Supporting Information Accompanying:

The Contribution of Ligand Flexibility to Metal Center Geometry Modulated Thermal Cyclization of Conjugated Pyridine and Quinoline Metalloenediynes of Cu(I) and Cu(II)

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Table 1S. Crystal data and structure refinement.

Identification code	zal06	
Empirical formula	$C_{26} H_{17} N_3$	
Formula weight	371.43	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pnma	
Unit cell dimensions	a = 8.3605(7) Å	α= 90°.
	b = 18.2233(15) Å	β= 90°.
	c = 12.9522(10) Å	γ = 90°.
Volume	1973.3(3) $Å^3$	
Z	4	
Density (calculated)	1.250 g/cm^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	776	
Crystal size	0.30 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.93 to 28.26°.	
Index ranges	-8<=h<=11, -23<=k<=24, -15<=l<=17	
Reflections collected	9043	
Independent reflections	2414 [R(int) = 0.0360]	
Completeness to theta = 28.26°	95.8 %	
Absorption correction	Empirical from SADABS	
Max. and min. transmission	0.9852 and 0.9779	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2414 / 0 / 147	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0385, wR2 = 0.0941	
R indices (all data)	R1 = 0.0642, wR2 = 0.1024	
Largest diff. peak and hole	0.164 and -0.167e^{-3} Å	

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

	x	y	z	U(eq)
N(1)	1552(1)	3939(1)	802(1)	35(1)
N(2)	5046(2)	7500	2039(1)	52(1)
C(1)	127(2)	3667(1)	929(1)	35(1)
C(2)	1756(1)	4669(1)	1026(1)	30(1)
C(3)	3284(2)	4976(1)	903(1)	35(1)
C(4)	3530(2)	5705(1)	1098(1)	39(1)
C(5)	2268(2)	6149(1)	1430(1)	40(1)
C(6)	780(2)	5866(1)	1564(1)	36(1)
C(7)	476(1)	5115(1)	1363(1)	30(1)
C(8)	-1038(1)	4793(1)	1482(1)	30(1)
C(9)	-1234(1)	4061(1)	1273(1)	30(1)
C(10)	-2710(2)	3677(1)	1390(1)	32(1)
C(11)	-3878(1)	3302(1)	1485(1)	32(1)
C(12)	-5266(2)	2869(1)	1608(1)	33(1)
C(13)	7491(3)	7500	821(2)	44(1)
C(14)	6116(2)	7500	1497(1)	37(1)

Table 3S. Bond lengths [Å] and angles [°].

N(1)-C(1)	1.3012(15)
N(1)-C(2)	1.3719(15)
N(2)-C(14)	1.137(2)
C(1)-C(9)	1.4161(17)
C(2)-C(3)	1.4031(16)
C(2)-C(7)	1.4132(16)
C(3)-C(4)	1.3673(19)
C(4)-C(5)	1.3981(18)
C(5)-C(6)	1.3585(18)
C(6)-C(7)	1.4152(17)
C(7)-C(8)	1.4039(16)
C(8)-C(9)	1.3721(17)
C(9)-C(10)	1.4267(17)
C(10)-C(11)	1.1980(17)
C(11)-C(12)	1.4126(17)
C(12)-C(12)#1	1.344(2)
C(13)-C(14)	1.446(3)

C(1)-N(1)-C(2)	117.19(10)
N(1)-C(1)-C(9)	125.60(11)
N(1)-C(2)-C(3)	118.39(11)
N(1)-C(2)-C(7)	121.92(11)
C(3)-C(2)-C(7)	119.68(11)
C(4)-C(3)-C(2)	120.18(12)
C(3)-C(4)-C(5)	120.43(12)
C(6)-C(5)-C(4)	120.65(12)
C(5)-C(6)-C(7)	120.55(12)
C(8)-C(7)-C(2)	118.43(11)
C(8)-C(7)-C(6)	123.07(11)
C(2)-C(7)-C(6)	118.50(11)
C(9)-C(8)-C(7)	119.53(11)
C(8)-C(9)-C(1)	117.32(11)
C(8)-C(9)-C(10)	123.96(11)
C(1)-C(9)-C(10)	118.72(11)
C(11)-C(10)-C(9)	174.50(13)
C(10)-C(11)-C(12)	179.01(14)
C(12)#1-C(12)-C(11)	123.97(7)
N(2)-C(14)-C(13)	179.2(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 4S. Anisotropic displacement parameters ($Å^2 x\ 10^3$). 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}
N(1)	34(1)	33(1)	38(1)	-1(1)	1(1)	4(1)
N(2)	53(1)	43(1)	59(1)	0	12(1)	0
C(1)	37(1)	29(1)	38(1)	-1(1)	2(1)	0(1)
C(2)	33(1)	33(1)	24(1)	2(1)	-2(1)	1(1)
C(3)	30(1)	44(1)	31(1)	1(1)	1(1)	1(1)
C(4)	35(1)	47(1)	33(1)	3(1)	-1(1)	-11(1)
C(5)	48(1)	35(1)	36(1)	-1(1)	0(1)	-9(1)
C(6)	41(1)	32(1)	34(1)	-2(1)	2(1)	1(1)
C(7)	32(1)	33(1)	24(1)	1(1)	0(1)	0(1)
C(8)	30(1)	34(1)	27(1)	1(1)	1(1)	3(1)
C(9)	30(1)	34(1)	27(1)	3(1)	-2(1)	-1(1)
C(10)	33(1)	34(1)	31(1)	1(1)	-1(1)	1(1)
C(11)	31(1)	33(1)	32(1)	0(1)	-2(1)	5(1)
C(12)	24(1)	40(1)	36(1)	-1(1)	-1(1)	3(1)
C(13)	43(1)	49(1)	40(1)	0	4(1)	0
C(14)	41(1)	30(1)	39(1)	0	-4(1)	0

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

	x	y	z	U(eq)
H(1A)	-13	3161	779	42
H(3A)	4150	4676	685	42
H(4A)	4564	5910	1006	46
H(5A)	2454	6655	1564	48
H(6A)	-64	6174	1794	43
H(8A)	-1921	5080	1706	36
H(12)	-6277(16)	3124(7)	1677(9)	45(4)
H(1)	8520(30)	7500	1237(18)	67(7)
H(2)	7440(16)	7056(8)	393(11)	59(4)