Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Heavier carbene analogues and their derivatives as κ-*El*, κ^2-*El, N*, and κ^2-*N, N'* ligands: Different reactivity patterns for acyclic and cyclic diamidogermylenes and -stannylenes

Joseph K. West,[a] *Gregory L. Fondong,*[a] *Bruce C. Noll,*[b] *and Lothar Stahl*[a]

Department of Chemistry, University of North Dakota, Grand Forks, ND 58201 USA

[b]*Bruker, AXS Inc., Madison, WI 53711 USA*

Table 1. Crystal data and structure refinement for **E**.

Identification code	joe52_0m	
Empirical formula	$C_{24}H_{72}Cu_4N_4Si_8$	
Formula weight	223.93	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2/n	
Unit cell dimensions	a = 9.2974(2) Å	α = 90°.
	b = 13.4245(3) Å	β = 90.4290(10)°.
	c = 17.7591(4) Å	γ = 90°.
Volume	2216.50(8) $Å^3$	
Z	2	
Density (calculated)	1.342 Mg/m^3	
Absorption coefficient	2.129 mm^{-1}	
F(000)	944	
Crystal size	0.19 x 0.19 x 0.56 mm^3	
Theta range for data collection	1.52 to 40.25°.	
Index ranges	-15 <= h <= 16, -24 <= k <= 24, -32<= l <= 28	
Reflections collected	49521	
Independent reflections	13684 [R(int) = 0.0226]	
Completeness to theta = 40.25°	98.0 %	
Absorption correction	SADABS	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13684 / 0 / 194	
Goodness-of-fit on F^2	1.000	
Final R indices [I>2sigma(I)]	R1 = 0.0253, wR2 = 0.0645	
R indices (all data)	R1 = 0.0454, wR2 = 0.0742	
Largest diff. peak and hole	0.551 and -0.483 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **E**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	2053(1)	3509(1)	3218(1)	17(1)
Cu(2)	2058(1)	1514(1)	3220(1)	17(1)
Si(1)	4051(1)	5206(1)	2763(1)	20(1)
Si(2)	3983(1)	-183(1)	2848(1)	27(1)
Si(3)	2797(1)	2597(1)	4729(1)	24(1)
Si(4)	-252(1)	2444(1)	4139(1)	21(1)
N(1)	2500	4535(1)	2500	18(1)
N(2)	2500	493(1)	2500	19(1)
N(3)	1606(1)	2510(1)	3958(1)	17(1)
C(1)	5031(1)	5693(1)	1919(1)	34(1)
C(2)	3621(1)	6288(1)	3389(1)	32(1)
C(3)	5336(1)	4416(1)	3311(1)	29(1)
C(4)	3625(2)	-658(1)	3822(1)	44(1)
C(5)	4452(2)	-1266(1)	2231(1)	50(1)
C(6)	5637(1)	599(1)	2888(1)	42(1)
C(7)	4660(1)	2211(1)	4475(1)	35(1)
C(8)	2862(1)	3906(1)	5099(1)	39(1)
C(9)	2270(2)	1763(1)	5528(1)	45(1)
C(10)	-1312(1)	2796(1)	3289(1)	32(1)
C(11)	-808(1)	1154(1)	4419(1)	38(1)
C(12)	-831(2)	3320(1)	4896(1)	47(1)

Table 3. Bond lengths [Å] and angles [°] for **E**.

