Supporting Information

A Trimethylene versus an Ethylene Cross-bridged Tetraazamacrocycle and *in vitro*/*in vivo* Comparisons of their Copper(II) Complexes

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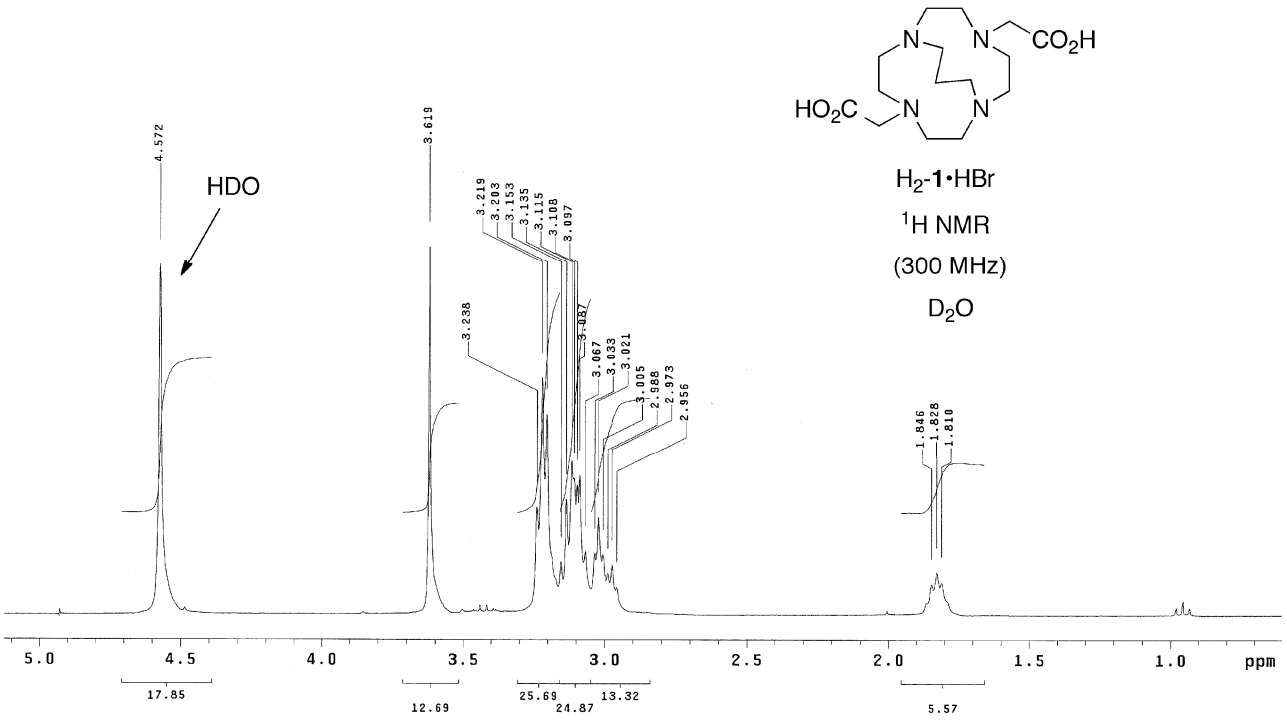
NMR Spectra of H_2-**1**•HBr



H_2-**1**•HBr

^{1}H NMR

(300 MHz)

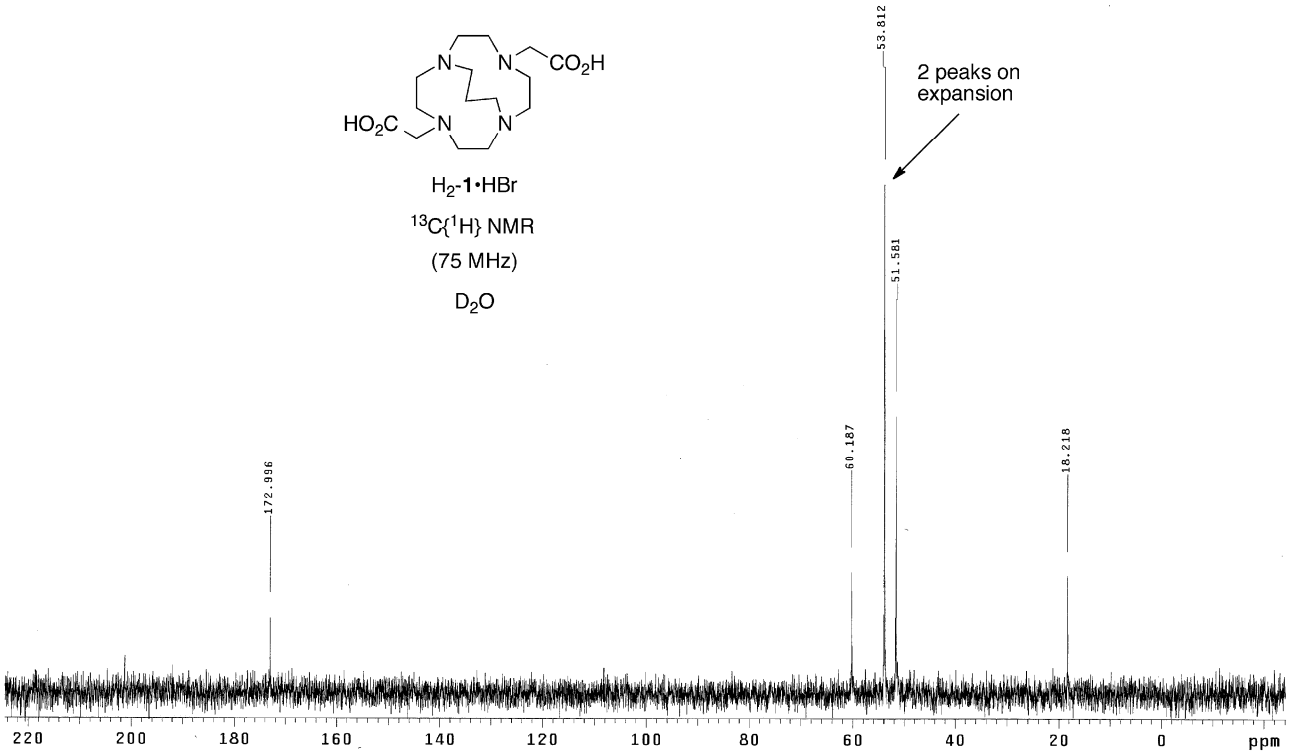
D_2O

H_2-**1**•HBr

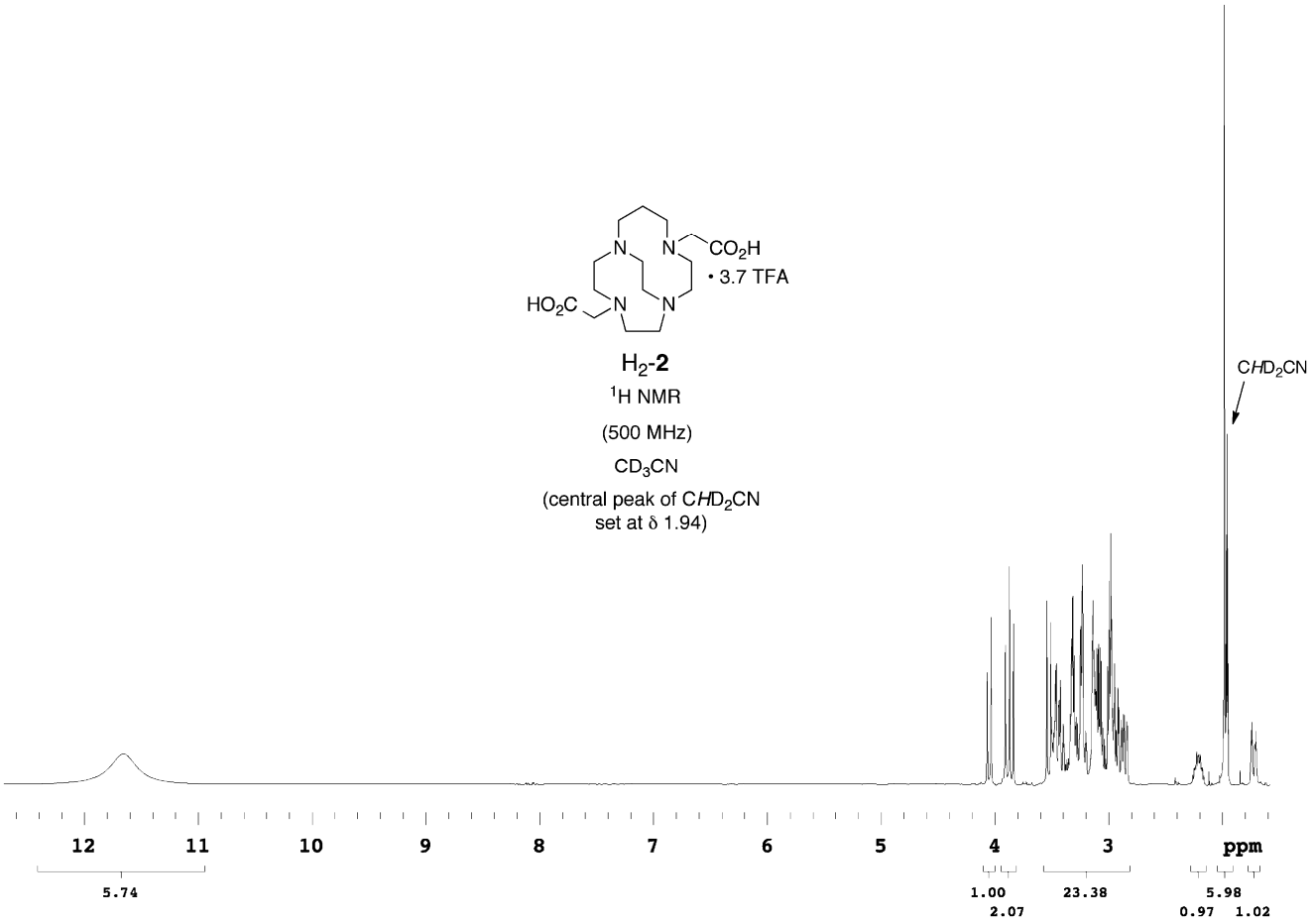
$^{13}C\{^1H\}$ NMR

(75 MHz)

