Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1998, 37(16), 3935-3942, DOI:10.1021/ic970840n

Table S1. Bond lengths [A] and angles [deg] for $[Cu(\mathbf{L7})(H_2O)](ClO_4)_2$.

Cu(1)-N(2)	2.006(9)
Cu(1)-N(4)	2.013(9)
Cu(1)-N(3)	2.056(11)
Cu(1)-N(1)	2.073(10)
Cu(1)-O(1)#1	2.415(9)
Cl(1)-O(11)	1.393(10)
Cl(1)-O(14)	1.421(10)
Cl(1)-O(12)	1.419(9)
Cl(1)-O(13)	1.451(8)
Cl(2)-O(22)	1.34
Cl(2)-O(24)	1.38
Cl(2)-O(21)	1.42
Cl(2)-O(23)	1.44
O(1)-Cu(1)#2	2.415(9)
O(1)-H(10)	1.080(11)
O(1)-H(11)	1.08
N(1)-C(1)	1.45(2)
N(1)-C(2)	1.54(2)
N(1)-H(1)	0.91
N(2)-C(5)	1.47(2)
N(2)-C(4)	1.47(2)
N(2)-H(2)	0.91
N(3)-C(6)	1.44(2)
N(3)-C(8)	1.47(2)
N(3)-H(3)	0.91
N(4)-C(9)	1.45(2)
N(4)-H(4)	0.90
N(4)-H(5)	0.90
C(1)-C(11)	1.51(2)
C(1)-H(100)	0.97
C(1)-H(101)	0.97
C(2)-C(3)	1.47(2)
C(2)-H(200)	0.97
C(2)-H(201)	0.97
C(3)-C(4)	1.48(2)
C(3)-H(300)	0.97
C(3)-H(301)	0.97
C(4)-H(400)	0.97
C(4)-H(401)	0.97
C(5)-C(6)	1.52(2)
C(5)-H(500)	0.97
C(5)-H(501)	0.97
C(6)-H(600)	0.97
C(6)-H(601)	0.97
C(7)-C(8)	1.47(2)
C(7)-C(9)	1.49(2)
C(7)-H(700)	0.97
C(7)-H(701)	0.97
C(8)-H(800)	0.97
C(8)-H(801)	0.97
C(9)-H(900)	0.97
C(9)-H(901)	0.97
C(11)-C(12)	1.36(2)
C(11)-C(16)	1.39(2)
C(12)-C(13)	1.34(2)
C(12)-H(12)	0.93

C(13)-C(14)	1.40(2)
C(13)-H(13)	0.93
C(14)-C(15)	1.31(2)
C(14)-H(14)	0.93
C(15)-C(16)	1.44(2)
C(15)-H(15)	0.93
C(16)-H(16)	0.93
N(2)-Cu(1)-N(4)	172.6(4)
N(2)-Cu(1)-N(3)	84.3(4)
N(4)-Cu(1)-N(3)	93.1(4)
N(2)-Cu(1)-N(1)	90.8(4)
N(4)-Cu(1)-N(1)	91.4(4)
N(3)-Cu(1)-N(1)	174.5(5)
N(2)-Cu(1)-O(1)#1	93.1(4)
N(4)-Cu(1)-O(1)#1	93.7(4)
N(3)-Cu(1)-O(1)#1	88.4(4)
N(1)-Cu(1)-O(1)#1	94.5(4)
O(11)-Cl(1)-O(14)	108.5(7)
O(11)-Cl(1)-O(12)	111.1(6)
O(14)-Cl(1)-O(12)	110.8(7)
O(11)-Cl(1)-O(13)	108.3(6)
O(14)-Cl(1)-O(13)	109.2(7)
O(12)-Cl(1)-O(13)	109.0(6)
O(22)-Cl(2)-O(24)	128.9
O(22)-Cl(2)-O(21)	104.3
O(24)-Cl(2)-O(21)	113.2
O(22)-Cl(2)-O(23)	107.7
O(24)-Cl(2)-O(23)	97.3
O(21)-Cl(2)-O(23)	101.9
Cu(1)#2-O(1)-H(10)	94(10)
Cu(1)#2-O(1)-H(11)	139(10)
H(10)-O(1)-H(11)	109.46(7)
C(1)-N(1)-C(2)	113.3(9)
C(1)-N(1)-Cu(1)	112.8(7)
C(2)-N(1)-Cu(1)	112.2(8)
C(1)-N(1)-H(1)	105.6(6)
C(2)-N(1)-H(1)	106.1(7)
Cu(1)-N(1)-H(1)	106.1(3)
C(5)-N(2)-C(4)	109.7(11)
C(5)-N(2)-Cu(1)	109.6(8)
C(4)-N(2)-Cu(1)	117.1(8)
C(5)-N(2)-H(2)	106.5(7)
C(4)-N(2)-H(2)	106.8(7)
Cu(1)-N(2)-H(2)	106.6(3)
C(6)-N(3)-C(8)	114.6(11)
C(6)-N(3)-Cu(1)	105.7(9)
C(8)-N(3)-Cu(1)	117.9(9)
C(6)-N(3)-H(3)	105.7(8)
C(8)-N(3)-H(3)	106.0(8)
Cu(1)-N(3)-H(3)	105.9(3)
C(9)-N(4)-Cu(1)	120.5(8)
C(9)-N(4)-H(4)	107.6(8)
Cu(1)-N(4)-H(4)	107.2(3)
C(9)-N(4)-H(5)	107.0(7)
Cu(1)-N(4)-H(5)	107.0(3)
H(4)-N(4)-H(5)	106.8
N(1)-C(1)-C(11)	117.5(9)
N(1)-C(1)-H(100)	107.1(6)
C(11)-C(1)-H(100)	107.8(6)
N(1)-C(1)-H(101)	108.3(6)

