Inorganic Chemistry
including bioinorganic chemistry
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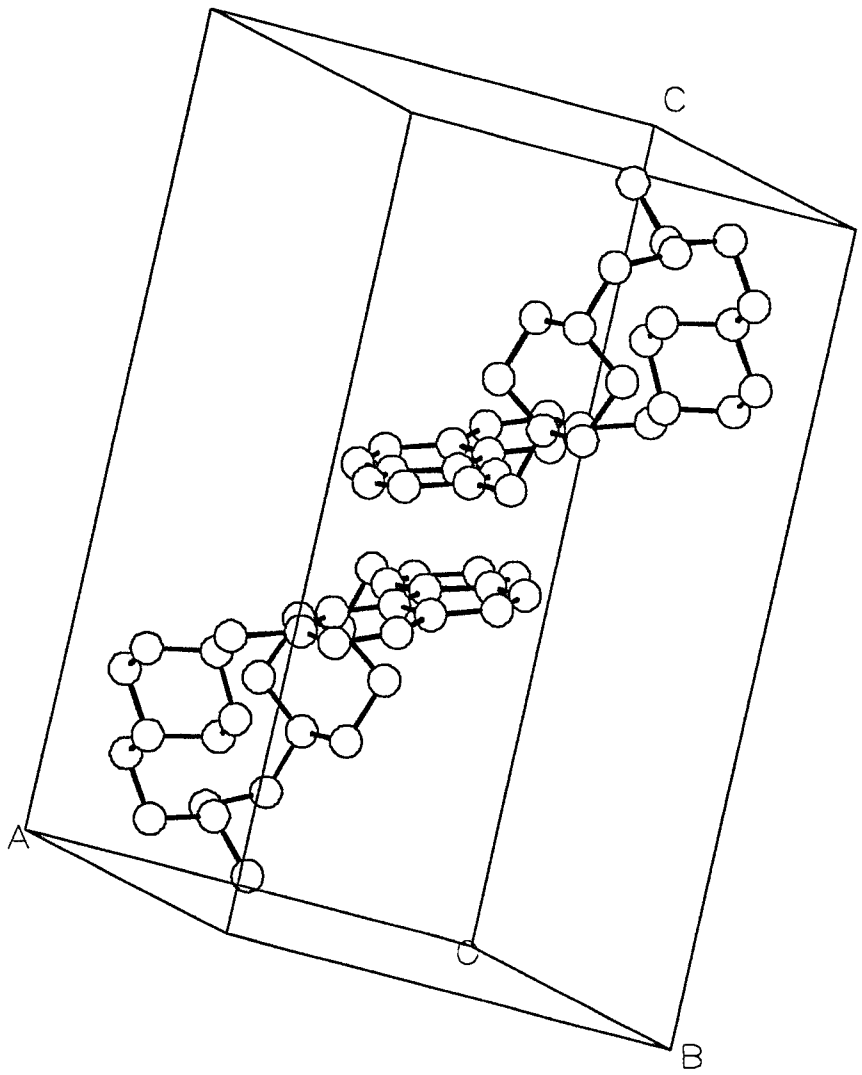

Figure S1. Crystal packing for $[H_2\mathbf{L2}Cu(NCS)_2](ClO_4)_2 \cdot 3H_2O$. In order to evidence the π-π interactions between two phenanthroline moiety, only the macrocyclic framework has been drawn.