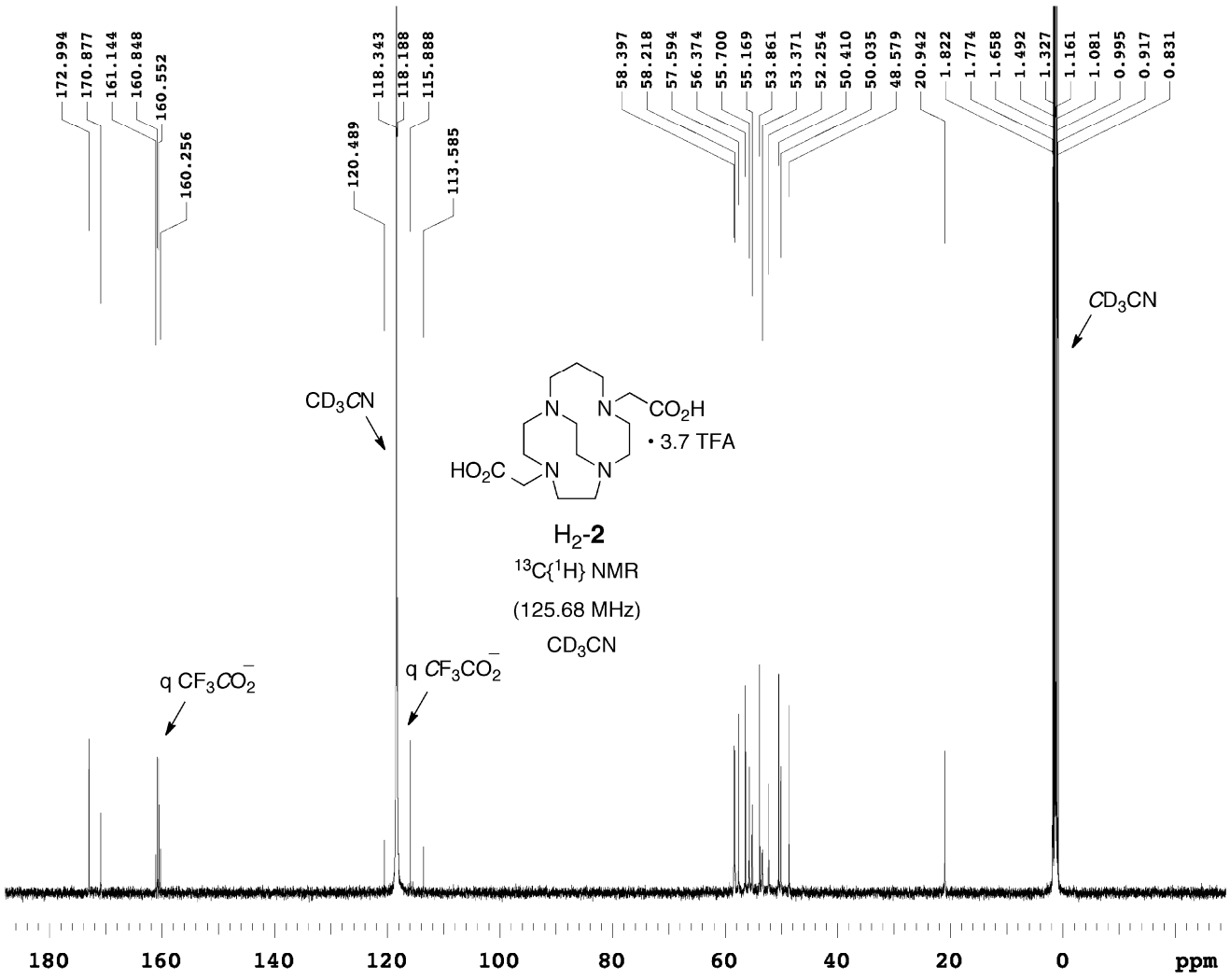
D_2O



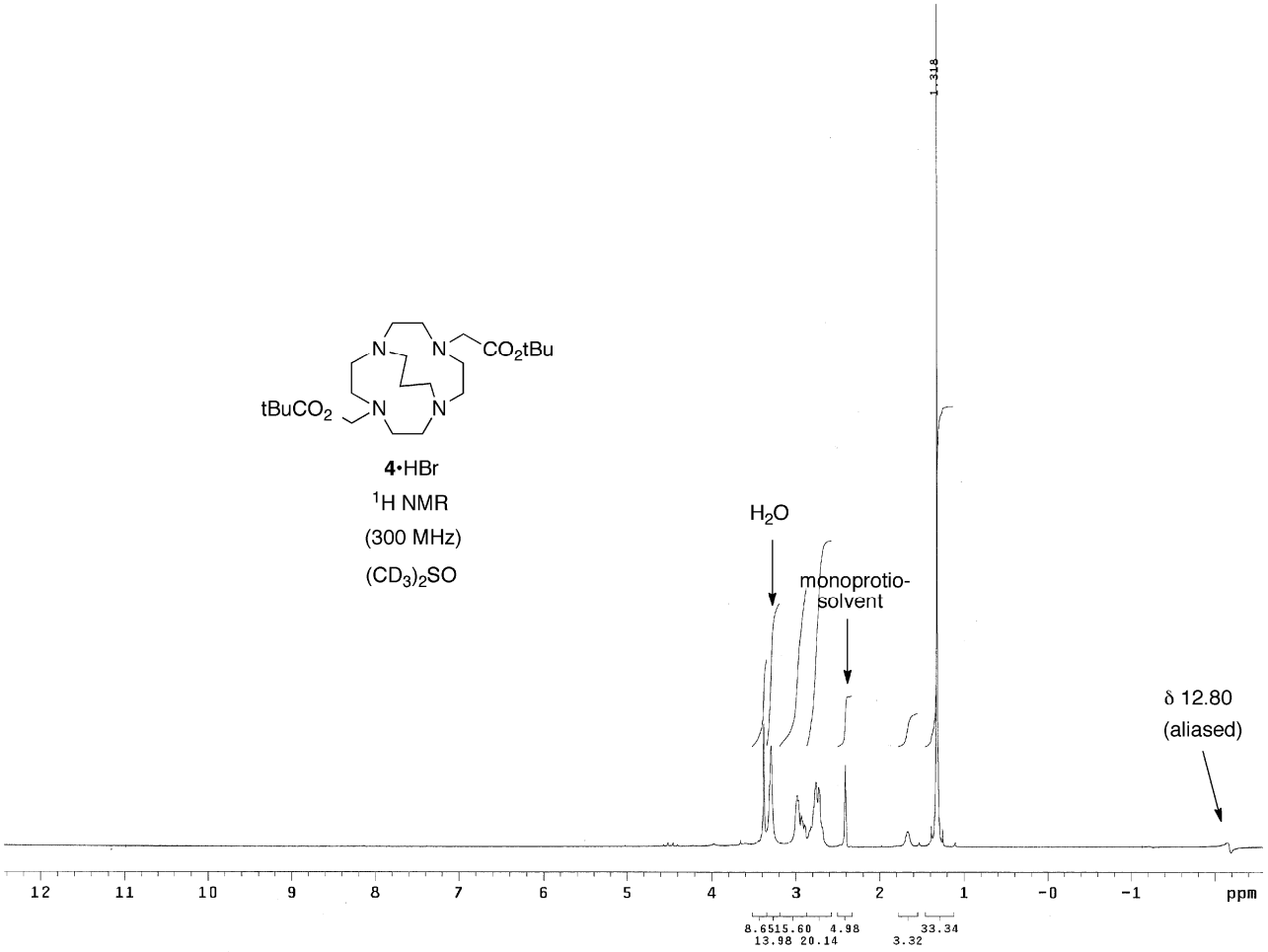
NMR Spectra of H_2-**2**•3.7TFA



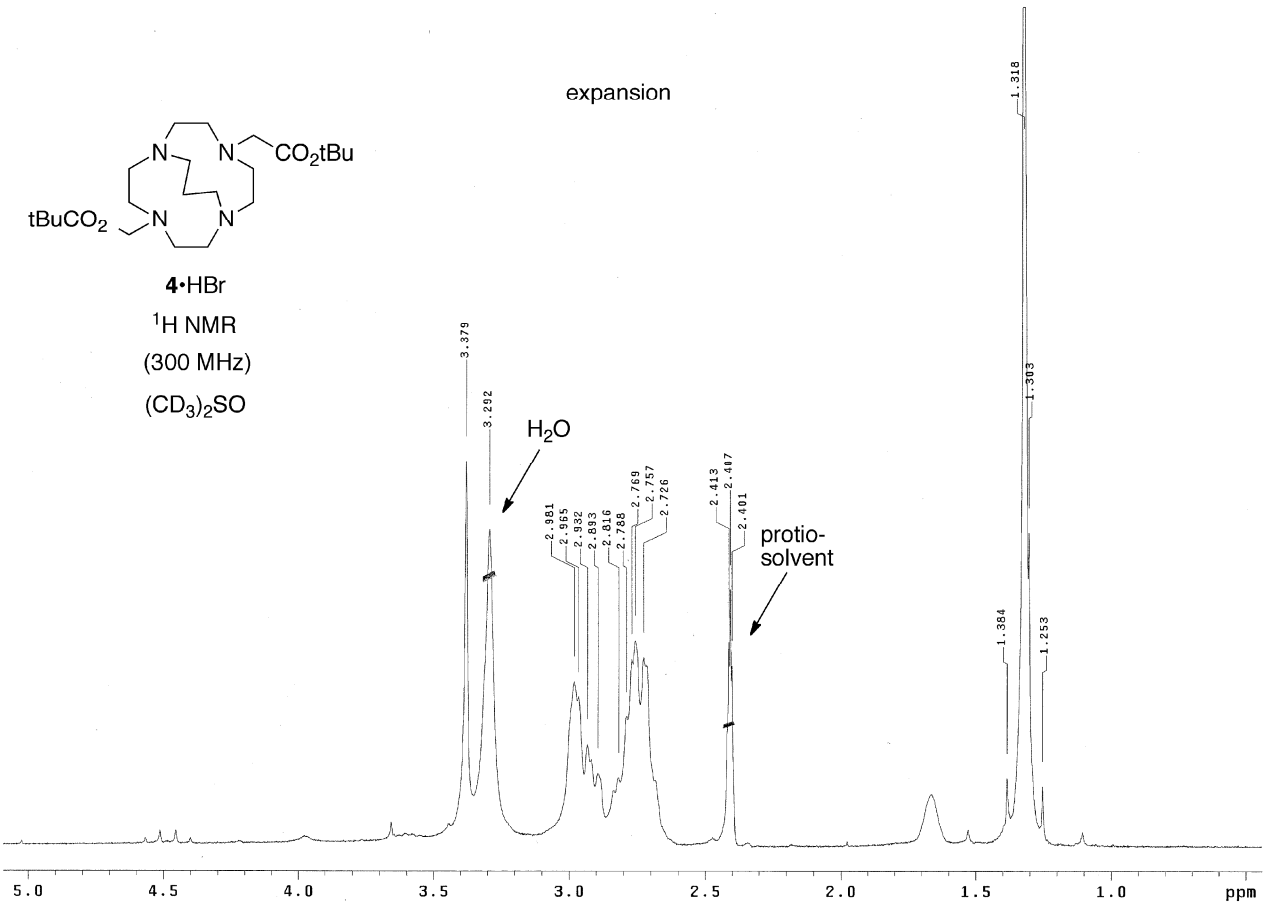
cont. - NMR Spectra of H_2-**2**•3.7TFA



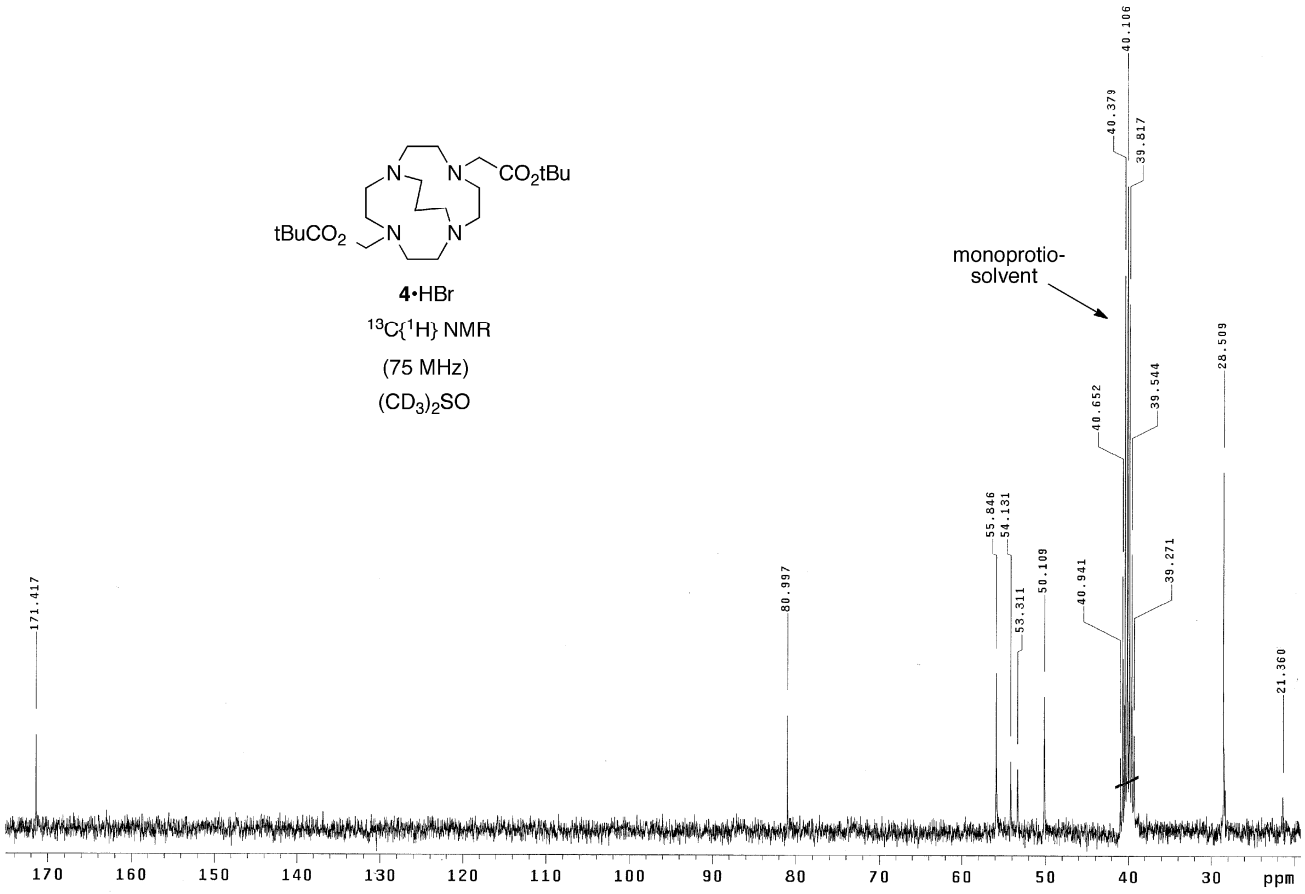
NMR Spectra of **4**•HBr



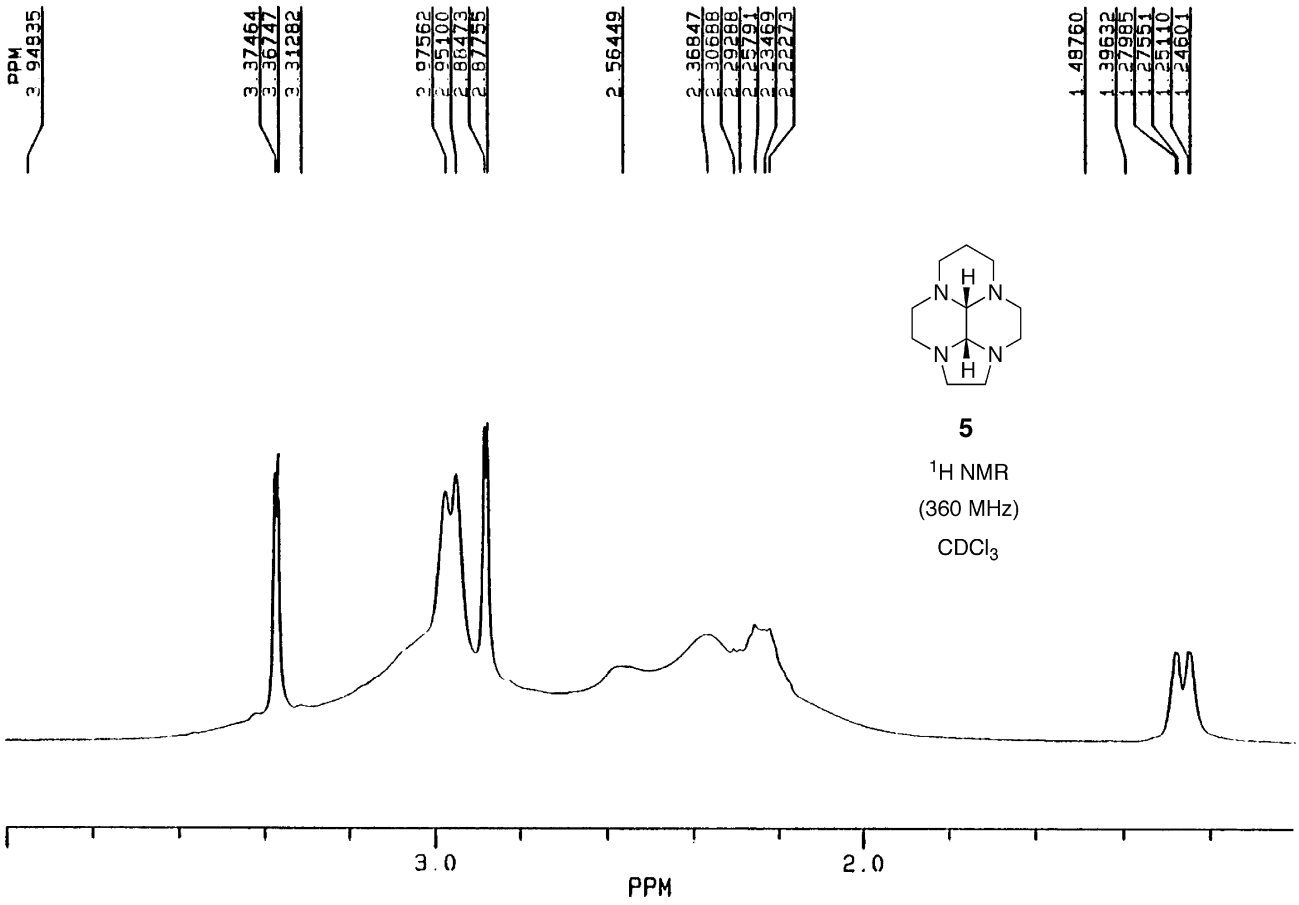
cont. - NMR Spectra of **4**•HBr



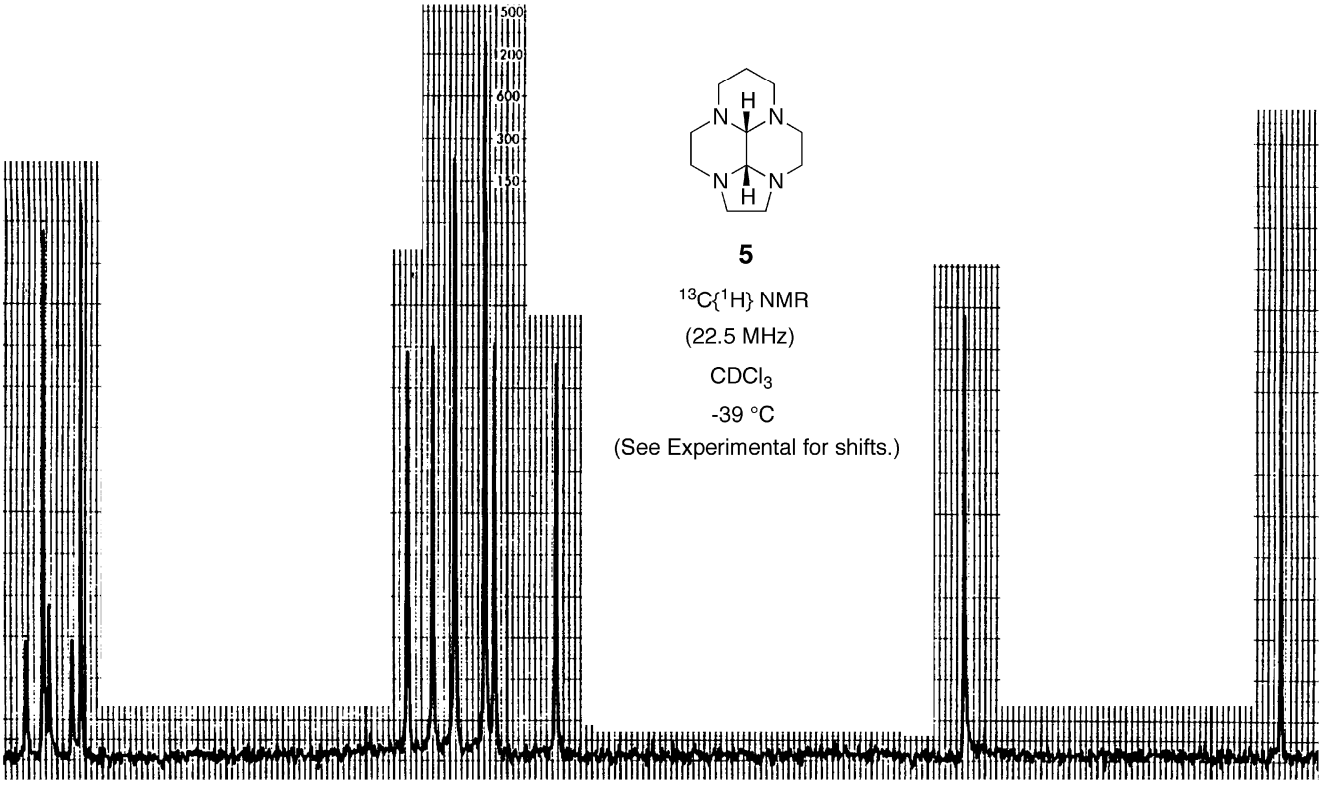
cont. - NMR Spectra of **4**•HBr



NMR Spectra of **5**



cont. - NMR Spectra of **5**



5

$^{13}C\{^{1}H\}$ NMR

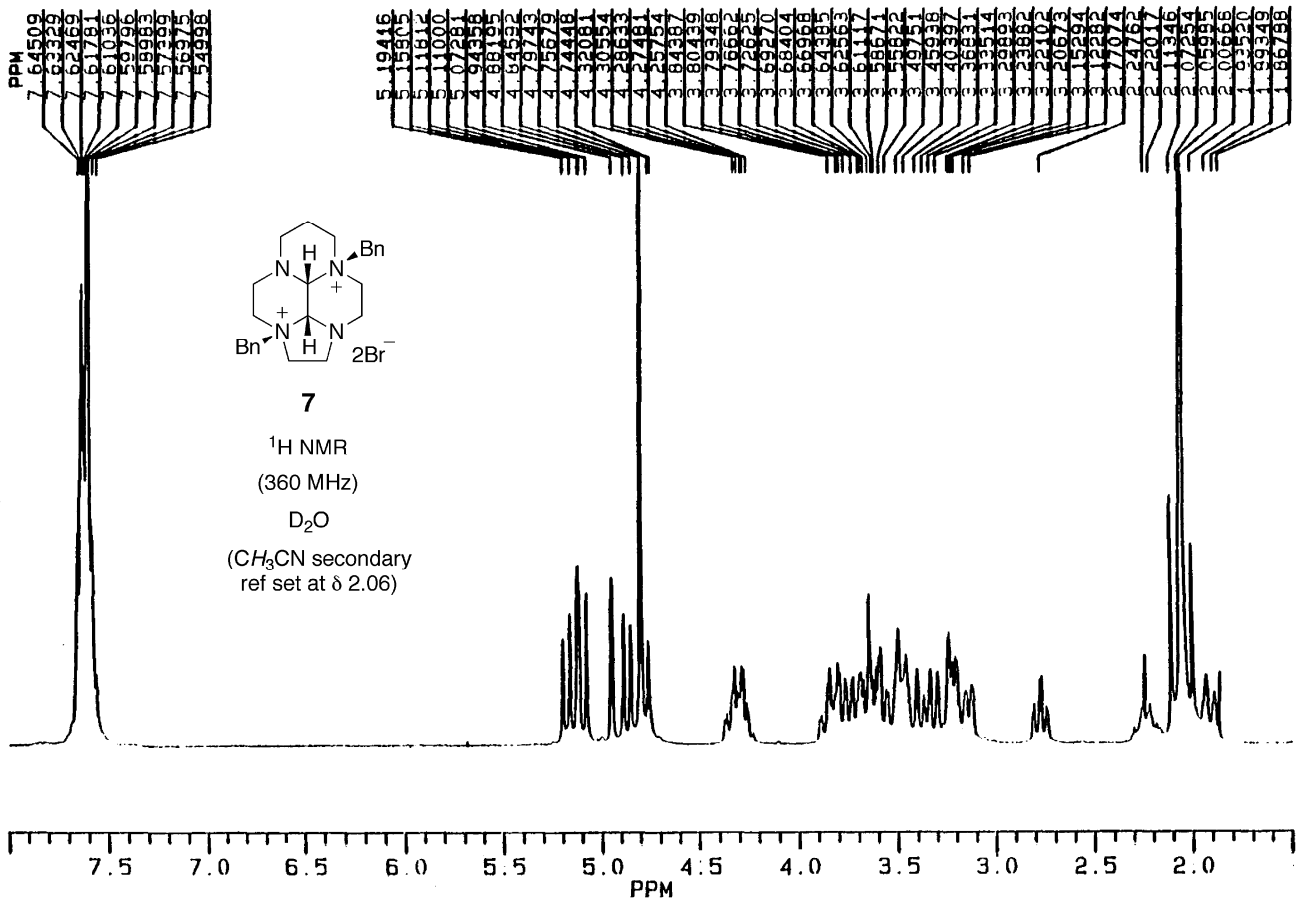
(22.5 MHz)