C(11)-C(1)-H(101)	108.3(7)
H(100)-C(1)-H(101)	107.3
C(3)-C(2)-N(1)	112.6(11)
C(3)-C(2)-H(200)	109.4(8)
N(1)-C(2)-H(200)	109.4(6)
C(3)-C(2)-H(201)	108.6(8)
N(1)-C(2)-H(201)	109.0(7)
H(200)-C(2)-H(201)	107.8
C(2)-C(3)-C(4)	115.3(12)
C(2)-C(3)-H(300)	108.5(8)
C(4)-C(3)-H(300)	108.9(9)
C(2)-C(3)-H(301)	108.2(8)
C(4)-C(3)-H(301)	108.4(8)
H(300)-C(3)-H(301)	107.3
N(2)-C(4)-C(3)	112.1(11)
N(2)-C(4)-H(400)	109.4(7)
C(3)-C(4)-H(400)	110.1(9)
N(2)-C(4)-H(401)	108.8(6)
C(3)-C(4)-H(401)	108.4(8)
H(400)-C(4)-H(401)	107.9
N(2)-C(5)-C(6)	109.3(11)
N(2)-C(5)-H(500)	109.9(6)
C(6)-C(5)-H(500)	109.8(7)
N(2)-C(5)-H(501)	109.8(7)
C(6)-C(5)-H(501)	109.8(7)
H(500)-C(5)-H(501)	108.2
N(3)-C(6)-C(5)	108.0(11)
N(3)-C(6)-H(600)	109.8(7)
C(5)-C(6)-H(600)	110.3(7)
N(3)-C(6)-H(601)	110.0(8)
C(5)-C(6)-H(601)	110.3(7)
H(600)-C(6)-H(601)	108.5
C(8)-C(7)-C(9)	115.0(13)
C(8)-C(7)-H(700)	108.3(7)
C(9)-C(7)-H(700)	108.7(8)
C(8)-C(7)-H(701)	108.5(10)
C(9)-C(7)-H(701)	108.6(9)
H(700)-C(7)-H(701)	107.56(6)
C(7)-C(8)-N(3)	115.9(11)
C(7)-C(8)-H(800)	108.7(8)
N(3)-C(8)-H(800)	108.1(7)
C(7)-C(8)-H(801)	108.2(10)
N(3)-C(8)-H(801)	108.3(8)
H(800)-C(8)-H(801)	107.4
N(4)-C(9)-C(7)	118.2(13)
N(4)-C(9)-H(900)	107.7(7)
C(7)-C(9)-H(900)	107.8(8)
N(4)-C(9)-H(901)	107.6(8)
C(7)-C(9)-H(901)	107.9(9)
H(900)-C(9)-H(901)	107.2
C(12)-C(11)-C(16)	116.9(11)
C(12)-C(11)-C(1)	121.9(11)
C(16)-C(11)-C(1)	121.1(11)
C(13)-C(12)-C(11)	123.5(11)
C(13)-C(12)-H(12)	118.4(7)
C(11)-C(12)-H(12)	118.2(7)
C(12)-C(13)-C(14)	119.5(12)
C(12)-C(13)-H(13)	120.3(7)
C(14)-C(13)-H(13)	120.2(8)
C(15)-C(14)-C(13)	119.8(13)
C(15)-C(14)-H(14)	119.9(9)