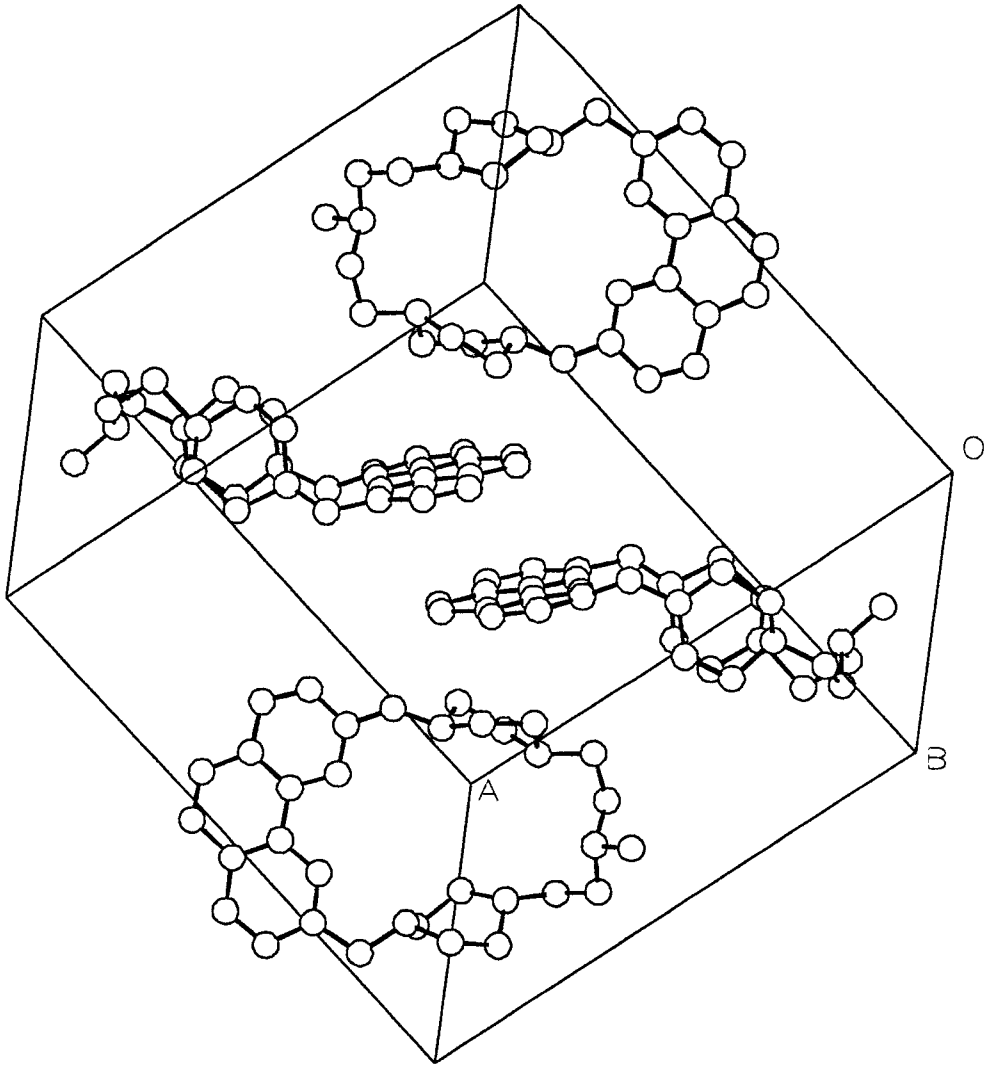

Figure S2. Crystal packing for $[Cu_2\mathbf{L2}(\mu\text{-}OH)(H_2O)(ClO_4)](ClO_4)_2 \cdot 2H_2O$. In order to evidence the π-π interactions between two phenanthroline moiety, only the macrocyclic framework has been drawn.

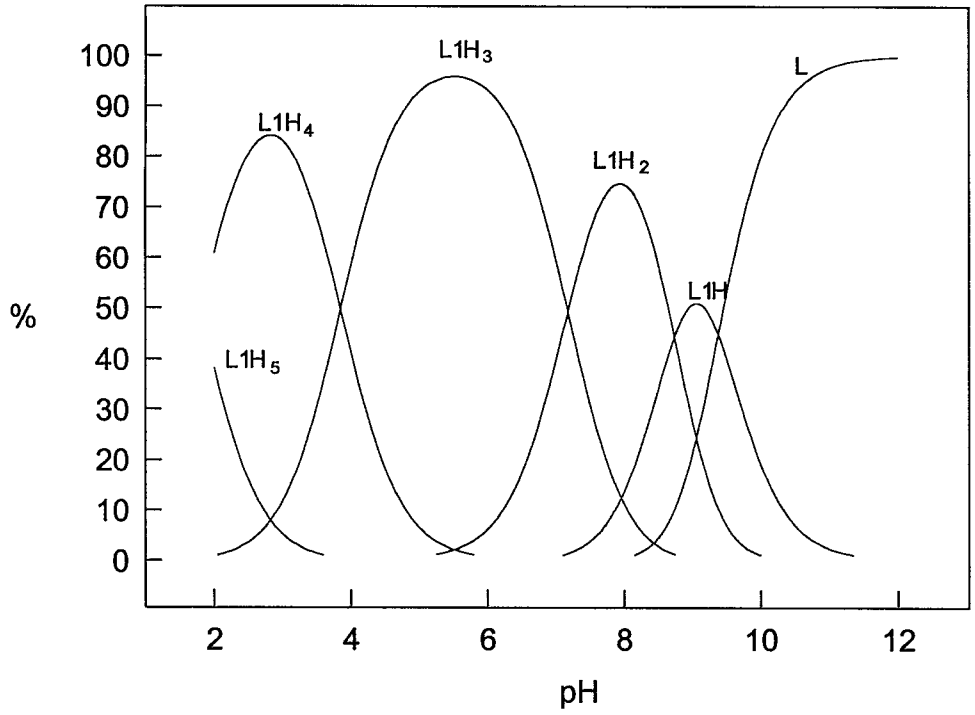

Figure S3. Distribution diagram of protonated forms of **L1** as a function of pH ([**L1**] = $1 \cdot 10^{-3}$ mol dm^{-3}) (charges omitted).