$CDCl_3$

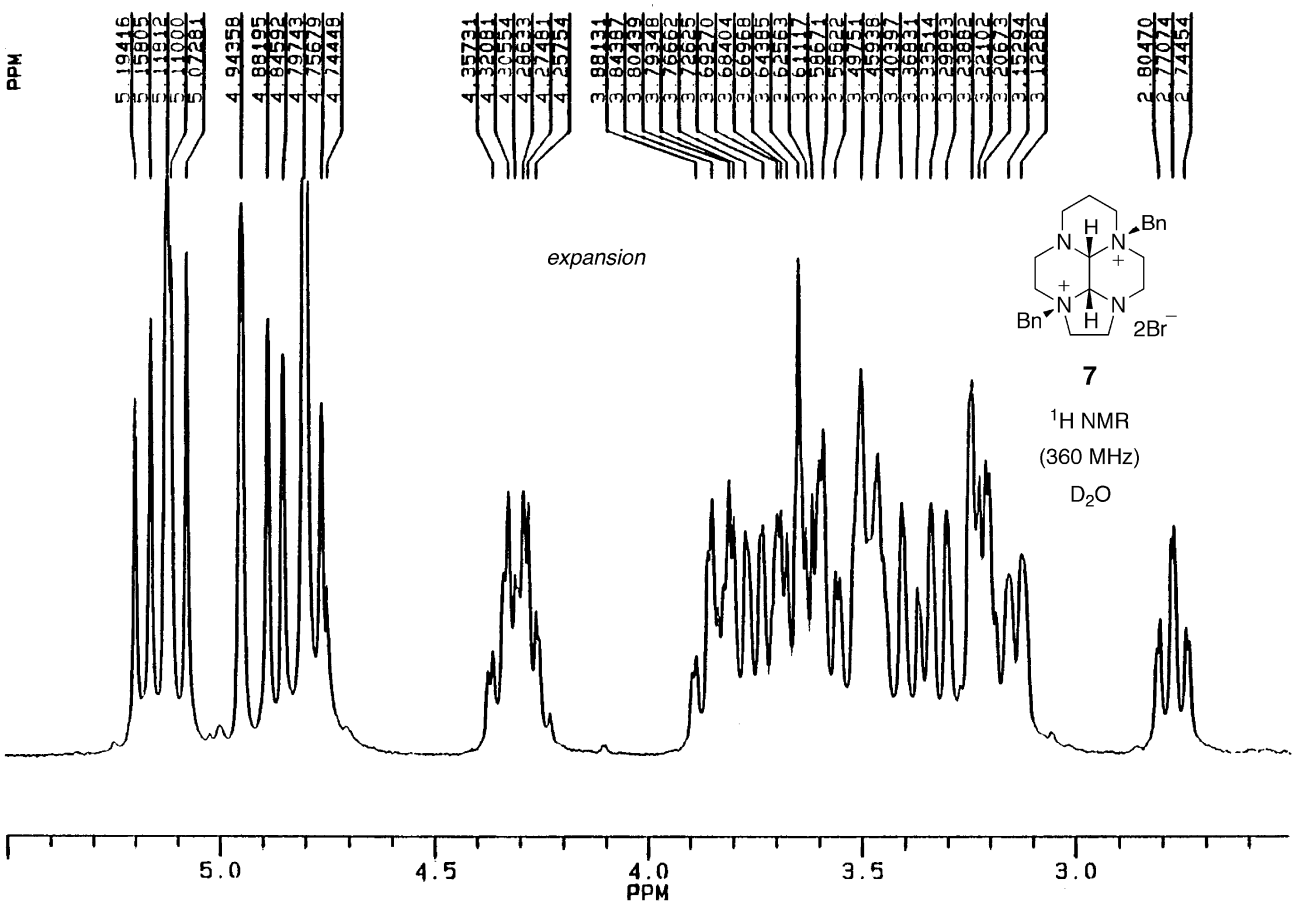
-39 °C

(See Experimental for shifts.)

