	N(3)-Ge(1)-N(2)	95.03(11)
Ge(1)-N(2)	2.017(2)	N(3)-Ge(1)-N(1)	97.09(13)
Ge(1)-N(1)	2.021(2)	N(2)-Ge(1)-N(1)	89.32(10)
N(1)-C(1)	1.349(4)	C(1)-N(1)-C(14)	121.9(2)
N(1)-C(14)	1.448(4)	C(1)-N(1)-Ge(1)	125.3(2)
C(1)-C(2)	1.395(4)	C(14)-N(1)-Ge(1)	112.86(17)
C(1)-C(8)	1.499(4)	N(1)-C(1)-C(2)	123.3(3)
N(2)-C(3)	1.336(4)	N(1)-C(1)-C(8)	119.1(3)
N(2)-C(26)	1.452(4)	C(2)-C(1)-C(8)	117.5(2)
C(2)-C(3)	1.417(4)	C(3)-N(2)-C(26)	120.2(2)
C(2)-C(7)	1.521(4)	C(3)-N(2)-Ge(1)	124.7(2)
C(3)-C(4)	1.509(4)	C(26)-N(2)-Ge(1)	114.49(18)
C(4)-C(5)	1.535(5)	C(1)-C(2)-C(3)	125.3(3)
		C(1)-C(2)-C(7)	121.1(3)
		C(3)-C(2)-C(7)	113.4(3)
		N(2)-C(3)-C(2)	124.6(3)
		N(2)-C(3)-C(4)	120.6(3)
		C(2)-C(3)-C(4)	114.7(3)
		C(3)-C(4)-C(5)	111.0(3)
		C(6)-C(5)-C(4)	111.9(3)

Crystallographic data for compound 4:

Empirical formula	C37 H48 Ge N2 O

Formula weight	609.36	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 11.7560(3) Å	α= 90°.
	b = 17.4116(5) Å	β= 106.992(3)°.
	c = 16.6421(4) Å	γ = 90°.
Volume	3257.78(15) $Å^3$	
Z	4	
Density (calculated)	1.242 Mg/m^3	
Absorption coefficient	0.971 mm^{-1}	
F(000)	1296	
Crystal size	0.31 x 0.14 x 0.05 mm^3	
Theta range for data collection	3.43 to 25.00°.	
Index ranges	-13<=h<=13, -20<=k<=20, -19<=l<=19	
Reflections collected	23624	
Independent reflections	5720 [R(int) = 0.0371]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.83390	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5720 / 0 / 379	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0336, wR2 = 0.0752	
R indices (all data)	R1 = 0.0516, wR2 = 0.0789	
Largest diff. peak and hole	0.521 and -0.366 $e.Å^{-3}$	

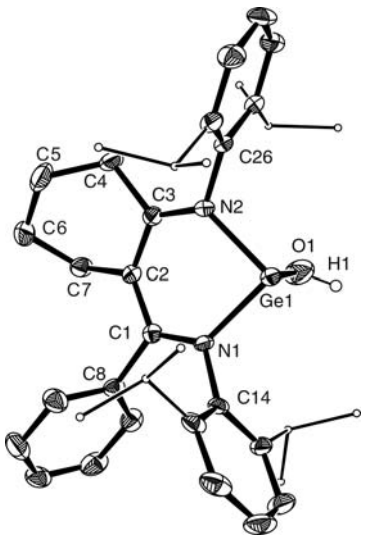

Figure 3. Molecular structure of compound **4.** Thermal ellipsoids are drawn at 50% probability level. Hydrogen atoms are omitted for clarity.

Table 3. Selected interatomic distances and angles of compound **4**

Interatomic distances (Å)		Angles(°)	
Ge(1)-O(1)	1.8249(18)	O(1)-Ge(1)-N(2)	93.87(8)
Ge(1)-N(2)	2.0054(17)	O(1)-Ge(1)-N(1)	95.29(8)
Ge(1)-N(1)	2.0071(16)	N(2)-Ge(1)-N(1)	89.43(7)
N(1)-C(1)	1.340(3)	C(1)-N(1)-C(14)	121.78(17)
N(1)-C(14)	1.452(3)	C(1)-N(1)-Ge(1)	125.97(14)
C(1)-C(2)	1.402(3)	C(14)-N(1)-Ge(1)	112.24(12)
C(1)-C(8)	1.503(3)	N(1)-C(1)-C(2)	123.35(18)
N(2)-C(3)	1.331(3)	N(1)-C(1)-C(8)	119.70(18)
N(2)-C(26)	1.457(3)	C(2)-C(1)-C(8)	116.90(17)
C(2)-C(3)	1.419(3)	C(3)-N(2)-C(26)	120.24(17)
C(2)-C(7)	1.519(3)	C(3)-N(2)-Ge(1)	125.15(14)
C(3)-C(4)	1.509(3)	C(26)-N(2)-Ge(1)	114.02(12)
		C(1)-C(2)-C(3)	124.72(18)
		C(1)-C(2)-C(7)	121.30(18)
		C(3)-C(2)-C(7)	113.81(18)
		N(2)-C(3)-C(2)	124.61(19)
		N(2)-C(3)-C(4)	120.81(18)
		C(2)-C(3)-C(4)	114.55(18)
		C(3)-C(4)-C(5)	111.40(19)

Reference

1. Sheldrick, G. M. *SHELX-97 Program for Crystal Structure Determination*, Universität Göttingen (Germany) **1997**.