C(13)-C(14)-H(14)	120.3(8)
C(14)-C(15)-C(16)	119.9(13)
C(14)-C(15)-H(15)	119.8(8)
C(16)-C(15)-H(15)	120.2(7)
C(11)-C(16)-C(15)	119.4(12)
C(11)-C(16)-H(16)	120.6(7)
C(15)-C(16)-H(16)	120.0(8)

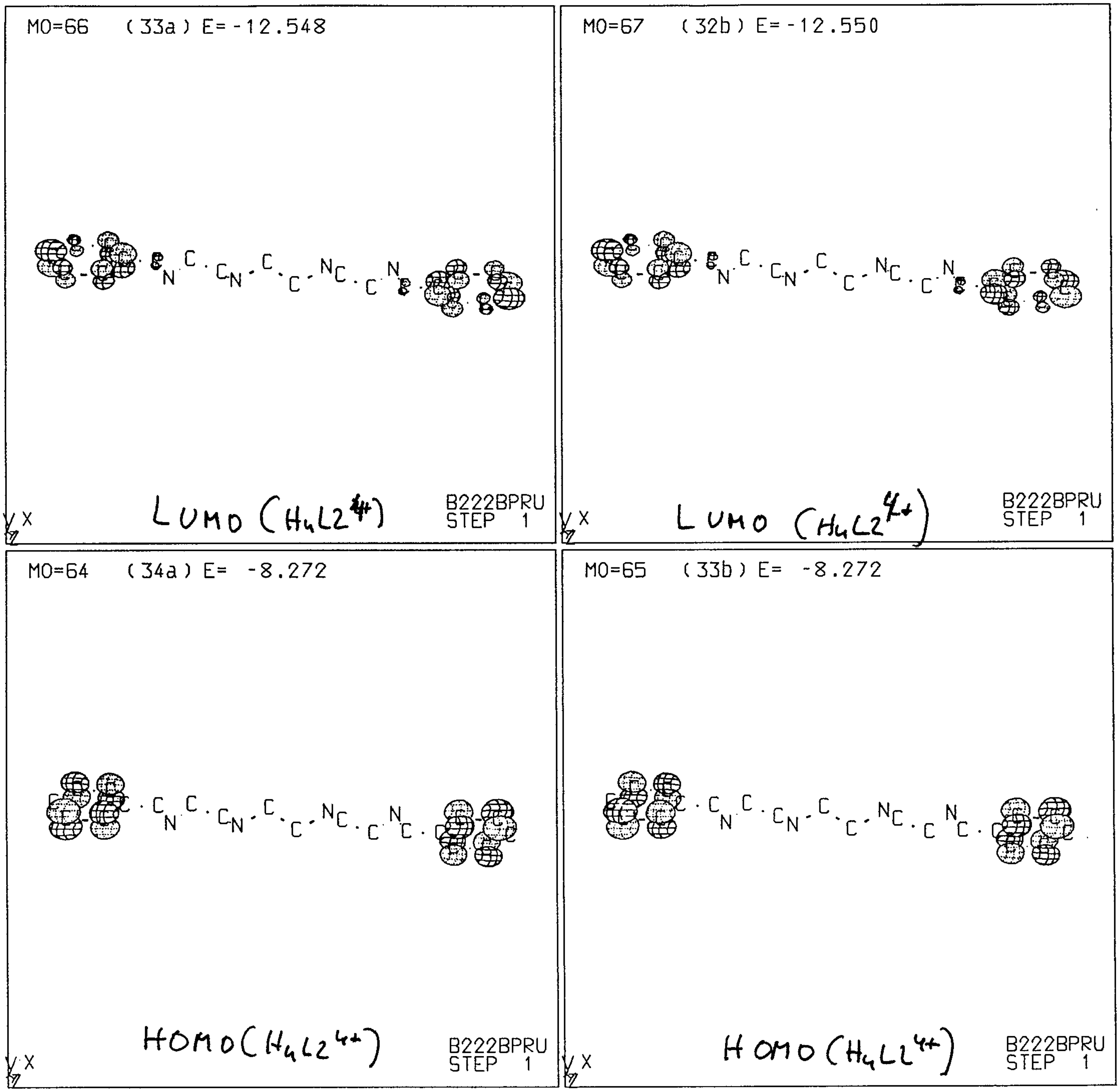
Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z   #2 x-1,y,z