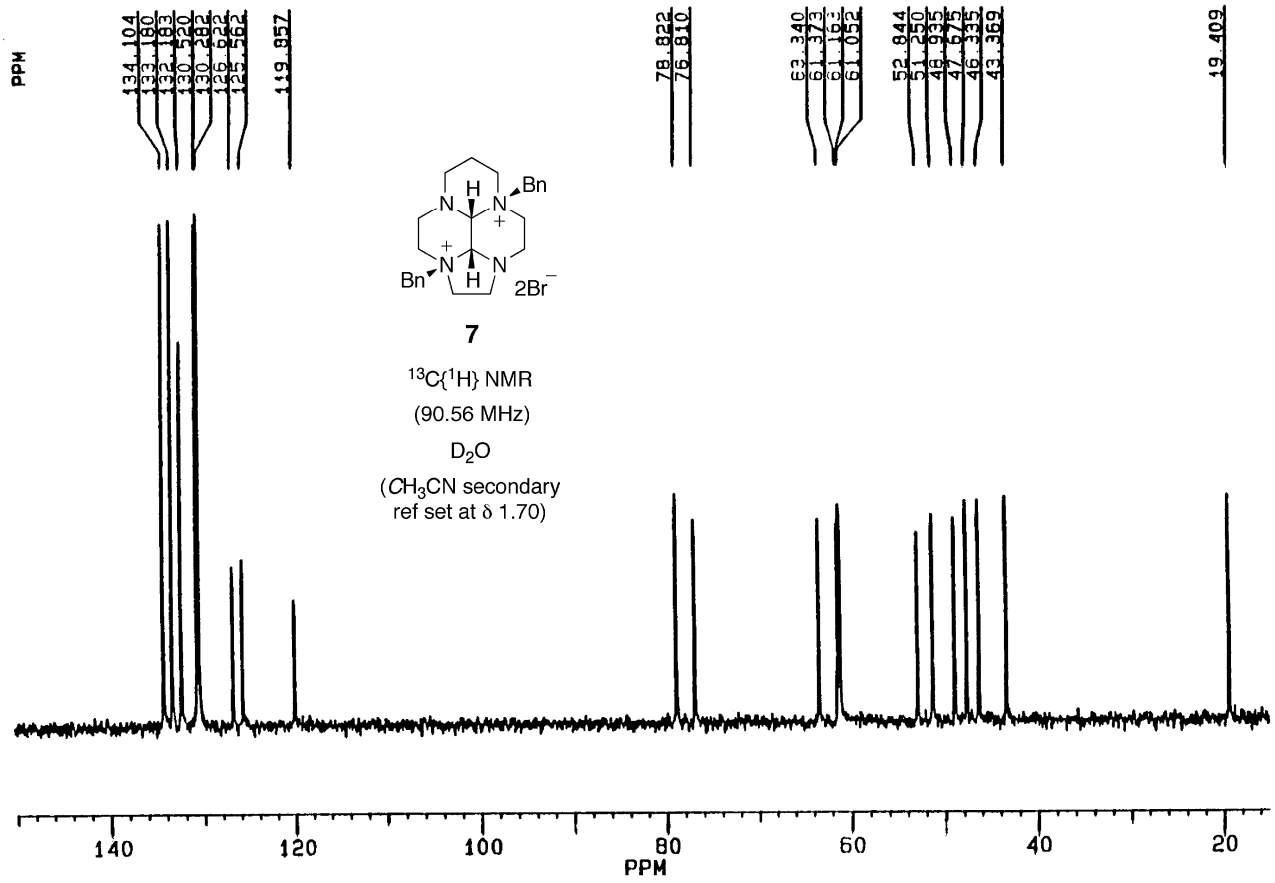
NMR Spectra of **7**



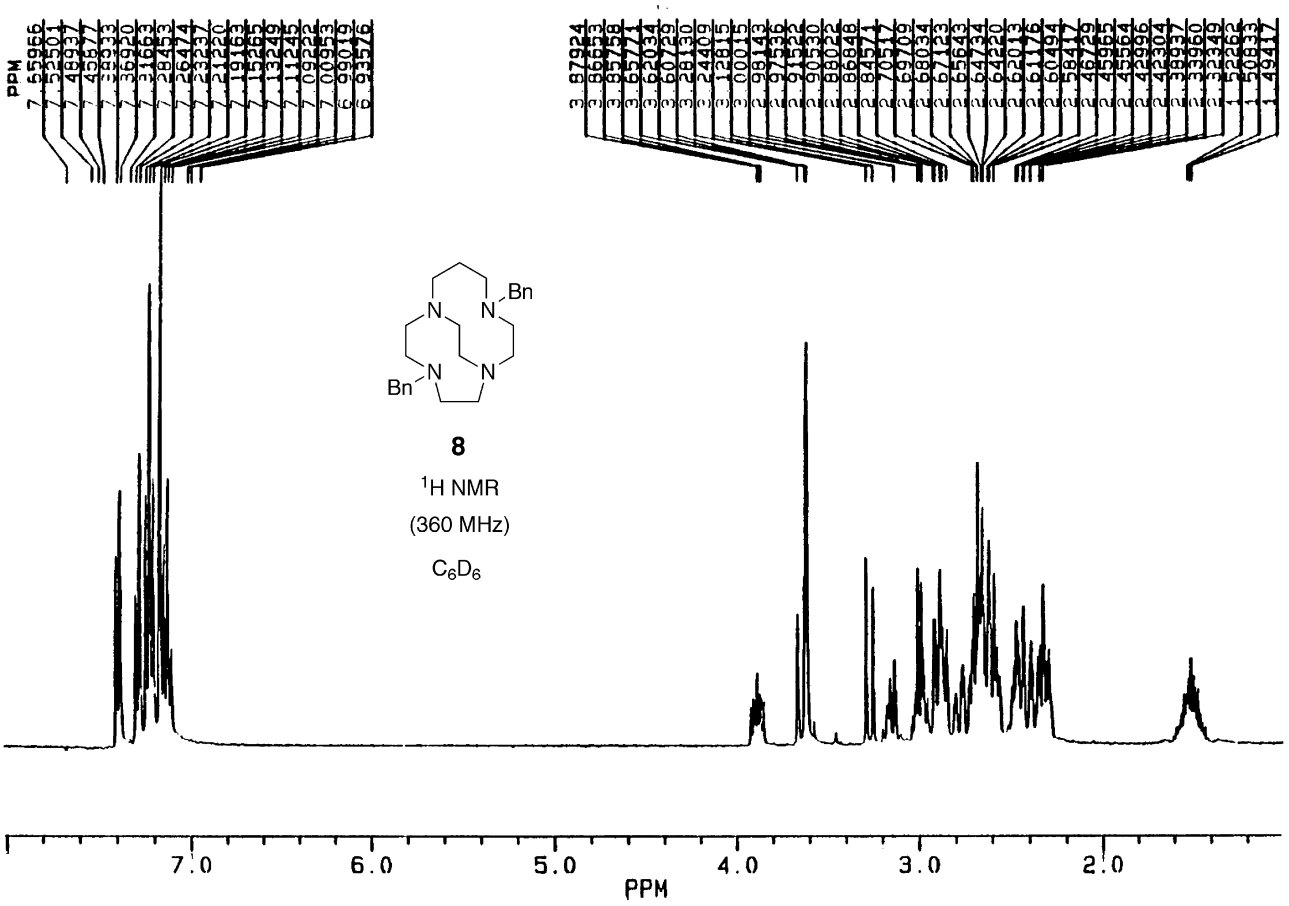
cont. - NMR Spectra of **7**



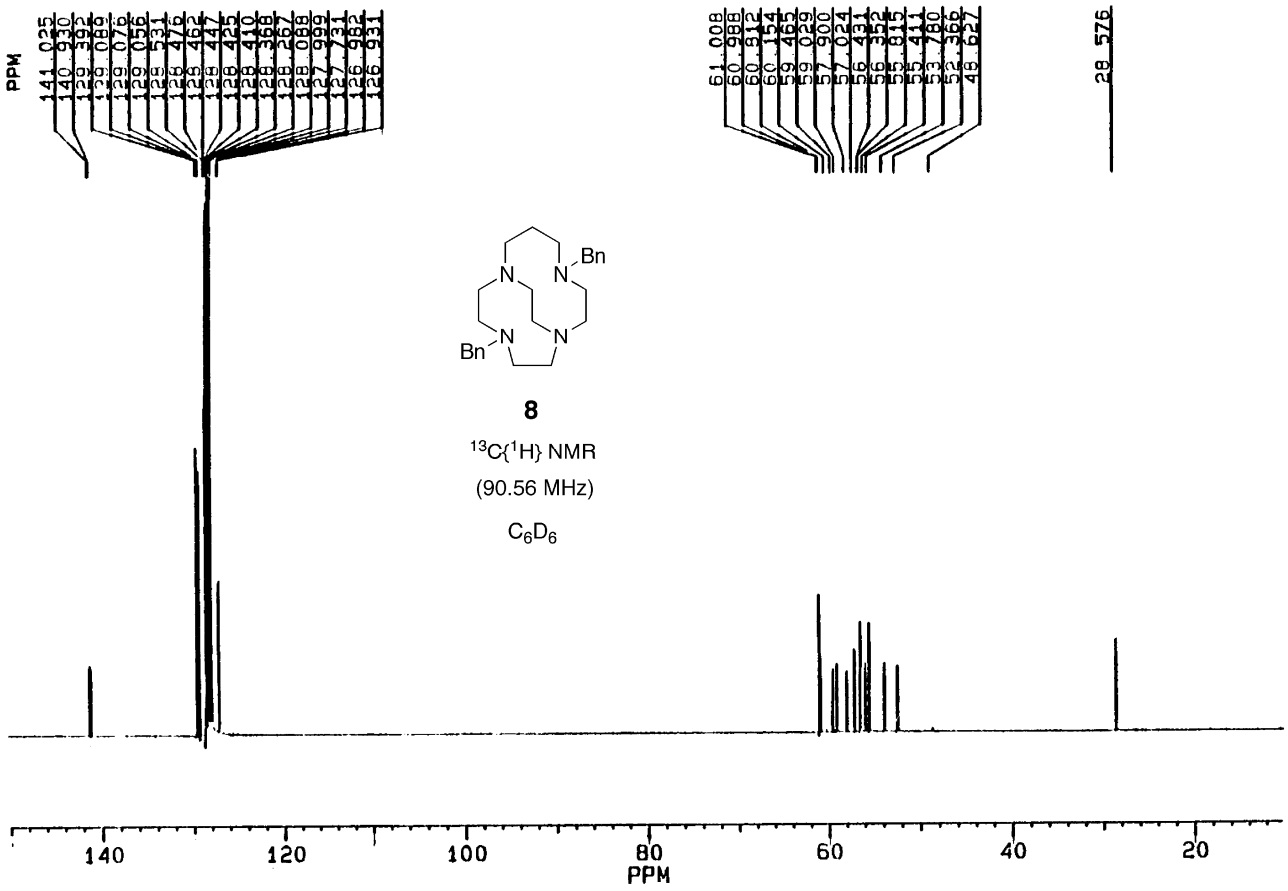
cont. - NMR Spectra of **7**



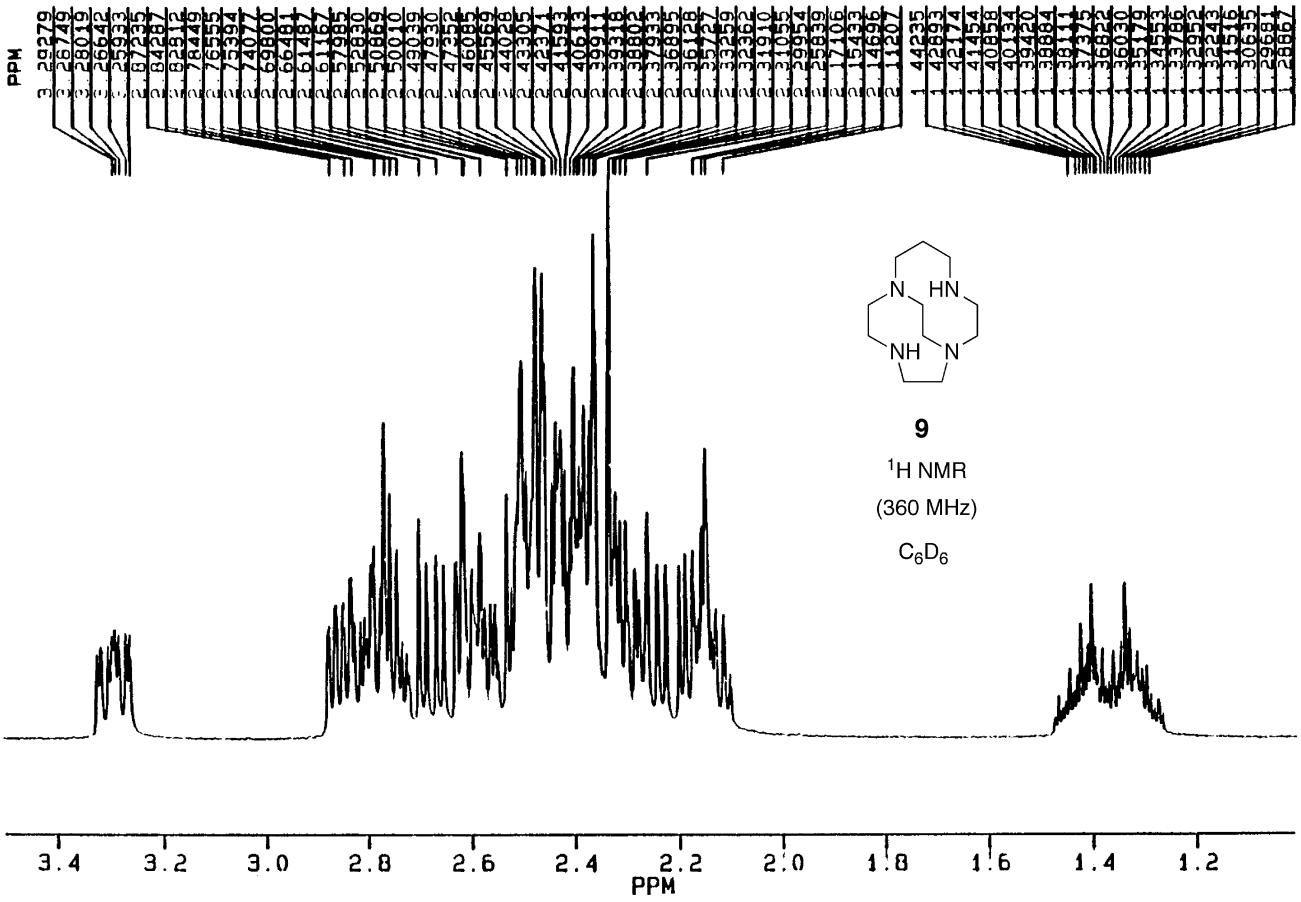
NMR Spectra of **8**



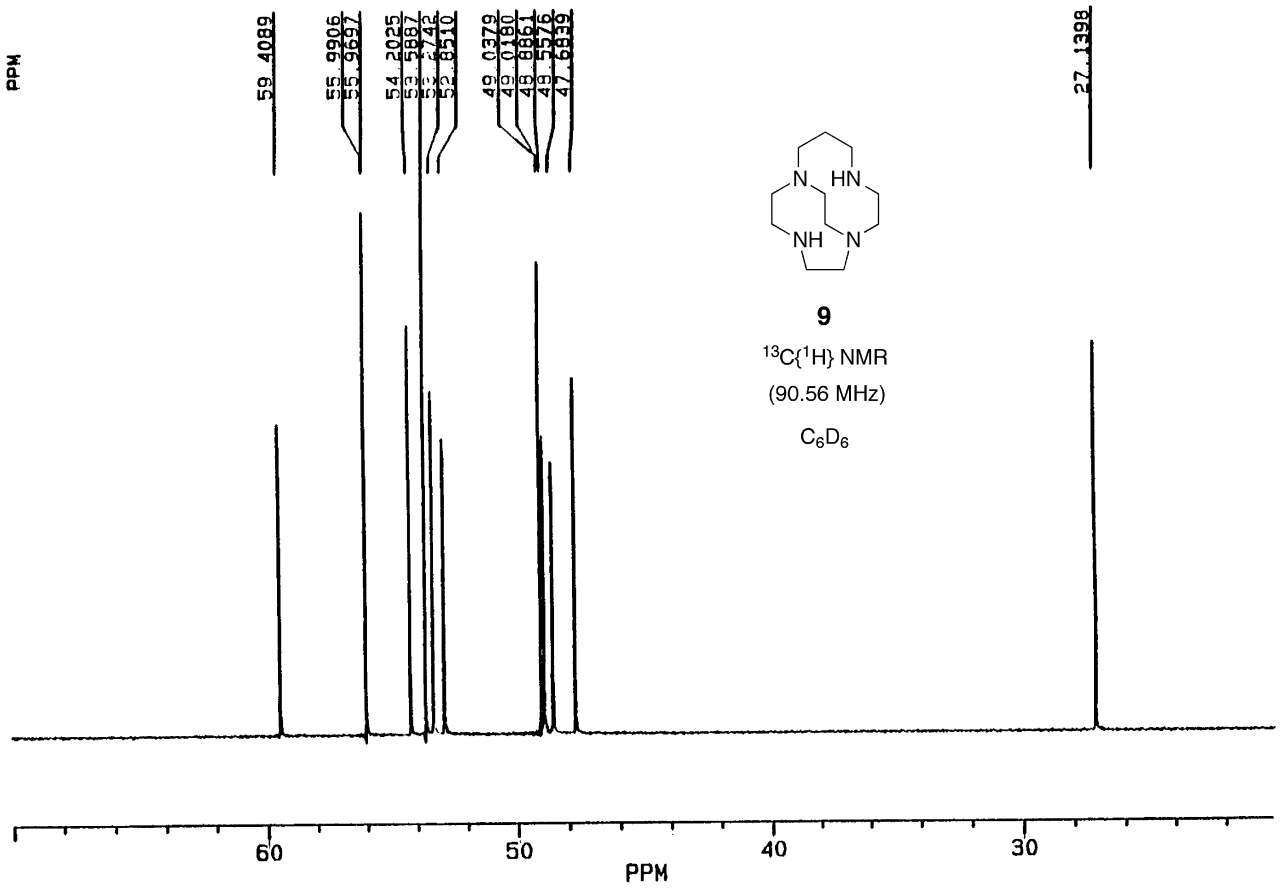
cont. - NMR Spectra of **8**



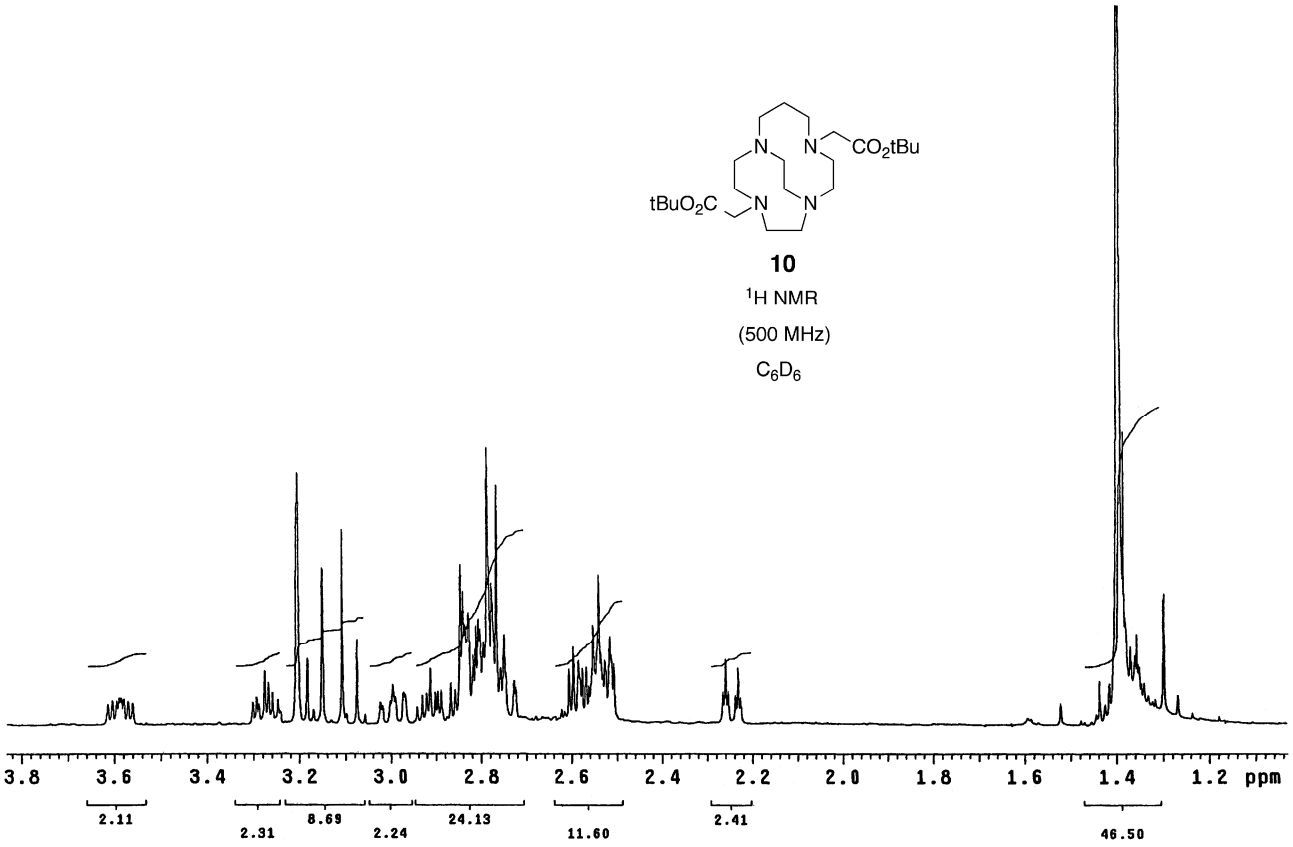
NMR Spectra of **9**



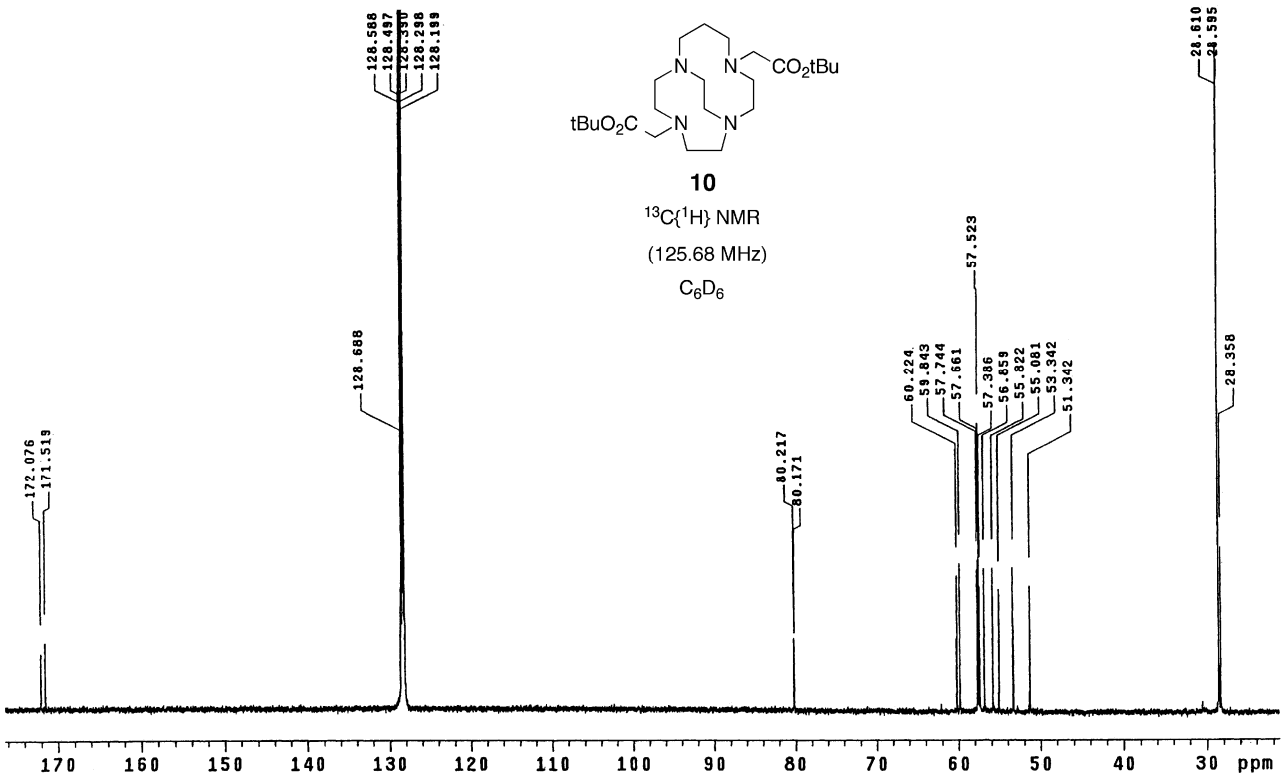
cont. - NMR Spectra of **9**



NMR Spectra of **10**



cont.- NMR Spectra of **10**



X-ray Data for C3B-DO2A (**11**)

Table S1. Crystal data and structure refinement for complex **11**.

Identification code	wong155	
Empirical formula	C21 H30 Cu F12 N4 O6	
Formula weight	726.03	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 12.2973(7) Å	α= 90°
	b = 13.3899(8) Å	β= 106.581(3)°
	c = 17.5444(10) Å	γ = 90°
Volume	2768.7(3) $Å^3$	
Z	4	
Density (calculated)	1.742 g/cm^3	
Absorption coefficient	2.293 mm^{-1}	
F(000)	1476	
Crystal size	0.15 x 0.10 x 0.10 mm^3	
Theta range for data collection	3.92 to 69.53°	
Index ranges	-14<=h<=14, -16<=k<=16, -21<=l<=16	
Reflections collected	26620	
Independent reflections	5164 [R(int) = 0.0299]	
Completeness to theta = 67.00°	99.8 %	
Max. and min. transmission	0.8031 and 0.7249	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5164 / 0 / 399	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0497, wR2 = 0.1253	
R indices (all data)	R1 = 0.0558, wR2 = 0.1299	
Largest diff. peak and hole	1.459 and -0.838 e $Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for **11**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	718(3)	1348(2)	4843(2)	27(1)
C(2)	-258(3)	1937(2)	5009(2)	27(1)
C(3)	2826(3)	1284(2)	5388(2)	26(1)
C(4)	3769(3)	1856(2)	5991(2)	25(1)
C(5)	617(3)	3987(2)	6428(2)	25(1)
C(6)	-374(3)	3377(2)	5901(2)	28(1)
C(7)	2717(3)	4044(2)	6842(2)	25(1)
C(8)	3719(3)	3350(2)	6853(2)	25(1)
C(9)	1889(3)	2713(3)	4561(2)	29(1)
C(10)	2300(4)	3711(3)	4936(2)	41(1)
C(11)	1630(3)	4198(2)	5421(2)	31(1)
C(12)	-439(3)	1630(2)	6358(2)	26(1)
C(13)	371(3)	746(2)	6617(2)	23(1)
C(14)	3741(3)	1640(2)	7377(2)	23(1)
C(15)	3070(3)	1836(2)	7976(2)	22(1)
C(16)	305(3)	1340(3)	9262(2)	34(1)
C(17)	1176(3)	2126(3)	9222(2)	27(1)
C(18)	996(3)	3099(3)	9621(2)	37(1)
C(19)	-2763(3)	3631(4)	7236(4)	65(2)
C(20)	-2788(3)	4643(3)	7611(2)	27(1)
C(21)	-1734(3)	5249(3)	7666(2)	42(1)
N(1)	1794(2)	1907(2)	5115(2)	23(1)
N(2)	-21(2)	2317(2)	5847(2)	22(1)
N(3)	3376(2)	2275(2)	6661(2)	21(1)
N(4)	1675(2)	3756(2)	6212(2)	21(1)
O(1)	1371(2)	858(2)	6579(1)	24(1)
O(2)	3(2)	-19(2)	6863(1)	28(1)
O(3)	2188(2)	2347(2)	7765(1)	27(1)
O(4)	3480(2)	1435(2)	8639(1)	24(1)
O(5)	2248(2)	1778(2)	9598(1)	32(1)
O(6)	-2884(2)	4520(2)	8367(2)	44(1)
Cu(1)	1667(1)	2267(1)	6311(1)	18(1)

F(1)	252(2)	1164(2)	9995(2)	47(1)
F(2)	555(2)	475(2)	8972(2)	54(1)
F(3)	-743(2)	1578(2)	8831(2)	54(1)
F(4)	1260(2)	3021(2)	10408(2)	51(1)
F(5)	1654(3)	3803(2)	9456(2)	69(1)
F(6)	-69(2)	3420(2)	9373(2)	53(1)
F(7)	-2796(3)	3720(4)	6479(2)	129(2)
F(8)	-3657(2)	3111(2)	7275(3)	124(2)
F(9)	-1844(2)	3102(2)	7586(2)	77(1)
F(10)	-1548(3)	5350(4)	6959(2)	112(2)
F(11)	-1838(3)	6139(2)	7937(3)	104(2)
F(12)	-797(2)	4865(2)	8130(2)	55(1)

Table S3. Bond lengths [Å] and angles [°] for **11**.

C(1)-N(1)	1.476(4)
C(1)-C(2)	1.532(5)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-N(2)	1.502(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-N(1)	1.480(4)
C(3)-C(4)	1.534(5)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-N(3)	1.501(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-N(4)	1.488(4)
C(5)-C(6)	1.537(4)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-N(2)	1.496(4)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-N(4)	1.484(4)
C(7)-C(8)	1.539(4)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-N(3)	1.511(4)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-N(1)	1.479(4)
C(9)-C(10)	1.511(5)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.494(5)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900

C(11)-N(4)	1.494(4)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-N(2)	1.476(4)
C(12)-C(13)	1.530(4)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-O(2)	1.245(4)
C(13)-O(1)	1.259(4)
C(14)-N(3)	1.477(4)
C(14)-C(15)	1.532(4)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-O(3)	1.247(4)
C(15)-O(4)	1.248(4)
C(16)-F(1)	1.328(4)
C(16)-F(3)	1.334(4)
C(16)-F(2)	1.336(4)
C(16)-C(17)	1.517(5)
C(17)-O(5)	1.376(4)
C(17)-C(18)	1.525(5)
C(17)-H(17)	1.0000
C(18)-F(4)	1.328(5)
C(18)-F(5)	1.328(4)
C(18)-F(6)	1.328(4)
C(19)-F(8)	1.319(6)
C(19)-F(7)	1.323(7)
C(19)-F(9)	1.327(6)
C(19)-C(20)	1.510(5)
C(20)-O(6)	1.375(4)
C(20)-C(21)	1.509(5)
C(20)-H(20)	1.0000
C(21)-F(11)	1.303(5)
C(21)-F(12)	1.312(4)
C(21)-F(10)	1.331(5)
N(1)-Cu(1)	2.201(3)
N(2)-Cu(1)	2.003(3)

N(3)-Cu(1)	2.014(3)
N(4)-Cu(1)	2.002(3)
O(1)-Cu(1)	2.003(2)
O(5)-H(5)	0.8400
O(6)-H(6)	0.8400

N(1)-C(1)-C(2)	110.8(3)
N(1)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1A)	109.5
N(1)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	108.1
N(2)-C(2)-C(1)	114.6(3)
N(2)-C(2)-H(2A)	108.6
C(1)-C(2)-H(2A)	108.6
N(2)-C(2)-H(2B)	108.6
C(1)-C(2)-H(2B)	108.6
H(2A)-C(2)-H(2B)	107.6
N(1)-C(3)-C(4)	110.5(3)
N(1)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3A)	109.5
N(1)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
N(3)-C(4)-C(3)	112.2(2)
N(3)-C(4)-H(4A)	109.2
C(3)-C(4)-H(4A)	109.2
N(3)-C(4)-H(4B)	109.2
C(3)-C(4)-H(4B)	109.2
H(4A)-C(4)-H(4B)	107.9
N(4)-C(5)-C(6)	109.7(3)
N(4)-C(5)-H(5A)	109.7
C(6)-C(5)-H(5A)	109.7
N(4)-C(5)-H(5B)	109.7
C(6)-C(5)-H(5B)	109.7
H(5A)-C(5)-H(5B)	108.2
N(2)-C(6)-C(5)	110.3(2)

N(2)-C(6)-H(6A)	109.6
C(5)-C(6)-H(6A)	109.6
N(2)-C(6)-H(6B)	109.6
C(5)-C(6)-H(6B)	109.6
H(6A)-C(6)-H(6B)	108.1
N(4)-C(7)-C(8)	111.8(3)
N(4)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7A)	109.3
N(4)-C(7)-H(7B)	109.3
C(8)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	107.9
N(3)-C(8)-C(7)	113.6(2)
N(3)-C(8)-H(8A)	108.8
C(7)-C(8)-H(8A)	108.8
N(3)-C(8)-H(8B)	108.8
C(7)-C(8)-H(8B)	108.8
H(8A)-C(8)-H(8B)	107.7
N(1)-C(9)-C(10)	116.0(3)
N(1)-C(9)-H(9A)	108.3
C(10)-C(9)-H(9A)	108.3
N(1)-C(9)-H(9B)	108.3
C(10)-C(9)-H(9B)	108.3
H(9A)-C(9)-H(9B)	107.4
C(11)-C(10)-C(9)	117.7(3)
C(11)-C(10)-H(10A)	107.9
C(9)-C(10)-H(10A)	107.9
C(11)-C(10)-H(10B)	107.9
C(9)-C(10)-H(10B)	107.9
H(10A)-C(10)-H(10B)	107.2
N(4)-C(11)-C(10)	118.4(3)
N(4)-C(11)-H(11A)	107.7
C(10)-C(11)-H(11A)	107.7
N(4)-C(11)-H(11B)	107.7
C(10)-C(11)-H(11B)	107.7
H(11A)-C(11)-H(11B)	107.1
N(2)-C(12)-C(13)	110.7(2)
N(2)-C(12)-H(12A)	109.5