Cu(1)-N(1)	1.9243(6)
Cu(1)-N(3)	1.9249(7)
Cu(1)-Cu(2)	2.67889(15)
Cu(1)-Cu(1)#1	2.6891(2)
Cu(2)-N(3)	1.9200(7)
Cu(2)-N(2)	1.9211(7)
Cu(2)-Cu(2)#1	2.6930(2)
Si(1)-N(1)	1.7601(5)
Si(1)-C(3)	1.8661(10)
Si(1)-C(2)	1.8748(10)
Si(1)-C(1)	1.8768(10)
Si(2)-N(2)	1.7590(5)
Si(2)-C(6)	1.8625(13)
Si(2)-C(5)	1.8749(12)
Si(2)-C(4)	1.8759(12)
Si(3)-N(3)	1.7586(8)
Si(3)-C(7)	1.8664(12)
Si(3)-C(9)	1.8752(12)
Si(3)-C(8)	1.8770(12)
Si(4)-N(3)	1.7620(8)
Si(4)-C(10)	1.8584(11)
Si(4)-C(12)	1.8682(11)
Si(4)-C(11)	1.8749(11)
N(1)-Si(1)#1	1.7601(5)
N(1)-Cu(1)#1	1.9243(6)
N(2)-Si(2)#1	1.7590(5)
N(2)-Cu(2)#1	1.9211(7)
N(1)-Cu(1)-N(3)	178.48(3)
N(1)-Cu(1)-Cu(2)	135.720(19)
N(3)-Cu(1)-Cu(2)	45.76(2)
N(1)-Cu(1)-Cu(1)#1	45.677(19)
N(3)-Cu(1)-Cu(1)#1	135.80(2)
Cu(2)-Cu(1)-Cu(1)#1	90.042(3)

N(3)-Cu(2)-N(2)	178.63(3)
N(3)-Cu(2)-Cu(1)	45.91(2)
N(2)-Cu(2)-Cu(1)	135.46(2)
N(3)-Cu(2)-Cu(2)#1	135.87(2)
N(2)-Cu(2)-Cu(2)#1	45.500(19)
Cu(1)-Cu(2)-Cu(2)#1	89.957(3)
N(1)-Si(1)-C(3)	111.57(4)
N(1)-Si(1)-C(2)	112.07(4)
C(3)-Si(1)-C(2)	105.62(5)
N(1)-Si(1)-C(1)	111.61(4)
C(3)-Si(1)-C(1)	107.57(5)
C(2)-Si(1)-C(1)	108.09(5)
N(2)-Si(2)-C(6)	111.53(5)
N(2)-Si(2)-C(5)	112.34(6)
C(6)-Si(2)-C(5)	105.27(7)
N(2)-Si(2)-C(4)	110.85(4)
C(6)-Si(2)-C(4)	107.99(6)
C(5)-Si(2)-C(4)	108.60(6)
N(3)-Si(3)-C(7)	111.93(5)
N(3)-Si(3)-C(9)	112.57(5)
C(7)-Si(3)-C(9)	105.37(6)
N(3)-Si(3)-C(8)	110.69(5)
C(7)-Si(3)-C(8)	108.43(6)
C(9)-Si(3)-C(8)	107.57(6)
N(3)-Si(4)-C(10)	110.66(4)
N(3)-Si(4)-C(12)	112.88(5)
C(10)-Si(4)-C(12)	105.69(6)
N(3)-Si(4)-C(11)	111.57(5)
C(10)-Si(4)-C(11)	107.73(5)
C(12)-Si(4)-C(11)	108.01(6)
Si(1)-N(1)-Si(1)#1	118.44(5)
Si(1)-N(1)-Cu(1)	111.783(13)
Si(1)#1-N(1)-Cu(1)	111.172(13)
Si(1)-N(1)-Cu(1)#1	111.172(13)
Si(1)#1-N(1)-Cu(1)#1	111.783(13)
Cu(1)-N(1)-Cu(1)#1	88.65(4)

