SUPPORTING INFORMATION

Metal-Mediated Polymerization of Acrylates: Relevance of Radical Traps?

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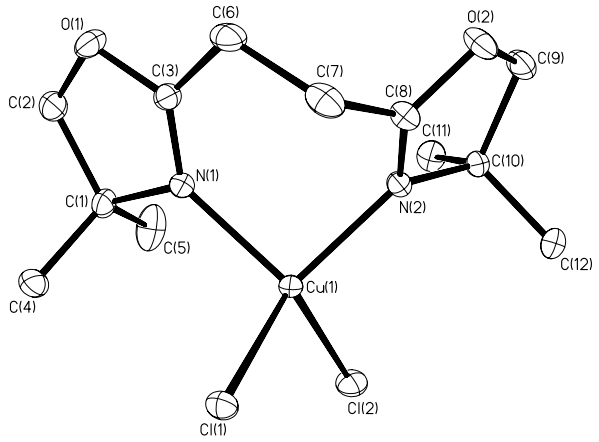

Table 1. Crystal data and structure refinement for sen18a.

Identification code	sen18a	
Empirical formula	C12 H20 Cl2 Cu N2 O2	
Formula weight	358.74	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 14.0146(7) Å	α= 90°.
	b = 9.5327(5) Å	β= 105.9800(10)°.
	c = 11.9678(6) Å	γ = 90°.
Volume	1537.08(14) $Å^3$	
Z	4	
Density (calculated)	1.550 Mg/m^3	
Absorption coefficient	1.767 mm^{-1}	
F(000)	740	
Crystal size	0.25 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.51 to 28.28°.	
Index ranges	-18<=h<=17, -12<=k<=11, -11<=l<=15	
Reflections collected	9377	
Independent reflections	3553 [R(int) = 0.0178]	
Completeness to theta = 28.28°	93.0 %	
Absorption correction	SADABS	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3553 / 0 / 172	
Goodness-of-fit on F^2	0.409	
Final R indices [I>2sigma(I)]	R1 = 0.0277, wR2 = 0.0767	
R indices (all data)	R1 = 0.0319, wR2 = 0.0916	
Largest diff. peak and hole	0.425 and -0.218 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sen18a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	2260(1)	463(1)	6326(1)	19(1)
Cl(1)	884(1)	-274(1)	6720(1)	27(1)
Cl(2)	3390(1)	-353(1)	7887(1)	32(1)
N(1)	1893(1)	80(2)	4624(1)	23(1)
N(2)	2839(1)	2340(2)	6173(1)	21(1)
O(1)	1525(1)	274(2)	2688(1)	39(1)
O(2)	2685(1)	4505(2)	5425(2)	32(1)
C(1)	2090(2)	-1365(2)	4228(2)	28(1)
C(2)	1934(2)	-1137(3)	2920(2)	43(1)
C(3)	1570(2)	858(3)	3728(2)	28(1)
C(4)	1335(2)	-2395(2)	4452(2)	32(1)
C(5)	3145(2)	-1799(3)	4848(3)	48(1)
C(6)	1232(2)	2339(3)	3660(2)	34(1)
C(7)	1241(2)	3024(2)	4819(2)	32(1)
C(8)	2282(2)	3259(2)	5532(2)	25(1)
C(9)	3741(2)	4373(2)	5992(2)	33(1)
C(10)	3851(2)	2964(2)	6655(2)	23(1)
C(11)	4618(2)	2005(3)	6365(2)	32(1)
C(12)	4059(2)	3187(3)	7962(2)	32(1)

Table 3. Bond lengths [Å] and angles [°] for sen18a.