C(13)-C(12)-H(12A)	109.5
N(2)-C(12)-H(12B)	109.5
C(13)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	108.1
O(2)-C(13)-O(1)	125.0(3)
O(2)-C(13)-C(12)	118.0(3)
O(1)-C(13)-C(12)	117.0(3)
N(3)-C(14)-C(15)	113.1(2)
N(3)-C(14)-H(14A)	109.0
C(15)-C(14)-H(14A)	109.0
N(3)-C(14)-H(14B)	109.0
C(15)-C(14)-H(14B)	109.0
H(14A)-C(14)-H(14B)	107.8
O(3)-C(15)-O(4)	126.8(3)
O(3)-C(15)-C(14)	118.9(3)
O(4)-C(15)-C(14)	114.3(3)
F(1)-C(16)-F(3)	106.6(3)
F(1)-C(16)-F(2)	107.2(3)
F(3)-C(16)-F(2)	106.3(3)
F(1)-C(16)-C(17)	113.5(3)
F(3)-C(16)-C(17)	112.9(3)
F(2)-C(16)-C(17)	110.0(3)
O(5)-C(17)-C(16)	109.6(3)
O(5)-C(17)-C(18)	108.3(3)
C(16)-C(17)-C(18)	112.0(3)
O(5)-C(17)-H(17)	109.0
C(16)-C(17)-H(17)	109.0
C(18)-C(17)-H(17)	109.0
F(4)-C(18)-F(5)	107.4(3)
F(4)-C(18)-F(6)	107.0(3)
F(5)-C(18)-F(6)	107.7(3)
F(4)-C(18)-C(17)	112.7(3)
F(5)-C(18)-C(17)	109.2(3)
F(6)-C(18)-C(17)	112.6(3)
F(8)-C(19)-F(7)	108.2(4)
F(8)-C(19)-F(9)	107.9(5)
F(7)-C(19)-F(9)	106.9(4)

F(8)-C(19)-C(20)	109.3(3)
F(7)-C(19)-C(20)	110.9(5)
F(9)-C(19)-C(20)	113.5(4)
O(6)-C(20)-C(21)	108.1(3)
O(6)-C(20)-C(19)	109.3(4)
C(21)-C(20)-C(19)	112.8(3)
O(6)-C(20)-H(20)	108.9
C(21)-C(20)-H(20)	108.9
C(19)-C(20)-H(20)	108.9
F(11)-C(21)-F(12)	107.0(4)
F(11)-C(21)-F(10)	107.9(4)
F(12)-C(21)-F(10)	105.3(4)
F(11)-C(21)-C(20)	110.1(4)
F(12)-C(21)-C(20)	114.6(3)
F(10)-C(21)-C(20)	111.5(3)
C(1)-N(1)-C(9)	112.9(3)
C(1)-N(1)-C(3)	115.1(3)
C(9)-N(1)-C(3)	113.8(3)
C(1)-N(1)-Cu(1)	96.78(18)
C(9)-N(1)-Cu(1)	120.5(2)
C(3)-N(1)-Cu(1)	95.92(18)
C(12)-N(2)-C(6)	113.3(3)
C(12)-N(2)-C(2)	112.3(2)
C(6)-N(2)-C(2)	113.9(2)
C(12)-N(2)-Cu(1)	103.41(18)
C(6)-N(2)-Cu(1)	106.95(18)
C(2)-N(2)-Cu(1)	106.03(19)
C(14)-N(3)-C(4)	111.3(2)
C(14)-N(3)-C(8)	111.2(2)
C(4)-N(3)-C(8)	113.5(2)
C(14)-N(3)-Cu(1)	107.10(18)
C(4)-N(3)-Cu(1)	107.47(18)
C(8)-N(3)-Cu(1)	105.88(18)
C(7)-N(4)-C(5)	112.8(2)
C(7)-N(4)-C(11)	112.6(3)
C(5)-N(4)-C(11)	110.5(2)
C(7)-N(4)-Cu(1)	102.58(18)

C(5)-N(4)-Cu(1)	99.09(18)
C(11)-N(4)-Cu(1)	118.4(2)
C(13)-O(1)-Cu(1)	111.72(19)
C(17)-O(5)-H(5)	109.5
C(20)-O(6)-H(6)	109.5
N(4)-Cu(1)-N(2)	87.81(10)
N(4)-Cu(1)-O(1)	164.72(10)
N(2)-Cu(1)-O(1)	83.69(10)
N(4)-Cu(1)-N(3)	89.47(10)
N(2)-Cu(1)-N(3)	173.64(11)
O(1)-Cu(1)-N(3)	100.19(9)
N(4)-Cu(1)-N(1)	97.56(10)
N(2)-Cu(1)-N(1)	88.08(10)
O(1)-Cu(1)-N(1)	94.83(9)
N(3)-Cu(1)-N(1)	86.57(10)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **11**. 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}
C(1)	32(2)	23(2)	23(2)	-4(1)	5(1)	-2(1)
C(2)	25(2)	27(2)	25(2)	-2(1)	2(1)	-1(1)
C(3)	32(2)	23(2)	27(2)	-2(1)	14(1)	6(1)
C(4)	23(2)	29(2)	26(2)	2(1)	13(1)	6(1)
C(5)	25(2)	20(2)	29(2)	-1(1)	7(1)	4(1)
C(6)	22(2)	19(2)	39(2)	-1(1)	5(1)	4(1)
C(7)	23(2)	21(2)	30(2)	-3(1)	5(1)	-2(1)
C(8)	21(2)	21(2)	31(2)	0(1)	7(1)	-2(1)
C(9)	37(2)	30(2)	22(2)	3(1)	11(1)	2(1)
C(10)	50(2)	39(2)	37(2)	8(2)	15(2)	2(2)
C(11)	43(2)	22(2)	30(2)	7(1)	13(2)	3(1)
C(12)	22(2)	28(2)	31(2)	1(1)	9(1)	-1(1)
C(13)	25(2)	24(2)	21(2)	-2(1)	7(1)	-3(1)
C(14)	22(1)	21(2)	25(2)	2(1)	5(1)	3(1)
C(15)	23(2)	19(1)	23(2)	-2(1)	6(1)	-3(1)
C(16)	30(2)	34(2)	40(2)	-7(2)	13(2)	-1(1)
C(17)	23(2)	36(2)	23(2)	4(1)	8(1)	3(1)
C(18)	36(2)	31(2)	48(2)	4(2)	18(2)	-1(2)
C(19)	20(2)	68(3)	103(4)	-53(3)	14(2)	-2(2)
C(20)	27(2)	29(2)	27(2)	0(1)	9(1)	4(1)
C(21)	42(2)	38(2)	39(2)	12(2)	4(2)	-5(2)
N(1)	26(1)	23(1)	22(1)	0(1)	8(1)	2(1)
N(2)	21(1)	19(1)	24(1)	1(1)	5(1)	1(1)
N(3)	21(1)	21(1)	23(1)	1(1)	9(1)	2(1)
N(4)	23(1)	18(1)	22(1)	0(1)	6(1)	1(1)
O(1)	24(1)	20(1)	28(1)	4(1)	8(1)	1(1)
O(2)	31(1)	25(1)	30(1)	4(1)	11(1)	-6(1)
O(3)	26(1)	29(1)	27(1)	3(1)	10(1)	6(1)
O(4)	27(1)	22(1)	21(1)	0(1)	2(1)	2(1)
O(5)	26(1)	44(1)	27(1)	6(1)	9(1)	5(1)
O(6)	38(1)	65(2)	35(1)	15(1)	19(1)	18(1)
Cu(1)	18(1)	16(1)	21(1)	1(1)	6(1)	1(1)

F(1)	55(1)	43(1)	51(1)	4(1)	30(1)	-11(1)
F(2)	56(2)	39(1)	77(2)	-22(1)	32(1)	-7(1)
F(3)	26(1)	66(2)	67(2)	-8(1)	6(1)	-5(1)
F(4)	63(2)	49(1)	43(1)	-14(1)	16(1)	0(1)
F(5)	78(2)	34(1)	112(3)	1(1)	54(2)	-16(1)
F(6)	51(1)	42(1)	71(2)	9(1)	24(1)	20(1)
F(7)	58(2)	238(5)	78(2)	-111(3)	-4(2)	30(3)
F(8)	35(2)	55(2)	283(6)	-76(3)	48(2)	-17(1)
F(9)	34(1)	43(2)	154(3)	-37(2)	26(2)	5(1)
F(10)	66(2)	213(5)	56(2)	58(2)	14(2)	-43(3)
F(11)	78(2)	29(2)	184(4)	-10(2)	5(2)	-10(1)
F(12)	33(1)	55(2)	66(2)	11(1)	-2(1)	-12(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **11**.

	x	y	z	U(eq)
H(1A)	798	697	5122	32
H(1B)	543	1216	4266	32
H(2A)	-438	2514	4641	33
H(2B)	-938	1504	4891	33
H(3A)	3091	1091	4926	31
H(3B)	2645	665	5636	31
H(4A)	4417	1401	6211	30
H(4B)	4036	2409	5716	30
H(5A)	446	4709	6353	30
H(5B)	721	3821	6994	30
H(6A)	-1024	3399	6128	33
H(6B)	-620	3674	5362	33
H(7A)	2564	4016	7366	30
H(7B)	2922	4740	6752	30
H(8A)	4099	3599	6463	30
H(8B)	4276	3380	7386	30
H(9A)	1134	2811	4173	35
H(9B)	2413	2488	4260	35
H(10A)	3087	3623	5279	49
H(10B)	2331	4178	4505	49
H(11A)	1885	4901	5510	37
H(11B)	826	4211	5098	37
H(12A)	-1201	1381	6064	32
H(12B)	-506	1993	6834	32
H(14A)	4557	1760	7640	27
H(14B)	3651	930	7214	27
H(17)	1119	2263	8652	33
H(20)	-3463	5021	7286	33
H(5)	2602	1679	9260	48
H(6)	-3537	4691	8377	66

X-ray Data for Cu-CB-TR2A (**12**)

Table S6. Crystal data and structure refinement for **12**.

Identification code	wong157	
Empirical formula	C45 H78 Cl3 Cu3 N12 Na3 O27	
Formula weight	1585.13	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 20.2068(19) Å	α= 90°.
	b = 24.613(2) Å	β= 105.8090(10)°.
	c = 13.0914(12) Å	γ = 90°.
Volume	6264.6(10) Å^3	
Z	4	
Density (calculated)	1.681 Mg/m^3	
Absorption coefficient	1.252 mm^{-1}	
F(000)	3276	
Crystal size	0.40 x 0.15 x 0.05 mm^3	
Theta range for data collection	1.33 to 27.82°.	
Index ranges	-25<=h<=26, -26<=k<=31, -16<=l<=17	
Reflections collected	37892	
Independent reflections	13599 [R(int) = 0.0675]	
Completeness to theta = 25.00°	98.8 %	
Absorption correction	multi-scan/sadabs	
Max. and min. transmission	0.9401 and 0.6344	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13599 / 44 / 797	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0784, wR2 = 0.1711	
R indices (all data)	R1 = 0.1396, wR2 = 0.2027	
Largest diff. peak and hole	1.332 and -1.200 e.Å^{-3}	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **12**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	4946(1)	1542(1)	-1621(1)	19(1)
Cu(2)	2141(1)	-38(1)	4979(1)	19(1)
Cu(3)	56(1)	1717(1)	310(1)	40(1)
Cl(1)	4716(1)	1020(1)	3373(1)	26(1)
Cl(3)	7502(1)	2399(1)	2126(2)	46(1)
Cl(2)	2558(1)	86(1)	-190(2)	44(1)
Na(1)	2743(1)	2472(1)	94(2)	26(1)
Na(2)	3075(1)	1205(1)	1397(2)	26(1)
Na(3)	2218(1)	2085(1)	2688(2)	27(1)
O(1)	3564(2)	1743(2)	340(4)	24(1)
O(2)	4308(2)	2042(2)	-521(3)	22(1)
O(3)	3993(2)	1447(2)	-2529(4)	24(1)
O(4)	3157(2)	2004(2)	-3409(4)	39(1)
O(5)	2541(2)	1140(2)	2753(4)	29(1)
O(6)	2179(2)	874(2)	4132(3)	24(1)
O(7)	1315(2)	-186(2)	3819(4)	27(1)
O(8)	198(2)	40(3)	3322(4)	47(2)
O(9)	2199(2)	1837(2)	825(4)	30(1)
O(10)	1226(2)	1848(2)	1308(4)	34(1)
O(11)	256(3)	2378(2)	-439(5)	40(1)
O(12)	734(4)	3171(3)	199(9)	109(4)
O(13)	1921(3)	93(4)	-908(5)	80(3)
O(14)	3055(4)	-188(3)	-578(5)	81(3)
O(15)	2822(8)	581(6)	97(13)	82(6)
O(16)	2463(7)	-171(6)	751(9)	63(5)
O(15A)	2795(8)	270(6)	810(11)	78(6)
O(16A)	2594(10)	670(6)	-579(17)	95(7)
O(17)	4098(3)	853(3)	2604(5)	52(2)
O(18)	5226(3)	1129(2)	2809(5)	50(2)
O(19)	4950(3)	584(2)	4087(5)	50(2)
O(20)	4589(3)	1499(2)	3900(5)	53(2)
O(21)	7603(6)	1897(5)	1729(10)	51(4)

O(22)	6910(6)	2538(6)	1412(11)	71(5)
O(23)	7944(7)	2705(6)	1938(13)	83(6)
O(24)	7406(10)	2370(8)	2986(11)	99(7)
O(21A)	8122(5)	2278(5)	2694(9)	60(4)
O(22A)	7351(6)	2364(5)	1134(8)	73(4)
O(23A)	7412(5)	2946(4)	2346(9)	58(4)
O(24A)	7047(5)	2184(5)	2594(9)	57(3)
O(25)	3354(2)	2147(2)	3941(4)	28(1)
O(26)	1825(2)	1941(2)	4238(4)	25(1)
O(27)	2328(7)	3043(5)	3116(11)	47(5)
O(27A)	2012(5)	3013(4)	2300(8)	37(3)
N(1)	4867(3)	992(2)	-569(4)	19(1)
N(2)	4999(3)	2118(2)	-2626(4)	23(1)
N(3)	5694(3)	1090(3)	-2297(5)	38(2)
N(4)	5849(3)	1810(2)	-626(4)	24(1)
N(5)	2822(3)	-132(2)	4159(4)	21(1)
N(6)	1503(3)	212(2)	5800(4)	25(1)
N(7)	2938(3)	156(2)	6273(4)	21(1)
N(8)	2204(3)	-817(2)	5867(4)	28(1)
N(9)	555(4)	1184(3)	-357(6)	53(2)
N(10)	-4(4)	1128(4)	1394(6)	57(2)
N(12)	-352(4)	2235(4)	1096(7)	72(3)
C(1)	4035(3)	1674(3)	-104(5)	18(1)
C(2)	4242(3)	1082(3)	-189(5)	23(2)
C(3)	3772(3)	1899(3)	-2966(5)	28(2)
C(4)	4296(3)	2353(3)	-2910(6)	29(2)
C(5)	5122(4)	1852(3)	-3576(6)	31(2)
C(6)	5694(5)	1439(4)	-3311(7)	45(2)
C(7)	5450(5)	559(4)	-2576(8)	54(2)
C(8)	5311(4)	268(3)	-1654(6)	35(2)
C(9)	4759(4)	463(3)	-1172(6)	28(2)
C(10)	5514(3)	1034(3)	316(5)	23(1)
C(11)	5786(4)	1619(3)	426(5)	26(2)
C(12)	6483(4)	1609(3)	-872(6)	35(2)
C(13)	6371(4)	1102(4)	-1521(6)	39(2)
C(14)	5742(4)	2409(3)	-881(6)	34(2)
C(15)	5548(4)	2508(3)	-2080(6)	31(2)

C(16)	2438(3)	790(3)	3379(5)	21(1)
C(17)	2612(3)	199(3)	3172(5)	24(2)
C(18)	775(4)	45(3)	3959(6)	32(2)
C(19)	879(3)	376(3)	4981(6)	32(2)
C(20)	1376(4)	-242(3)	6467(6)	32(2)
C(21)	1509(4)	-800(3)	6044(6)	34(2)
C(22)	2304(4)	-1246(3)	5157(6)	35(2)
C(23)	2918(4)	-1149(3)	4712(6)	32(2)
C(24)	2840(4)	-717(3)	3856(5)	28(2)
C(25)	3508(3)	67(3)	4847(5)	26(2)
C(26)	3423(3)	424(3)	5771(6)	29(2)
C(27)	3267(3)	-335(3)	6869(5)	29(2)
C(28)	2753(4)	-785(3)	6872(6)	34(2)
C(29)	2637(4)	516(3)	6953(6)	31(2)
C(30)	1894(4)	670(3)	6430(6)	30(2)
C(31)	1576(4)	1723(3)	682(6)	27(2)
C(32)	1230(4)	1420(3)	-331(7)	42(2)
C(33)	381(5)	2770(4)	226(10)	63(3)
C(34)	100(5)	2706(5)	1209(9)	77(4)
C(35)	-1055(3)	2359(2)	393(5)	111(6)
N(11)	-1039(3)	1506(2)	-307(5)	71(5)
C(36)	-1528(3)	1865(2)	-49(5)	53(5)
C(37)	-1141(3)	1434(2)	-1444(5)	135(7)
C(38)	-595(3)	1058(2)	-1629(5)	171(17)
C(43)	-1188(3)	980(2)	115(5)	130(12)
N(11A)	-914(3)	1319(2)	-661(5)	80(7)
C(36A)	-1329(3)	1788(2)	-271(5)	129(14)
C(37A)	-1177(3)	1480(2)	-1756(5)	135(7)
C(38A)	-557(3)	1085(2)	-1911(5)	51(6)
C(43A)	-910(3)	738(2)	-170(5)	55(7)
C(39)	173(3)	1075(2)	-1498(5)	113(6)
C(40)	641(7)	679(5)	285(10)	90(4)
C(41)	594(5)	763(4)	1369(8)	57(3)
C(42)	-674(5)	841(5)	1100(8)	82(4)
C(44)	80(5)	1450(5)	2339(9)	72(3)
C(45)	-363(6)	1943(6)	2162(11)	93(4)

Table S8. Bond lengths [Å] and angles [°] for **12**.