Si(2)-N(2)-Si(2)#1	117.87(5)
Si(2)-N(2)-Cu(2)	107.753(14)
Si(2)#1-N(2)-Cu(2)	115.541(13)
Si(2)-N(2)-Cu(2)#1	115.541(13)
Si(2)#1-N(2)-Cu(2)#1	107.753(14)
Cu(2)-N(2)-Cu(2)#1	89.00(4)
Si(3)-N(3)-Si(4)	118.21(4)
Si(3)-N(3)-Cu(2)	115.96(4)
Si(4)-N(3)-Cu(2)	108.05(4)
Si(3)-N(3)-Cu(1)	110.32(4)
Si(4)-N(3)-Cu(1)	112.14(4)
Cu(2)-N(3)-Cu(1)	88.33(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,y,-z+1/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **E**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	20(1)	16(1)	14(1)	1(1)	0(1)	0(1)
Cu(2)	18(1)	16(1)	17(1)	0(1)	2(1)	1(1)
Si(1)	24(1)	17(1)	19(1)	0(1)	-1(1)	-2(1)
Si(2)	26(1)	23(1)	32(1)	8(1)	9(1)	7(1)
Si(3)	25(1)	30(1)	16(1)	3(1)	-3(1)	-1(1)
Si(4)	20(1)	25(1)	17(1)	0(1)	3(1)	1(1)
N(1)	23(1)	14(1)	16(1)	0	0(1)	0
N(2)	22(1)	14(1)	22(1)	0	5(1)	0
N(3)	20(1)	19(1)	13(1)	1(1)	1(1)	1(1)
C(1)	37(1)	34(1)	32(1)	6(1)	6(1)	-7(1)
C(2)	42(1)	23(1)	32(1)	-9(1)	-4(1)	0(1)
C(3)	30(1)	30(1)	29(1)	0(1)	-6(1)	3(1)
C(4)	49(1)	42(1)	40(1)	21(1)	8(1)	9(1)
C(5)	57(1)	29(1)	65(1)	2(1)	26(1)	18(1)
C(6)	24(1)	59(1)	43(1)	13(1)	2(1)	-1(1)
C(7)	27(1)	38(1)	39(1)	8(1)	-4(1)	3(1)
C(8)	45(1)	43(1)	31(1)	-14(1)	-5(1)	-3(1)
C(9)	45(1)	66(1)	24(1)	20(1)	-4(1)	-5(1)
C(10)	26(1)	36(1)	34(1)	6(1)	-7(1)	2(1)
C(11)	37(1)	39(1)	37(1)	12(1)	3(1)	-9(1)
C(12)	40(1)	62(1)	38(1)	-21(1)	12(1)	7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **E**.

	x	y	z	U(eq)
H(1A)	5175	5150	1558	51
H(1B)	5966	5959	2077	51
H(1C)	4462	6222	1681	51
H(2A)	2964	6743	3124	48
H(2B)	4510	6642	3519	48
H(2C)	3164	6046	3849	48
H(3A)	4968	4317	3821	44
H(3B)	6274	4748	3338	44
H(3C)	5442	3769	3062	44
H(4A)	3293	-109	4140	65
H(4B)	4512	-938	4036	65
H(4C)	2884	-1177	3800	65
H(5A)	3634	-1726	2203	75
H(5B)	5289	-1614	2442	75
H(5C)	4679	-1026	1724	75
H(6A)	5997	703	2377	63
H(6B)	6373	261	3191	63
H(6C)	5409	1244	3116	63
H(7A)	4693	1486	4412	52
H(7B)	5328	2410	4877	52
H(7C)	4936	2535	4004	52
H(8A)	2948	4372	4677	59
H(8B)	3695	3981	5436	59
H(8C)	1979	4048	5376	59
H(9A)	1323	1961	5714	67
H(9B)	2982	1821	5936	67
H(9C)	2232	1072	5353	67
H(10A)	-1288	3522	3226	48
H(10B)	-2310	2576	3348	48
H(10C)	-896	2477	2844	48

H(11A)	-514	680	4029	56
H(11B)	-1856	1130	4474	56
H(11C)	-347	978	4898	56
H(12A)	-413	3109	5379	70
H(12B)	-1883	3314	4930	70
H(12C)	-502	3994	4777	70