Cu(1)-N(1)	1.9914(17)
Cu(1)-N(2)	1.9940(16)
Cu(1)-Cl(1)	2.2221(5)
Cu(1)-Cl(2)	2.2306(6)
N(1)-C(3)	1.280(3)
N(1)-C(1)	1.508(3)
N(2)-C(8)	1.279(3)
N(2)-C(10)	1.498(2)
O(1)-C(3)	1.349(3)
O(1)-C(2)	1.458(4)
O(2)-C(8)	1.336(2)
O(2)-C(9)	1.453(3)
C(1)-C(4)	1.520(3)
C(1)-C(5)	1.519(3)
C(1)-C(2)	1.535(3)
C(3)-C(6)	1.485(3)
C(6)-C(7)	1.530(4)
C(7)-C(8)	1.491(3)
C(9)-C(10)	1.546(3)
C(10)-C(11)	1.522(3)
C(10)-C(12)	1.525(3)
N(1)-Cu(1)-N(2)	93.91(7)
N(1)-Cu(1)-Cl(1)	99.42(5)
N(2)-Cu(1)-Cl(1)	134.57(5)
N(1)-Cu(1)-Cl(2)	135.82(6)
N(2)-Cu(1)-Cl(2)	100.18(5)
Cl(1)-Cu(1)-Cl(2)	99.75(2)
C(3)-N(1)-C(1)	108.56(18)
C(3)-N(1)-Cu(1)	133.11(16)
C(1)-N(1)-Cu(1)	118.10(13)
C(8)-N(2)-C(10)	108.38(16)
C(8)-N(2)-Cu(1)	118.25(14)
C(10)-N(2)-Cu(1)	133.36(13)
C(3)-O(1)-C(2)	106.81(18)
C(8)-O(2)-C(9)	106.35(16)
N(1)-C(1)-C(4)	109.76(17)
N(1)-C(1)-C(5)	109.46(18)
C(4)-C(1)-C(5)	111.7(2)
N(1)-C(1)-C(2)	101.82(18)
C(4)-C(1)-C(2)	111.16(18)
C(5)-C(1)-C(2)	112.5(2)
O(1)-C(2)-C(1)	105.24(19)
N(1)-C(3)-O(1)	116.7(2)
N(1)-C(3)-C(6)	129.1(2)
O(1)-C(3)-C(6)	114.18(19)
C(3)-C(6)-C(7)	115.68(18)
C(8)-C(7)-C(6)	110.22(18)
N(2)-C(8)-O(2)	117.50(19)
N(2)-C(8)-C(7)	125.44(19)
O(2)-C(8)-C(7)	116.89(18)
O(2)-C(9)-C(10)	105.03(17)
N(2)-C(10)-C(11)	109.07(16)

N(2)-C(10)-C(12)	110.09(17)
C(11)-C(10)-C(12)	111.71(18)
N(2)-C(10)-C(9)	101.40(16)
C(11)-C(10)-C(9)	112.41(19)
C(12)-C(10)-C(9)	111.67(18)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for sen18a. 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)	23(1)	17(1)	17(1)	1(1)	5(1)	-1(1)
Cl(1)	28(1)	28(1)	29(1)	1(1)	12(1)	-4(1)
Cl(2)	35(1)	32(1)	26(1)	10(1)	0(1)	1(1)
N(1)	24(1)	24(1)	20(1)	0(1)	6(1)	-5(1)
N(2)	22(1)	19(1)	22(1)	1(1)	5(1)	-2(1)
O(1)	44(1)	53(1)	18(1)	2(1)	6(1)	-15(1)
O(2)	33(1)	19(1)	43(1)	8(1)	7(1)	-2(1)
C(1)	32(1)	29(1)	23(1)	-8(1)	10(1)	-5(1)
C(2)	69(2)	39(1)	27(1)	-11(1)	22(1)	-22(1)
C(3)	25(1)	35(1)	21(1)	2(1)	4(1)	-11(1)
C(4)	45(1)	23(1)	31(1)	-2(1)	15(1)	-5(1)
C(5)	33(1)	54(2)	56(2)	-27(1)	10(1)	9(1)
C(6)	29(1)	36(1)	31(1)	14(1)	-3(1)	-7(1)
C(7)	22(1)	26(1)	44(1)	11(1)	5(1)	4(1)
C(8)	26(1)	20(1)	29(1)	2(1)	8(1)	-1(1)
C(9)	34(1)	26(1)	34(1)	4(1)	2(1)	-9(1)
C(10)	24(1)	23(1)	22(1)	-1(1)	5(1)	-6(1)
C(11)	26(1)	37(1)	35(1)	-4(1)	10(1)	-1(1)
C(12)	39(1)	31(1)	24(1)	-6(1)	6(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sen18a.

	x	y	z	U(eq)
H(2A)	2572	-1211	2719	52
H(2B)	1467	-1840	2464	52
H(4A)	1449	-2516	5291	48
H(4B)	1407	-3301	4097	48
H(4C)	664	-2031	4112	48
H(5A)	3208	-1929	5678	72
H(5B)	3607	-1067	4750	72
H(5C)	3303	-2681	4518	72
H(6A)	547	2384	3142	41
H(6B)	1659	2901	3294	41
H(7A)	885	3931	4674	38
H(7B)	894	2410	5248	38
H(9A)	3977	5161	6536	39
H(9B)	4125	4361	5411	39
H(11A)	4660	1128	6803	48
H(11B)	5266	2470	6576	48
H(11C)	4420	1800	5530	48
H(12A)	4122	2275	8354	47
H(12B)	3510	3713	8122	47
H(12C)	4677	3716	8250	47