Cu(1)-N(2)	1.955(6)
Cu(1)-N(1)	1.968(5)
Cu(1)-O(3)	1.981(4)
Cu(1)-N(4)	2.041(5)
Cu(1)-N(3)	2.244(6)
Cu(2)-O(7)	1.960(4)
Cu(2)-N(5)	1.975(5)
Cu(2)-N(6)	1.988(6)
Cu(2)-N(7)	2.051(5)
Cu(2)-N(8)	2.228(6)
Cu(3)-N(12)	1.956(9)
Cu(3)-N(9)	1.995(9)
Cu(3)-O(11)	1.997(6)
Cu(3)-N(10)	2.055(8)
Cu(3)-N(11)	2.202(5)
Cu(3)-N(11A)	2.250(5)
Cu(3)-O(10)	2.391(5)
Cl(1)-O(19)	1.417(5)
Cl(1)-O(20)	1.424(6)
Cl(1)-O(17)	1.434(6)
Cl(1)-O(18)	1.446(5)
Cl(3)-O(24)	1.196(12)
Cl(3)-O(23)	1.243(12)
Cl(3)-O(22A)	1.254(10)
Cl(3)-O(21A)	1.305(9)
Cl(3)-O(24A)	1.343(9)
Cl(3)-O(22)	1.347(11)
Cl(3)-O(21)	1.377(10)
Cl(3)-O(23A)	1.400(9)
Cl(2)-O(15)	1.341(12)
Cl(2)-O(15A)	1.344(13)
Cl(2)-O(13)	1.372(7)
Cl(2)-O(14)	1.414(6)
Cl(2)-O(16)	1.443(11)
Cl(2)-O(16A)	1.533(15)

Na(1)-O(9)	2.266(5)
Na(1)-O(4)#1	2.305(6)
Na(1)-O(26)#2	2.377(5)
Na(1)-O(25)#2	2.387(5)
Na(1)-O(1)	2.405(5)
Na(1)-O(27)#2	2.798(15)
Na(1)-Na(3)#2	3.226(4)
Na(1)-Na(2)	3.530(4)
Na(1)-Na(3)	3.940(4)
Na(2)-O(15)	2.246(12)
Na(2)-O(5)	2.320(5)
Na(2)-O(1)	2.322(5)
Na(2)-O(9)	2.322(5)
Na(2)-O(17)	2.397(6)
Na(2)-O(15A)	2.443(14)
Na(2)-O(16A)	2.83(2)
Na(2)-Na(3)	3.484(4)
Na(3)-O(27A)	2.352(9)
Na(3)-O(10)	2.377(5)
Na(3)-O(26)	2.399(5)
Na(3)-O(5)	2.411(6)
Na(3)-O(27)	2.419(12)
Na(3)-O(25)	2.434(5)
Na(3)-O(9)	2.504(6)
Na(3)-C(31)	2.742(8)
Na(3)-Na(1)#1	3.226(4)
O(1)-C(1)	1.254(7)
O(2)-C(1)	1.260(7)
O(3)-C(3)	1.275(8)
O(4)-C(3)	1.247(8)
O(4)-Na(1)#2	2.305(6)
O(5)-C(16)	1.246(8)
O(6)-C(16)	1.252(7)
O(7)-C(18)	1.286(8)
O(8)-C(18)	1.235(8)
O(9)-C(31)	1.253(8)
O(10)-C(31)	1.259(8)

O(11)-C(33)	1.278(11)
O(12)-C(33)	1.224(11)
O(25)-Na(1)#1	2.387(5)
O(26)-Na(1)#1	2.378(5)
O(27)-Na(1)#1	2.798(15)
N(1)-C(10)	1.495(8)
N(1)-C(2)	1.495(8)
N(1)-C(9)	1.508(8)
N(2)-C(4)	1.483(8)
N(2)-C(5)	1.485(8)
N(2)-C(15)	1.495(9)
N(3)-C(7)	1.410(11)
N(3)-C(13)	1.464(9)
N(3)-C(6)	1.581(11)
N(4)-C(12)	1.489(8)
N(4)-C(11)	1.493(8)
N(4)-C(14)	1.515(9)
N(5)-C(17)	1.489(8)
N(5)-C(24)	1.496(9)
N(5)-C(25)	1.515(8)
N(6)-C(19)	1.471(8)
N(6)-C(20)	1.482(9)
N(6)-C(30)	1.491(9)
N(7)-C(26)	1.477(8)
N(7)-C(27)	1.492(8)
N(7)-C(29)	1.496(9)
N(8)-C(22)	1.457(9)
N(8)-C(28)	1.474(9)
N(8)-C(21)	1.485(9)
N(9)-C(32)	1.474(10)
N(9)-C(40)	1.484(13)
N(9)-C(39)	1.506(9)
N(10)-C(44)	1.440(14)
N(10)-C(42)	1.484(11)
N(10)-C(41)	1.514(12)
N(12)-C(34)	1.458(15)
N(12)-C(35)	1.499(9)

N(12)-C(45)	1.575(14)
C(1)-C(2)	1.529(9)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.527(10)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.508(11)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.495(12)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.501(10)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.534(9)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.492(11)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.531(10)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.538(9)
C(17)-H(17A)	0.9900

C(17)-H(17B)	0.9900
C(18)-C(19)	1.532(10)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.531(11)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.526(10)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.523(10)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.542(10)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.518(10)
C(27)-H(27B)	0.9900
C(27)-H(27C)	0.9900
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(30)	1.520(10)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-C(32)	1.516(10)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-C(34)	1.550(15)
C(34)-H(34A)	0.9900

C(34)-H(34B)	0.9900
C(35)-C(36)	1.5573
C(35)-C(36A)	1.6645
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
N(11)-C(36)	1.4313
N(11)-C(37)	1.4571
N(11)-C(43)	1.4717
N(11)-H(36D)	1.4069
C(36)-H(36A)	0.9601
C(36)-H(36B)	0.9599
C(36)-H(36C)	1.0795
C(36)-H(36D)	0.7103
C(37)-C(38)	1.5096
C(37)-H(37A)	0.9599
C(37)-H(37B)	0.9601
C(37)-H(37C)	1.2041
C(37)-H(37D)	1.1386
C(38)-C(39)	1.5152
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	1.3437
C(38)-H(38D)	0.8351
C(43)-C(42)	1.460(9)
C(43)-H(43A)	0.9600
C(43)-H(43B)	0.9602
C(43)-H(43D)	1.1818
N(11A)-C(37A)	1.4426
N(11A)-C(43A)	1.5664
N(11A)-C(36A)	1.5930
C(36A)-H(36A)	1.1890
C(36A)-H(36B)	1.4325
C(36A)-H(36C)	0.9601
C(36A)-H(36D)	0.9601
C(37A)-C(38A)	1.6431
C(37A)-H(37A)	0.7474
C(37A)-H(37B)	0.9621

C(37A)-H(37C)	0.9600
C(37A)-H(37D)	0.9601
C(38A)-C(39)	1.4269
C(38A)-H(38A)	0.7064
C(38A)-H(38B)	1.2761
C(38A)-H(38C)	0.9600
C(38A)-H(38D)	0.9602
C(43A)-C(42)	1.620(11)
C(43A)-H(43A)	0.5877
C(43A)-H(43C)	0.9600
C(43A)-H(43D)	0.9600
C(39)-H(39A)	0.9899
C(39)-H(39B)	0.9901
C(40)-C(41)	1.462(15)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(44)-C(45)	1.489(16)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900

N(2)-Cu(1)-N(1)	176.8(2)
N(2)-Cu(1)-O(3)	84.5(2)
N(1)-Cu(1)-O(3)	95.1(2)
N(2)-Cu(1)-N(4)	89.5(2)
N(1)-Cu(1)-N(4)	90.2(2)
O(3)-Cu(1)-N(4)	167.0(2)
N(2)-Cu(1)-N(3)	85.8(3)
N(1)-Cu(1)-N(3)	97.3(2)
O(3)-Cu(1)-N(3)	110.7(2)
N(4)-Cu(1)-N(3)	80.2(2)
O(7)-Cu(2)-N(5)	97.4(2)

O(7)-Cu(2)-N(6)	86.3(2)
N(5)-Cu(2)-N(6)	168.7(2)
O(7)-Cu(2)-N(7)	174.0(2)
N(5)-Cu(2)-N(7)	88.3(2)
N(6)-Cu(2)-N(7)	87.7(2)
O(7)-Cu(2)-N(8)	99.2(2)
N(5)-Cu(2)-N(8)	103.4(2)
N(6)-Cu(2)-N(8)	86.4(2)
N(7)-Cu(2)-N(8)	81.3(2)
N(12)-Cu(3)-N(9)	174.1(3)
N(12)-Cu(3)-O(11)	84.2(3)
N(9)-Cu(3)-O(11)	97.3(3)
N(12)-Cu(3)-N(10)	89.1(4)
N(9)-Cu(3)-N(10)	88.3(3)
O(11)-Cu(3)-N(10)	166.3(3)
N(12)-Cu(3)-N(11)	79.6(3)
N(9)-Cu(3)-N(11)	105.2(3)
O(11)-Cu(3)-N(11)	109.2(2)
N(10)-Cu(3)-N(11)	81.0(2)
N(12)-Cu(3)-N(11A)	98.9(3)
N(9)-Cu(3)-N(11A)	86.1(3)
O(11)-Cu(3)-N(11A)	109.9(2)
N(10)-Cu(3)-N(11A)	82.9(3)
N(11)-Cu(3)-N(11A)	19.3
N(12)-Cu(3)-O(10)	96.9(3)
N(9)-Cu(3)-O(10)	77.6(2)
O(11)-Cu(3)-O(10)	81.8(2)
N(10)-Cu(3)-O(10)	87.3(2)
N(11)-Cu(3)-O(10)	167.9(2)
N(11A)-Cu(3)-O(10)	161.2(2)
O(19)-Cl(1)-O(20)	112.3(4)
O(19)-Cl(1)-O(17)	108.5(4)
O(20)-Cl(1)-O(17)	109.8(4)
O(19)-Cl(1)-O(18)	108.8(4)
O(20)-Cl(1)-O(18)	109.9(4)
O(17)-Cl(1)-O(18)	107.4(4)
O(24)-Cl(3)-O(23)	122.1(12)

O(24)-Cl(3)-O(22A)	156.3(11)
O(23)-Cl(3)-O(22A)	79.7(9)
O(24)-Cl(3)-O(21A)	80.1(10)
O(23)-Cl(3)-O(21A)	67.7(9)
O(22A)-Cl(3)-O(21A)	119.9(8)
O(24)-Cl(3)-O(24A)	40.6(9)
O(23)-Cl(3)-O(24A)	161.1(9)
O(22A)-Cl(3)-O(24A)	116.3(7)
O(21A)-Cl(3)-O(24A)	108.7(7)
O(24)-Cl(3)-O(22)	109.1(10)
O(23)-Cl(3)-O(22)	105.0(9)
O(22A)-Cl(3)-O(22)	51.6(8)
O(21A)-Cl(3)-O(22)	170.7(8)
O(24A)-Cl(3)-O(22)	80.1(8)
O(24)-Cl(3)-O(21)	112.4(10)
O(23)-Cl(3)-O(21)	106.3(9)
O(22A)-Cl(3)-O(21)	64.3(8)
O(21A)-Cl(3)-O(21)	78.0(7)
O(24A)-Cl(3)-O(21)	90.5(8)
O(22)-Cl(3)-O(21)	99.3(8)
O(24)-Cl(3)-O(23A)	78.5(10)
O(23)-Cl(3)-O(23A)	66.3(9)
O(22A)-Cl(3)-O(23A)	105.6(7)
O(21A)-Cl(3)-O(23A)	105.1(7)
O(24A)-Cl(3)-O(23A)	98.2(7)
O(22)-Cl(3)-O(23A)	75.9(8)
O(21)-Cl(3)-O(23A)	169.1(7)
O(15)-Cl(2)-O(15A)	54.0(8)
O(15)-Cl(2)-O(13)	114.1(9)
O(15A)-Cl(2)-O(13)	133.0(8)
O(15)-Cl(2)-O(14)	105.5(8)
O(15A)-Cl(2)-O(14)	114.3(8)
O(13)-Cl(2)-O(14)	112.6(4)
O(15)-Cl(2)-O(16)	107.1(9)
O(15A)-Cl(2)-O(16)	54.0(8)
O(13)-Cl(2)-O(16)	105.8(6)
O(14)-Cl(2)-O(16)	111.8(6)

O(15)-Cl(2)-O(16A)	36.0(8)
O(15A)-Cl(2)-O(16A)	88.3(10)
O(13)-Cl(2)-O(16A)	83.2(9)
O(14)-Cl(2)-O(16A)	103.0(8)
O(16)-Cl(2)-O(16A)	136.3(10)
O(9)-Na(1)-O(4)#1	97.6(2)
O(9)-Na(1)-O(26)#2	102.27(19)
O(4)#1-Na(1)-O(26)#2	96.7(2)
O(9)-Na(1)-O(25)#2	158.7(2)
O(4)#1-Na(1)-O(25)#2	100.8(2)
O(26)#2-Na(1)-O(25)#2	86.27(17)
O(9)-Na(1)-O(1)	79.96(18)
O(4)#1-Na(1)-O(1)	103.1(2)
O(26)#2-Na(1)-O(1)	159.7(2)
O(25)#2-Na(1)-O(1)	85.44(17)
O(9)-Na(1)-O(27)#2	91.2(3)
O(4)#1-Na(1)-O(27)#2	171.2(3)
O(26)#2-Na(1)-O(27)#2	80.9(3)
O(25)#2-Na(1)-O(27)#2	70.7(3)
O(1)-Na(1)-O(27)#2	78.9(3)
O(9)-Na(1)-Na(3)#2	125.25(16)
O(4)#1-Na(1)-Na(3)#2	125.99(19)
O(26)#2-Na(1)-Na(3)#2	47.79(13)
O(25)#2-Na(1)-Na(3)#2	48.63(13)
O(1)-Na(1)-Na(3)#2	114.44(15)
O(27)#2-Na(1)-Na(3)#2	46.7(3)
O(9)-Na(1)-Na(2)	40.29(13)
O(4)#1-Na(1)-Na(2)	96.09(17)
O(26)#2-Na(1)-Na(2)	141.82(15)
O(25)#2-Na(1)-Na(2)	126.12(15)
O(1)-Na(1)-Na(2)	40.80(12)
O(27)#2-Na(1)-Na(2)	91.0(3)
Na(3)#2-Na(1)-Na(2)	137.63(11)
O(9)-Na(1)-Na(3)	36.31(14)
O(4)#1-Na(1)-Na(3)	61.50(16)
O(26)#2-Na(1)-Na(3)	101.22(14)
O(25)#2-Na(1)-Na(3)	161.24(16)

O(1)-Na(1)-Na(3)	92.42(13)
O(27)#2-Na(1)-Na(3)	127.2(3)
Na(3)#2-Na(1)-Na(3)	146.01(11)
Na(2)-Na(1)-Na(3)	55.27(7)
O(15)-Na(2)-O(5)	118.4(4)
O(15)-Na(2)-O(1)	89.1(4)
O(5)-Na(2)-O(1)	149.0(2)
O(15)-Na(2)-O(9)	102.6(5)
O(5)-Na(2)-O(9)	79.66(18)
O(1)-Na(2)-O(9)	80.58(18)
O(15)-Na(2)-O(17)	103.3(5)
O(5)-Na(2)-O(17)	88.2(2)
O(1)-Na(2)-O(17)	99.7(2)
O(9)-Na(2)-O(17)	154.1(2)
O(15)-Na(2)-O(15A)	29.8(5)
O(5)-Na(2)-O(15A)	93.4(4)
O(1)-Na(2)-O(15A)	116.7(4)
O(9)-Na(2)-O(15A)	116.0(4)
O(17)-Na(2)-O(15A)	87.2(4)
O(15)-Na(2)-O(16A)	15.8(5)
O(5)-Na(2)-O(16A)	123.5(4)
O(1)-Na(2)-O(16A)	79.4(4)
O(9)-Na(2)-O(16A)	88.6(4)
O(17)-Na(2)-O(16A)	117.0(4)
O(15A)-Na(2)-O(16A)	44.1(5)
O(15)-Na(2)-Na(3)	138.8(4)
O(5)-Na(2)-Na(3)	43.58(14)
O(1)-Na(2)-Na(3)	106.44(15)
O(9)-Na(2)-Na(3)	45.90(14)
O(17)-Na(2)-Na(3)	111.00(18)
O(15A)-Na(2)-Na(3)	129.4(4)
O(16A)-Na(2)-Na(3)	129.8(4)
O(15)-Na(2)-Na(1)	105.3(5)
O(5)-Na(2)-Na(1)	111.33(15)
O(1)-Na(2)-Na(1)	42.59(13)
O(9)-Na(2)-Na(1)	39.13(13)
O(17)-Na(2)-Na(1)	130.89(19)

O(15A)-Na(2)-Na(1)	133.0(4)
O(16A)-Na(2)-Na(1)	89.8(3)
Na(3)-Na(2)-Na(1)	68.36(8)
O(27A)-Na(3)-O(10)	90.6(3)
O(27A)-Na(3)-O(26)	104.3(3)
O(10)-Na(3)-O(26)	101.59(18)
O(27A)-Na(3)-O(5)	167.1(3)
O(10)-Na(3)-O(5)	87.4(2)
O(26)-Na(3)-O(5)	88.64(18)
O(27A)-Na(3)-O(27)	26.3(3)
O(10)-Na(3)-O(27)	114.9(4)
O(26)-Na(3)-O(27)	88.8(4)
O(5)-Na(3)-O(27)	157.7(4)
O(27A)-Na(3)-O(25)	99.4(3)
O(10)-Na(3)-O(25)	166.5(2)
O(26)-Na(3)-O(25)	84.74(17)
O(5)-Na(3)-O(25)	80.79(18)
O(27)-Na(3)-O(25)	76.9(4)
O(27A)-Na(3)-O(9)	94.1(3)
O(10)-Na(3)-O(9)	54.13(16)
O(26)-Na(3)-O(9)	150.1(2)
O(5)-Na(3)-O(9)	74.43(18)
O(27)-Na(3)-O(9)	116.0(4)
O(25)-Na(3)-O(9)	115.65(18)
O(27A)-Na(3)-C(31)	95.7(3)
O(10)-Na(3)-C(31)	27.30(18)
O(26)-Na(3)-C(31)	125.6(2)
O(5)-Na(3)-C(31)	76.9(2)
O(27)-Na(3)-C(31)	121.9(4)
O(25)-Na(3)-C(31)	141.1(2)
O(9)-Na(3)-C(31)	27.15(17)
O(27A)-Na(3)-Na(1)#1	82.8(3)
O(10)-Na(3)-Na(1)#1	144.03(16)
O(26)-Na(3)-Na(1)#1	47.23(13)
O(5)-Na(3)-Na(1)#1	106.12(15)
O(27)-Na(3)-Na(1)#1	57.3(4)
O(25)-Na(3)-Na(1)#1	47.38(12)