Table S2. Anisotropic displacement parameters (A^2 x 10^3) for 1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	37(1)	35(1)	30(1)	3(1)	1(1)	-5(1)
Cl(1)	35(1)	50(2)	33(1)	5(1)	1(1)	-4(2)
O(11)	80(7)	61(6)	85(6)	-5(6)	-14(6)	-17(7)
O(12)	58(6)	95(8)	62(5)	22(5)	-15(5)	15(6)
O(13)	62(7)	145(10)	38(5)	34(5)	12(5)	-15(7)
O(14)	106(9)	87(7)	67(6)	-27(6)	28(6)	5(8)
Cl(2)	66(2)	89(3)	57(2)	26(2)	-14(2)	-16(2)
O(21)	116(9)	105(8)	33(4)	29(5)	-6(5)	14(8)
O(1)	61(6)	43(5)	61(5)	-6(4)	-7(4)	10(4)
N(1)	53(7)	28(5)	38(6)	-3(4)	3(6)	-15(6)
N(2)	39(6)	57(7)	34(5)	-16(5)	-6(5)	8(6)
N(3)	38(7)	66(7)	56(7)	17(6)	-12(5)	-13(6)
N(4)	47(6)	49(5)	37(5)	-4(4)	10(5)	-6(5)
C(1)	48(7)	38(6)	42(6)	7(5)	-13(6)	-5(6)
C(2)	50(9)	41(7)	102(11)	29(8)	-36(8)	1(7)
C(3)	40(8)	46(8)	139(15)	-4(11)	-10(11)	5(7)
C(4)	34(7)	93(12)	71(8)	-29(8)	-3(7)	10(9)
C(5)	40(7)	109(13)	43(7)	-9(8)	18(6)	-13(9)
C(6)	55(9)	107(13)	40(8)	10(8)	-5(7)	-35(10)
C(7)	80(12)	35(7)	109(12)	3(8)	-26(10)	-4(9)
C(8)	82(13)	54(8)	62(8)	27(7)	-8(8)	-2(9)
C(9)	61(10)	49(8)	74(9)	-5(7)	-11(8)	14(8)
C(11)	39(7)	23(5)	60(7)	11(6)	-4(6)	2(6)
C(12)	59(8)	41(7)	44(6)	-17(6)	2(6)	-14(6)
C(13)	55(9)	37(7)	75(8)	-6(6)	-9(7)	6(7)
C(14)	69(9)	34(6)	70(8)	9(6)	12(8)	-13(8)
C(15)	99(12)	86(11)	49(7)	10(8)	6(8)	-42(12)
C(16)	109(13)	41(7)	53(7)	4(6)	21(8)	-13(8)

Table S3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Cu(**L7**)(H_2O)](ClO_4)$_2$.

	x	y	z	U(eq)
H(10)	-3313(1246)	2519(788)	7940(185)	60(7)
H(11)	-5102(157)	3236(124)	8233(98)	60(7)
H(1)	7129(16)	890(9)	9393(4)	60(7)
H(2)	8800(14)	812(10)	8086(3)	60(7)
H(3)	10842(15)	3694(11)	8554(4)	60(7)
H(4)	6647(14)	2977(9)	9406(3)	60(7)
H(5)	8448(14)	3286(9)	9525(3)	60(7)
H(100)	6072(17)	26(10)	8543(4)	60(7)
H(101)	4989(17)	910(10)	8874(4)	60(7)
H(200)	9764(19)	-104(13)	9356(6)	60(7)
H(201)	8254(19)	-1101(13)	9330(6)	60(7)
H(300)	8530(21)	-1088(13)	8504(7)	60(7)
H(301)	10178(21)	-1622(13)	8769(7)	60(7)
H(400)	11588(19)	303(14)	8662(5)	60(7)
H(401)	11200(19)	-401(14)	8184(5)	60(7)
H(500)	10894(18)	1512(14)	7659(4)	60(7)
H(501)	11994(18)	1908(14)	8108(4)	60(7)
H(600)	10890(20)	3729(15)	7778(4)	60(7)
H(601)	8970(20)	3174(15)	7763(4)	60(7)
H(700)	8196(26)	6208(13)	8900(6)	60(7)
H(701)	9702(26)	5363(13)	9103(6)	60(7)
H(800)	9758(23)	5467(11)	8287(5)	60(7)
H(801)	7874(23)	4877(11)	8267(5)	60(7)
H(900)	7113(22)	5031(12)	9502(5)	60(7)
H(901)	6168(22)	4669(12)	9029(5)	60(7)
H(12)	4891(17)	-1963(10)	8514(4)	60(7)
H(13)	3625(18)	-3676(12)	8830(5)	60(7)
H(14)	2520(19)	-3608(11)	9606(5)	60(7)
H(15)	3348(24)	-2039(14)	10085(5)	60(7)
H(16)	4375(24)	-153(13)	9735(4)	60(7)



Frontier molecular orbitals for H_4**L2**$^{4+}$ in elongated conformatiom.