O(9)-Na(3)-Na(1)#1	161.22(16)
C(31)-Na(3)-Na(1)#1	171.33(18)
O(27A)-Na(3)-Na(2)	125.5(3)
O(10)-Na(3)-Na(2)	84.63(15)
O(26)-Na(3)-Na(2)	129.89(16)
O(5)-Na(3)-Na(2)	41.57(12)
O(27)-Na(3)-Na(2)	133.8(3)
O(25)-Na(3)-Na(2)	82.18(14)
O(9)-Na(3)-Na(2)	41.75(12)
C(31)-Na(3)-Na(2)	60.07(16)
Na(1)#1-Na(3)-Na(2)	127.52(10)
O(27A)-Na(3)-Na(1)	69.7(2)
O(10)-Na(3)-Na(1)	76.91(14)
O(26)-Na(3)-Na(1)	173.62(16)
O(5)-Na(3)-Na(1)	97.45(14)
O(27)-Na(3)-Na(1)	86.3(3)
O(25)-Na(3)-Na(1)	98.06(14)
O(9)-Na(3)-Na(1)	32.40(13)
C(31)-Na(3)-Na(1)	54.63(15)
Na(1)#1-Na(3)-Na(1)	131.75(10)
Na(2)-Na(3)-Na(1)	56.37(7)
C(1)-O(1)-Na(2)	134.3(4)
C(1)-O(1)-Na(1)	128.5(4)
Na(2)-O(1)-Na(1)	96.60(18)
C(3)-O(3)-Cu(1)	109.3(4)
C(3)-O(4)-Na(1)#2	126.6(5)
C(16)-O(5)-Na(2)	138.4(4)
C(16)-O(5)-Na(3)	126.7(4)
Na(2)-O(5)-Na(3)	94.85(19)
C(18)-O(7)-Cu(2)	112.6(4)
C(31)-O(9)-Na(1)	132.4(4)
C(31)-O(9)-Na(2)	122.9(5)
Na(1)-O(9)-Na(2)	100.6(2)
C(31)-O(9)-Na(3)	87.1(4)
Na(1)-O(9)-Na(3)	111.3(2)
Na(2)-O(9)-Na(3)	92.35(18)
C(31)-O(10)-Na(3)	92.7(4)

C(31)-O(10)-Cu(3)	105.0(4)
Na(3)-O(10)-Cu(3)	162.2(2)
C(33)-O(11)-Cu(3)	108.0(6)
Cl(2)-O(15)-Na(2)	145.6(11)
Cl(2)-O(15A)-Na(2)	127.9(10)
Cl(2)-O(16A)-Na(2)	99.7(10)
Cl(1)-O(17)-Na(2)	142.1(4)
Na(1)#1-O(25)-Na(3)	84.00(17)
Na(1)#1-O(26)-Na(3)	84.98(17)
Na(3)-O(27)-Na(1)#1	76.0(4)
C(10)-N(1)-C(2)	111.8(5)
C(10)-N(1)-C(9)	115.9(5)
C(2)-N(1)-C(9)	106.7(5)
C(10)-N(1)-Cu(1)	106.0(4)
C(2)-N(1)-Cu(1)	111.5(4)
C(9)-N(1)-Cu(1)	104.8(4)
C(4)-N(2)-C(5)	109.2(5)
C(4)-N(2)-C(15)	113.8(6)
C(5)-N(2)-C(15)	114.3(5)
C(4)-N(2)-Cu(1)	103.1(4)
C(5)-N(2)-Cu(1)	107.3(4)
C(15)-N(2)-Cu(1)	108.3(4)
C(7)-N(3)-C(13)	113.2(7)
C(7)-N(3)-C(6)	111.4(7)
C(13)-N(3)-C(6)	111.1(7)
C(7)-N(3)-Cu(1)	109.6(5)
C(13)-N(3)-Cu(1)	108.6(4)
C(6)-N(3)-Cu(1)	102.5(4)
C(12)-N(4)-C(11)	112.9(6)
C(12)-N(4)-C(14)	110.8(6)
C(11)-N(4)-C(14)	117.8(5)
C(12)-N(4)-Cu(1)	115.3(4)
C(11)-N(4)-Cu(1)	101.6(4)
C(14)-N(4)-Cu(1)	97.2(4)
C(17)-N(5)-C(24)	108.6(5)
C(17)-N(5)-C(25)	109.7(5)
C(24)-N(5)-C(25)	112.6(5)

C(17)-N(5)-Cu(2)	109.3(4)
C(24)-N(5)-Cu(2)	109.2(4)
C(25)-N(5)-Cu(2)	107.4(4)
C(19)-N(6)-C(20)	112.6(5)
C(19)-N(6)-C(30)	114.5(6)
C(20)-N(6)-C(30)	113.3(5)
C(19)-N(6)-Cu(2)	104.1(4)
C(20)-N(6)-Cu(2)	109.1(4)
C(30)-N(6)-Cu(2)	102.0(4)
C(26)-N(7)-C(27)	109.9(5)
C(26)-N(7)-C(29)	115.2(5)
C(27)-N(7)-C(29)	111.3(5)
C(26)-N(7)-Cu(2)	101.7(4)
C(27)-N(7)-Cu(2)	112.4(4)
C(29)-N(7)-Cu(2)	105.9(4)
C(22)-N(8)-C(28)	114.0(6)
C(22)-N(8)-C(21)	114.9(6)
C(28)-N(8)-C(21)	111.8(6)
C(22)-N(8)-Cu(2)	106.8(4)
C(28)-N(8)-Cu(2)	110.0(4)
C(21)-N(8)-Cu(2)	97.7(4)
C(32)-N(9)-C(40)	110.6(8)
C(32)-N(9)-C(39)	108.3(6)
C(40)-N(9)-C(39)	111.2(7)
C(32)-N(9)-Cu(3)	107.8(5)
C(40)-N(9)-Cu(3)	107.4(7)
C(39)-N(9)-Cu(3)	111.6(5)
C(44)-N(10)-C(42)	111.7(9)
C(44)-N(10)-C(41)	116.0(8)
C(42)-N(10)-C(41)	112.9(9)
C(44)-N(10)-Cu(3)	101.0(7)
C(42)-N(10)-Cu(3)	112.3(6)
C(41)-N(10)-Cu(3)	101.9(5)
C(34)-N(12)-C(35)	111.3(8)
C(34)-N(12)-C(45)	115.6(10)
C(35)-N(12)-C(45)	113.4(7)
C(34)-N(12)-Cu(3)	103.2(5)

C(35)-N(12)-Cu(3)	105.9(6)
C(45)-N(12)-Cu(3)	106.2(7)
O(1)-C(1)-O(2)	125.6(6)
O(1)-C(1)-C(2)	114.8(6)
O(2)-C(1)-C(2)	119.5(5)
N(1)-C(2)-C(1)	116.0(5)
N(1)-C(2)-H(2A)	108.3
C(1)-C(2)-H(2A)	108.3
N(1)-C(2)-H(2B)	108.3
C(1)-C(2)-H(2B)	108.3
H(2A)-C(2)-H(2B)	107.4
O(4)-C(3)-O(3)	124.9(7)
O(4)-C(3)-C(4)	117.5(7)
O(3)-C(3)-C(4)	117.6(6)
N(2)-C(4)-C(3)	109.3(6)
N(2)-C(4)-H(4A)	109.8
C(3)-C(4)-H(4A)	109.8
N(2)-C(4)-H(4B)	109.8
C(3)-C(4)-H(4B)	109.8
H(4A)-C(4)-H(4B)	108.3
N(2)-C(5)-C(6)	113.4(6)
N(2)-C(5)-H(5A)	108.9
C(6)-C(5)-H(5A)	108.9
N(2)-C(5)-H(5B)	108.9
C(6)-C(5)-H(5B)	108.9
H(5A)-C(5)-H(5B)	107.7
C(5)-C(6)-N(3)	112.6(6)
C(5)-C(6)-H(6A)	109.1
N(3)-C(6)-H(6A)	109.1
C(5)-C(6)-H(6B)	109.1
N(3)-C(6)-H(6B)	109.1
H(6A)-C(6)-H(6B)	107.8
N(3)-C(7)-C(8)	111.4(8)
N(3)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7A)	109.3
N(3)-C(7)-H(7B)	109.3
C(8)-C(7)-H(7B)	109.3

H(7A)-C(7)-H(7B)	108.0
C(7)-C(8)-C(9)	120.7(7)
C(7)-C(8)-H(8A)	107.2
C(9)-C(8)-H(8A)	107.2
C(7)-C(8)-H(8B)	107.2
C(9)-C(8)-H(8B)	107.2
H(8A)-C(8)-H(8B)	106.8
C(8)-C(9)-N(1)	118.6(6)
C(8)-C(9)-H(9A)	107.7
N(1)-C(9)-H(9A)	107.7
C(8)-C(9)-H(9B)	107.7
N(1)-C(9)-H(9B)	107.7
H(9A)-C(9)-H(9B)	107.1
N(1)-C(10)-C(11)	110.6(5)
N(1)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10A)	109.5
N(1)-C(10)-H(10B)	109.5
C(11)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	108.1
N(4)-C(11)-C(10)	109.1(5)
N(4)-C(11)-H(11A)	109.9
C(10)-C(11)-H(11A)	109.9
N(4)-C(11)-H(11B)	109.9
C(10)-C(11)-H(11B)	109.9
H(11A)-C(11)-H(11B)	108.3
C(13)-C(12)-N(4)	113.3(6)
C(13)-C(12)-H(12A)	108.9
N(4)-C(12)-H(12A)	108.9
C(13)-C(12)-H(12B)	108.9
N(4)-C(12)-H(12B)	108.9
H(12A)-C(12)-H(12B)	107.7
N(3)-C(13)-C(12)	112.3(6)
N(3)-C(13)-H(13A)	109.1
C(12)-C(13)-H(13A)	109.1
N(3)-C(13)-H(13B)	109.1
C(12)-C(13)-H(13B)	109.1
H(13A)-C(13)-H(13B)	107.9

N(4)-C(14)-C(15)	111.2(6)
N(4)-C(14)-H(14A)	109.4
C(15)-C(14)-H(14A)	109.4
N(4)-C(14)-H(14B)	109.4
C(15)-C(14)-H(14B)	109.4
H(14A)-C(14)-H(14B)	108.0
N(2)-C(15)-C(14)	109.7(6)
N(2)-C(15)-H(15A)	109.7
C(14)-C(15)-H(15A)	109.7
N(2)-C(15)-H(15B)	109.7
C(14)-C(15)-H(15B)	109.7
H(15A)-C(15)-H(15B)	108.2
O(5)-C(16)-O(6)	125.8(6)
O(5)-C(16)-C(17)	116.8(6)
O(6)-C(16)-C(17)	117.3(6)
N(5)-C(17)-C(16)	112.9(5)
N(5)-C(17)-H(17A)	109.0
C(16)-C(17)-H(17A)	109.0
N(5)-C(17)-H(17B)	109.0
C(16)-C(17)-H(17B)	109.0
H(17A)-C(17)-H(17B)	107.8
O(8)-C(18)-O(7)	125.6(7)
O(8)-C(18)-C(19)	118.3(7)
O(7)-C(18)-C(19)	116.1(6)
N(6)-C(19)-C(18)	112.1(6)
N(6)-C(19)-H(19A)	109.2
C(18)-C(19)-H(19A)	109.2
N(6)-C(19)-H(19B)	109.2
C(18)-C(19)-H(19B)	109.2
H(19A)-C(19)-H(19B)	107.9
N(6)-C(20)-C(21)	112.8(6)
N(6)-C(20)-H(20A)	109.0
C(21)-C(20)-H(20A)	109.0
N(6)-C(20)-H(20B)	109.0
C(21)-C(20)-H(20B)	109.0
H(20A)-C(20)-H(20B)	107.8
N(8)-C(21)-C(20)	110.5(6)

N(8)-C(21)-H(21A)	109.6
C(20)-C(21)-H(21A)	109.6
N(8)-C(21)-H(21B)	109.6
C(20)-C(21)-H(21B)	109.6
H(21A)-C(21)-H(21B)	108.1
N(8)-C(22)-C(23)	113.5(6)
N(8)-C(22)-H(22A)	108.9
C(23)-C(22)-H(22A)	108.9
N(8)-C(22)-H(22B)	108.9
C(23)-C(22)-H(22B)	108.9
H(22A)-C(22)-H(22B)	107.7
C(24)-C(23)-C(22)	117.2(6)
C(24)-C(23)-H(23A)	108.0
C(22)-C(23)-H(23A)	108.0
C(24)-C(23)-H(23B)	108.0
C(22)-C(23)-H(23B)	108.0
H(23A)-C(23)-H(23B)	107.2
N(5)-C(24)-C(23)	118.8(6)
N(5)-C(24)-H(24A)	107.6
C(23)-C(24)-H(24A)	107.6
N(5)-C(24)-H(24B)	107.6
C(23)-C(24)-H(24B)	107.6
H(24A)-C(24)-H(24B)	107.0
N(5)-C(25)-C(26)	111.8(5)
N(5)-C(25)-H(25A)	109.3
C(26)-C(25)-H(25A)	109.3
N(5)-C(25)-H(25B)	109.3
C(26)-C(25)-H(25B)	109.3
H(25A)-C(25)-H(25B)	107.9
N(7)-C(26)-C(25)	108.9(5)
N(7)-C(26)-H(26A)	109.9
C(25)-C(26)-H(26A)	109.9
N(7)-C(26)-H(26B)	109.9
C(25)-C(26)-H(26B)	109.9
H(26A)-C(26)-H(26B)	108.3
N(7)-C(27)-C(28)	112.6(5)
N(7)-C(27)-H(27B)	109.1

C(28)-C(27)-H(27B)	109.1
N(7)-C(27)-H(27C)	109.1
C(28)-C(27)-H(27C)	109.1
H(27B)-C(27)-H(27C)	107.8
N(8)-C(28)-C(27)	112.6(6)
N(8)-C(28)-H(28A)	109.1
C(27)-C(28)-H(28A)	109.1
N(8)-C(28)-H(28B)	109.1
C(27)-C(28)-H(28B)	109.1
H(28A)-C(28)-H(28B)	107.8
N(7)-C(29)-C(30)	113.1(6)
N(7)-C(29)-H(29A)	109.0
C(30)-C(29)-H(29A)	109.0
N(7)-C(29)-H(29B)	109.0
C(30)-C(29)-H(29B)	109.0
H(29A)-C(29)-H(29B)	107.8
N(6)-C(30)-C(29)	111.7(6)
N(6)-C(30)-H(30A)	109.3
C(29)-C(30)-H(30A)	109.3
N(6)-C(30)-H(30B)	109.3
C(29)-C(30)-H(30B)	109.3
H(30A)-C(30)-H(30B)	107.9
O(9)-C(31)-O(10)	124.6(7)
O(9)-C(31)-C(32)	116.6(7)
O(10)-C(31)-C(32)	118.8(6)
O(9)-C(31)-Na(3)	65.8(4)
O(10)-C(31)-Na(3)	60.0(4)
C(32)-C(31)-Na(3)	169.4(5)
N(9)-C(32)-C(31)	114.7(7)
N(9)-C(32)-H(32A)	108.6
C(31)-C(32)-H(32A)	108.6
N(9)-C(32)-H(32B)	108.6
C(31)-C(32)-H(32B)	108.6
H(32A)-C(32)-H(32B)	107.6
O(12)-C(33)-O(11)	126.7(10)
O(12)-C(33)-C(34)	117.1(11)
O(11)-C(33)-C(34)	116.0(9)

N(12)-C(34)-C(33)	111.0(9)
N(12)-C(34)-H(34A)	109.4
C(33)-C(34)-H(34A)	109.4
N(12)-C(34)-H(34B)	109.4
C(33)-C(34)-H(34B)	109.4
H(34A)-C(34)-H(34B)	108.0
N(12)-C(35)-C(36)	116.9(5)
N(12)-C(35)-C(36A)	105.9(5)
C(36)-C(35)-C(36A)	20.6
N(12)-C(35)-H(35A)	108.1
C(36)-C(35)-H(35A)	108.1
C(36A)-C(35)-H(35A)	97.2
N(12)-C(35)-H(35B)	108.1
C(36)-C(35)-H(35B)	108.1
C(36A)-C(35)-H(35B)	128.7
H(35A)-C(35)-H(35B)	107.3
C(36)-N(11)-C(37)	113.7
C(36)-N(11)-C(43)	103.3
C(37)-N(11)-C(43)	106.8
C(36)-N(11)-Cu(3)	117.25(17)
C(37)-N(11)-Cu(3)	104.56(17)
C(43)-N(11)-Cu(3)	110.99(15)
C(36)-N(11)-H(36D)	29.0
C(37)-N(11)-H(36D)	123.0
C(43)-N(11)-H(36D)	74.3
Cu(3)-N(11)-H(36D)	128.9
N(11)-C(36)-C(35)	100.1
N(11)-C(36)-H(36A)	111.8
C(35)-C(36)-H(36A)	111.7
N(11)-C(36)-H(36B)	111.8
C(35)-C(36)-H(36B)	111.8
H(36A)-C(36)-H(36B)	109.5
N(11)-C(36)-H(36C)	79.2
C(35)-C(36)-H(36C)	105.7
H(36A)-C(36)-H(36C)	35.4
H(36B)-C(36)-H(36C)	137.7
N(11)-C(36)-H(36D)	73.6

C(35)-C(36)-H(36D)	135.2
H(36A)-C(36)-H(36D)	111.6
H(36B)-C(36)-H(36D)	41.2
H(36C)-C(36)-H(36D)	116.0
N(11)-C(37)-C(38)	109.5
N(11)-C(37)-H(37A)	109.8
C(38)-C(37)-H(37A)	109.8
N(11)-C(37)-H(37B)	109.8
C(38)-C(37)-H(37B)	109.8
H(37A)-C(37)-H(37B)	108.2
N(11)-C(37)-H(37C)	112.1
C(38)-C(37)-H(37C)	109.4
H(37A)-C(37)-H(37C)	2.5
H(37B)-C(37)-H(37C)	106.2
N(11)-C(37)-H(37D)	129.7
C(38)-C(37)-H(37D)	107.6
H(37A)-C(37)-H(37D)	87.7
H(37B)-C(37)-H(37D)	23.6
H(37C)-C(37)-H(37D)	85.5
C(37)-C(38)-C(39)	137.4
C(37)-C(38)-H(38A)	102.8
C(39)-C(38)-H(38A)	102.8
C(37)-C(38)-H(38B)	102.8
C(39)-C(38)-H(38B)	102.8
H(38A)-C(38)-H(38B)	105.0
C(37)-C(38)-H(38C)	107.6
C(39)-C(38)-H(38C)	82.8
H(38A)-C(38)-H(38C)	26.4
H(38B)-C(38)-H(38C)	126.9
C(37)-C(38)-H(38D)	118.0
C(39)-C(38)-H(38D)	103.7
H(38A)-C(38)-H(38D)	64.3
H(38B)-C(38)-H(38D)	41.5
H(38C)-C(38)-H(38D)	85.5
C(42)-C(43)-N(11)	111.7(5)
C(42)-C(43)-H(43A)	109.3
N(11)-C(43)-H(43A)	109.4

C(42)-C(43)-H(43B)	109.0
N(11)-C(43)-H(43B)	109.4
H(43A)-C(43)-H(43B)	108.0
C(42)-C(43)-H(43D)	108.7
N(11)-C(43)-H(43D)	126.2
H(43A)-C(43)-H(43D)	21.3
H(43B)-C(43)-H(43D)	88.8
C(37A)-N(11A)-C(43A)	128.2
C(37A)-N(11A)-C(36A)	91.9
C(43A)-N(11A)-C(36A)	118.3
C(37A)-N(11A)-Cu(3)	118.05(15)
C(43A)-N(11A)-Cu(3)	105.10(14)
C(36A)-N(11A)-Cu(3)	87.51(17)
N(11A)-C(36A)-C(35)	130.5
N(11A)-C(36A)-H(36A)	130.0
C(35)-C(36A)-H(36A)	93.9
N(11A)-C(36A)-H(36B)	124.2
C(35)-C(36A)-H(36B)	85.6
H(36A)-C(36A)-H(36B)	72.8
N(11A)-C(36A)-H(36C)	104.6
C(35)-C(36A)-H(36C)	104.6
H(36A)-C(36A)-H(36C)	31.9
H(36B)-C(36A)-H(36C)	103.6
N(11A)-C(36A)-H(36D)	104.6
C(35)-C(36A)-H(36D)	104.6
H(36A)-C(36A)-H(36D)	79.7
H(36B)-C(36A)-H(36D)	20.7
H(36C)-C(36A)-H(36D)	105.7
N(11A)-C(37A)-C(38A)	82.6
N(11A)-C(37A)-H(37A)	106.2
C(38A)-C(37A)-H(37A)	116.0
N(11A)-C(37A)-H(37B)	87.0
C(38A)-C(37A)-H(37B)	112.8
H(37A)-C(37A)-H(37B)	130.6
N(11A)-C(37A)-H(37C)	114.9
C(38A)-C(37A)-H(37C)	114.9
H(37A)-C(37A)-H(37C)	8.7

H(37B)-C(37A)-H(37C)	129.4
N(11A)-C(37A)-H(37D)	114.9
C(38A)-C(37A)-H(37D)	114.9
H(37A)-C(37A)-H(37D)	117.0
H(37B)-C(37A)-H(37D)	27.9
H(37C)-C(37A)-H(37D)	111.9
C(39)-C(38A)-C(37A)	135.1
C(39)-C(38A)-H(38A)	131.1
C(37A)-C(38A)-H(38A)	92.3
C(39)-C(38A)-H(38B)	93.1
C(37A)-C(38A)-H(38B)	92.9
H(38A)-C(38A)-H(38B)	96.2
C(39)-C(38A)-H(38C)	103.4
C(37A)-C(38A)-H(38C)	103.4
H(38A)-C(38A)-H(38C)	42.2
H(38B)-C(38A)-H(38C)	134.8
C(39)-C(38A)-H(38D)	103.4
C(37A)-C(38A)-H(38D)	103.4
H(38A)-C(38A)-H(38D)	68.4
H(38B)-C(38A)-H(38D)	29.5
H(38C)-C(38A)-H(38D)	105.2
N(11A)-C(43A)-C(42)	104.2(5)
N(11A)-C(43A)-H(43A)	91.9
C(42)-C(43A)-H(43A)	122.0
N(11A)-C(43A)-H(43C)	111.0
C(42)-C(43A)-H(43C)	111.2
H(43A)-C(43A)-H(43C)	113.8
N(11A)-C(43A)-H(43D)	110.9
C(42)-C(43A)-H(43D)	110.5
H(43A)-C(43A)-H(43D)	19.6
H(43C)-C(43A)-H(43D)	109.0
C(38A)-C(39)-C(38)	15.3
C(38A)-C(39)-N(9)	124.8(4)
C(38)-C(39)-N(9)	110.5(4)
C(38A)-C(39)-H(39A)	106.0
C(38)-C(39)-H(39A)	109.5

N(9)-C(39)-H(39A)	109.5
C(38A)-C(39)-H(39B)	97.3
C(38)-C(39)-H(39B)	109.5
N(9)-C(39)-H(39B)	109.8
H(39A)-C(39)-H(39B)	108.1
C(41)-C(40)-N(9)	113.8(10)
C(41)-C(40)-H(40A)	108.8
N(9)-C(40)-H(40A)	108.8
C(41)-C(40)-H(40B)	108.8
N(9)-C(40)-H(40B)	108.8
H(40A)-C(40)-H(40B)	107.7
C(40)-C(41)-N(10)	111.6(9)
C(40)-C(41)-H(41A)	109.3
N(10)-C(41)-H(41A)	109.3
C(40)-C(41)-H(41B)	109.3
N(10)-C(41)-H(41B)	109.3
H(41A)-C(41)-H(41B)	108.0
C(43)-C(42)-N(10)	119.8(8)
C(43)-C(42)-C(43A)	35.9(2)
N(10)-C(42)-C(43A)	109.4(8)
C(43)-C(42)-H(42A)	107.4
N(10)-C(42)-H(42A)	107.4
C(43A)-C(42)-H(42A)	79.4
C(43)-C(42)-H(42B)	107.4
N(10)-C(42)-H(42B)	107.4
C(43A)-C(42)-H(42B)	138.6
H(42A)-C(42)-H(42B)	106.9
N(10)-C(44)-C(45)	112.9(10)
N(10)-C(44)-H(44A)	109.0
C(45)-C(44)-H(44A)	109.0
N(10)-C(44)-H(44B)	109.0
C(45)-C(44)-H(44B)	109.0
H(44A)-C(44)-H(44B)	107.8
C(44)-C(45)-N(12)	110.9(9)
C(44)-C(45)-H(45A)	109.5
N(12)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5

N(12)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	108.0

Symmetry transformations used to generate equivalent atoms:

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

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **12**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	21(1)	20(1)	19(1)	5(1)	9(1)	3(1)
Cu(2)	19(1)	22(1)	18(1)	1(1)	6(1)	0(1)
Cu(3)	23(1)	50(1)	45(1)	17(1)	4(1)	-8(1)
Cl(1)	25(1)	24(1)	30(1)	1(1)	8(1)	3(1)
Cl(3)	42(1)	53(1)	43(1)	-4(1)	10(1)	-12(1)
Cl(2)	39(1)	60(1)	28(1)	-16(1)	3(1)	8(1)
Na(1)	24(1)	29(2)	27(1)	6(1)	8(1)	-1(1)
Na(2)	24(1)	32(2)	23(1)	7(1)	11(1)	5(1)
Na(3)	29(1)	28(2)	25(1)	1(1)	10(1)	1(1)
O(1)	28(2)	25(3)	23(2)	2(2)	14(2)	-1(2)
O(2)	27(2)	19(2)	24(2)	2(2)	13(2)	-2(2)
O(3)	29(2)	18(2)	24(2)	-1(2)	6(2)	-2(2)
O(4)	26(3)	51(4)	36(3)	13(3)	3(2)	4(2)
O(5)	37(3)	25(3)	28(3)	6(2)	16(2)	7(2)
O(6)	32(3)	22(3)	24(2)	2(2)	16(2)	5(2)
O(7)	25(2)	34(3)	24(2)	-3(2)	7(2)	-1(2)
O(8)	21(3)	79(5)	36(3)	-2(3)	1(2)	4(3)
O(9)	23(2)	32(3)	38(3)	11(2)	12(2)	3(2)
O(10)	20(2)	54(4)	28(3)	2(3)	8(2)	-2(2)
O(11)	32(3)	41(3)	50(3)	9(3)	17(3)	-5(3)
O(12)	103(6)	46(5)	219(11)	-50(6)	114(7)	-26(5)
O(13)	53(4)	136(8)	47(4)	-10(5)	7(3)	1(5)
O(14)	106(6)	105(6)	32(3)	7(4)	20(4)	78(5)
O(17)	36(3)	59(4)	49(4)	5(3)	-9(3)	4(3)
O(18)	56(4)	39(4)	70(4)	-7(3)	45(3)	-8(3)
O(19)	46(3)	42(4)	56(4)	27(3)	7(3)	12(3)
O(20)	66(4)	38(3)	60(4)	-17(3)	28(3)	13(3)
O(25)	27(2)	30(3)	31(3)	-7(2)	12(2)	-3(2)
O(26)	29(2)	23(3)	23(2)	0(2)	8(2)	1(2)
N(1)	26(3)	16(3)	15(3)	0(2)	7(2)	3(2)
N(2)	23(3)	29(3)	19(3)	2(3)	9(2)	0(2)
N(3)	26(3)	51(4)	32(4)	-18(3)	-1(3)	11(3)

N(4)	26(3)	24(3)	25(3)	-3(3)	13(2)	0(2)
N(5)	22(3)	22(3)	19(3)	0(2)	7(2)	2(2)
N(6)	20(3)	31(3)	26(3)	4(3)	9(2)	2(2)
N(7)	28(3)	18(3)	18(3)	-2(2)	7(2)	-5(2)
N(8)	34(3)	23(3)	24(3)	-1(3)	3(3)	-3(3)
N(9)	59(5)	43(5)	49(5)	6(4)	2(4)	-18(4)
N(10)	39(4)	72(6)	54(5)	22(5)	4(4)	-14(4)
N(12)	35(4)	119(9)	77(6)	37(6)	39(4)	27(5)
C(1)	22(3)	20(3)	12(3)	-4(3)	3(2)	1(3)
C(2)	28(3)	22(4)	23(3)	1(3)	12(3)	-2(3)
C(3)	29(4)	32(4)	22(4)	-1(3)	7(3)	-4(3)
C(4)	23(3)	35(4)	30(4)	7(3)	9(3)	4(3)
C(5)	48(4)	28(4)	25(4)	0(3)	24(3)	-1(3)
C(6)	57(5)	37(5)	49(5)	0(4)	26(4)	11(4)
C(7)	41(5)	50(6)	74(7)	-9(5)	21(5)	9(4)
C(8)	37(4)	37(5)	30(4)	-7(4)	10(3)	8(4)
C(9)	41(4)	17(4)	26(4)	-1(3)	8(3)	-1(3)
C(10)	25(3)	25(4)	20(3)	4(3)	9(3)	1(3)
C(11)	30(4)	32(4)	17(3)	-5(3)	9(3)	0(3)
C(12)	23(4)	45(5)	38(4)	1(4)	12(3)	-1(3)
C(13)	28(4)	57(6)	32(4)	-13(4)	6(3)	14(4)
C(14)	37(4)	30(4)	38(4)	-4(4)	16(3)	-6(3)
C(15)	32(4)	31(4)	35(4)	2(3)	15(3)	-2(3)
C(16)	25(3)	22(4)	18(3)	3(3)	8(3)	2(3)
C(17)	30(4)	23(4)	20(3)	4(3)	9(3)	1(3)
C(18)	27(4)	40(5)	30(4)	2(4)	11(3)	-4(3)
C(19)	26(4)	42(5)	30(4)	5(4)	9(3)	2(3)
C(20)	26(4)	37(4)	36(4)	4(4)	14(3)	-1(3)
C(21)	39(4)	33(4)	32(4)	3(4)	15(3)	-9(3)
C(22)	48(5)	22(4)	34(4)	1(3)	8(4)	-2(3)
C(23)	42(4)	22(4)	30(4)	1(3)	8(3)	6(3)
C(24)	37(4)	22(4)	27(4)	-1(3)	11(3)	4(3)
C(25)	17(3)	36(4)	27(4)	0(3)	5(3)	1(3)
C(26)	24(3)	29(4)	30(4)	1(3)	3(3)	-8(3)
C(27)	27(4)	34(4)	21(3)	6(3)	-3(3)	3(3)
C(28)	44(4)	27(4)	26(4)	3(3)	3(3)	-3(3)
C(29)	37(4)	30(4)	28(4)	-5(3)	13(3)	-7(3)

C(30)	39(4)	24(4)	31(4)	-4(3)	15(3)	-1(3)
C(31)	33(4)	23(4)	27(4)	15(3)	9(3)	2(3)
C(32)	47(5)	35(5)	40(5)	-2(4)	6(4)	-5(4)
C(33)	37(5)	49(6)	116(9)	-22(7)	42(6)	-7(4)
C(34)	55(6)	108(10)	77(8)	-31(7)	32(6)	24(7)
C(35)	43(6)	89(9)	225(17)	94(11)	78(8)	42(6)
C(39)	94(10)	150(14)	76(9)	-55(9)	-11(7)	-44(10)
C(40)	131(11)	44(7)	100(10)	14(7)	40(9)	-23(7)
C(41)	52(6)	48(6)	71(7)	18(5)	14(5)	-1(5)
C(42)	56(6)	89(9)	86(8)	44(7)	-7(6)	-34(6)
C(44)	56(6)	92(9)	71(8)	28(7)	23(6)	7(6)
C(45)	78(8)	120(12)	103(10)	8(9)	61(8)	34(8)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **12**.

	x	y	z	U(eq)
H(2A)	4320	911	519	28
H(2B)	3850	891	-677	28
H(4A)	4204	2539	-3605	35
H(4B)	4258	2624	-2370	35
H(5A)	5235	2134	-4039	37
H(5B)	4693	1671	-3979	37
H(6A)	6141	1629	-3187	54
H(6B)	5646	1192	-3925	54
H(7A)	5795	354	-2831	65
H(7B)	5021	577	-3164	65
H(8A)	5747	262	-1081	41
H(8B)	5201	-114	-1876	41
H(9A)	4685	176	-684	34
H(9B)	4328	495	-1750	34
H(10A)	5866	788	175	28
H(10B)	5422	919	989	28
H(11A)	5466	1858	672	31
H(11B)	6241	1633	956	31
H(12A)	6659	1895	-1259	42
H(12B)	6839	1539	-197	42
H(13A)	6732	1072	-1898	47
H(13B)	6414	784	-1043	47
H(14A)	6170	2610	-539	41
H(14B)	5373	2550	-588	41
H(15A)	5381	2886	-2235	38
H(15B)	5958	2460	-2347	38
H(17A)	2205	30	2677	28
H(17B)	2989	199	2823	28
H(19A)	913	766	4818	39
H(19B)	474	328	5260	39
H(20A)	893	-226	6501	38

H(20B)	1677	-198	7198	38
H(21A)	1474	-1084	6560	41
H(21B)	1157	-874	5368	41
H(22A)	1883	-1278	4559	42
H(22B)	2370	-1595	5546	42
H(23A)	3318	-1050	5311	38
H(23B)	3031	-1498	4420	38
H(24A)	3224	-762	3529	33
H(24B)	2410	-795	3297	33
H(25A)	3742	280	4406	32
H(25B)	3802	-249	5137	32
H(26A)	3874	474	6299	35
H(26B)	3245	786	5501	35
H(27B)	3498	-231	7611	35
H(27C)	3623	-474	6545	35
H(28A)	2999	-1137	7002	40
H(28B)	2542	-722	7462	40
H(29A)	2917	851	7119	37
H(29B)	2663	327	7631	37
H(30A)	1670	779	6984	36
H(30B)	1882	986	5957	36
H(32A)	1170	1673	-937	50
H(32B)	1538	1124	-430	50
H(34A)	489	2664	1854	93
H(34B)	-158	3037	1294	93
H(35A)	-1001	2574	-218	133
H(35B)	-1295	2592	795	133
H(36A)	-1890	1961	-666	63
H(36B)	-1723	1711	478	63
H(37A)	-1114	1779	-1771	162
H(37B)	-1588	1283	-1757	162
H(38A)	-776	957	-2361	205
H(38B)	-647	739	-1234	205
H(43A)	-1199	701	-403	157
H(43B)	-1633	994	245	157
H(36C)	-1665	1906	-902	155
H(36D)	-1584	1605	148	155

H(37C)	-1122	1858	-1891	162
H(37D)	-1634	1354	-2096	162
H(38C)	-624	1083	-2666	61
H(38D)	-695	730	-1743	61
H(43C)	-593	503	-384	67
H(43D)	-1360	578	-381	67
H(39A)	326	723	-1721	136
H(39B)	278	1363	-1959	136
H(40A)	283	415	-75	108
H(40B)	1095	518	314	108
H(41A)	1027	927	1800	69
H(41B)	537	407	1687	69
H(42A)	-577	447	1073	99
H(42B)	-889	894	1688	99
H(44A)	567	1563	2602	86
H(44B)	-31	1224	2895	86
H(45A)	-198	2198	2763	112
H(45B)	-841	1839	2132	112

Crystal mounted on a CryoLoop© with Paratone-N© oil and immediately placed under a stream of N_2 on a Bruker SMART APEX CCD system. Data collected at -100 ^{o}C with Mo Kα radiation and corrected for absorption using the APEX2 SADABS program. Structure solved by direct methods, developed by successive difference Fourier syntheses, and refined by full matrix least squares on all F^2 data. Following atoms were disordered over two positions, refined as isotropic with fixed bond distances to neighboring atoms yielding ratio occupancy of: carbon and nitrogen atoms C36, C37, C38, C43, N11 (55.53/44.47) and oxygen atoms O15, O16 (52.20/47.80), O21, O22, O23, O24 (43.88/56.12) , and O27 (43.20/56.90). Carbon C37 and C37A were treated with fixed displacement parameters. All other non-hydrogen atoms were refined as being anisotropic and hydrogen atoms were placed in calculated positions with temperature factors fixed at 1.2 or 1.5 times the equivalent isotropic U of the C atoms to which they were bonded.

APEX2 (SMART, SAINT, SADABS) and SHELXTL programs were obtained from Bruker AXS Madison , WI.