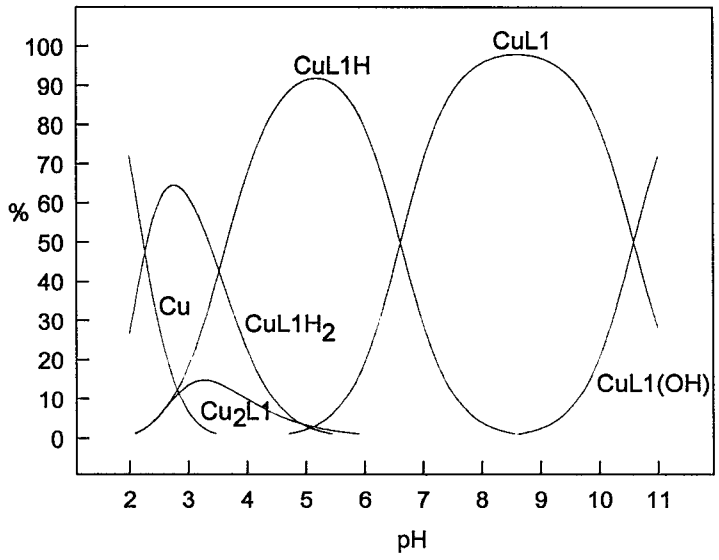

Figure S4. Distribution diagram of the species for the system **L1**\Cu(II) (NMe_4Cl 0.1 mol dm^{-3}, 298.1 K, [**L1**] = $1 \cdot 10^{-3}$ $1 \cdot 10^{-3}$ mol dm^{-3}, $[Cu^{2+}] = 1 \cdot 10^{-3}$ $1 \cdot 10^{-3}$ mol dm^{-3}) as a function of pH.

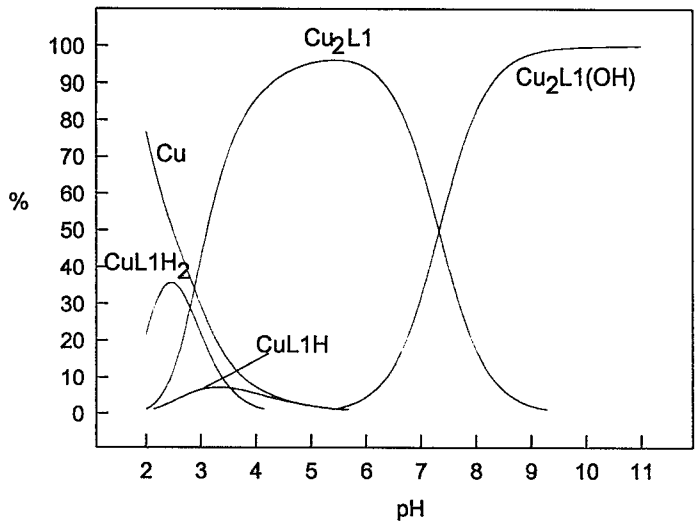

Figure S5. Distribution diagram of the species for the system **L1**\Cu(II) (NMe_4Cl 0.1 mol dm^{-3}, 298.1 K, [**L1**] = $1 \cdot 10^{-3}$ $1 \cdot 10^{-3}$ mol dm^{-3}, $[Cu^{2+}] = 2 \cdot 10^{-3}$ $1 \cdot 10^{-3}$ mol dm^{-3}) as a function of pH.

Table S1. Crystal data and structure refinement for $[H_2\mathbf{L2}Cu(NCS)_2](ClO_4)_2 \cdot 3H_2O$.

Empirical formula	$C_{29}H_{45}Cl_2CuN_9O_{11}S_2$
Formula weight	894.30
Temperature	298 K
Wavelength	0.71069 Å
Crystal system	triclinic
Space group	P -1
Unit cell dimensions	a = 9.770(10) Å α = 106.87(3) deg.
	b = 12.027(5) Å β = 90.22(8) deg.
	c = 18.006(7) Å γ = 104.48(8) deg.
Volume	1954(2) $Å^3$
Z	2
Density (calculated)	1.520 Mg/m^3
Absorption coefficient	0.870 mm^{-1}
F(000)	930
Crystal size	0.2 x 0.17 x 0.06 mm
Theta range for data collection	2.52 to 20.00 deg.
Index ranges	$-9 \le h \le 9, -11 \le k \le 11, 0 \le l \le 17$
Scan rate	4.1 deg min^{-1}
Scan mode	θ - 2θ
Scan width	0.6 + 0.35 tg θ
Reflections collected	3804
Independent reflections	3648 [R(int) = 0.0852]
Refinement method	Full-matrix least-squares on F^2
Data/restraints/Parameters	3646 / 0 / 509
Goodness-of-fit on F^2	1.055
Transmission factors	0.85 - 0.95
w	$1 / [\sigma^2(Fo^2) + (0.0813\ P)^2 + 7.97\ P]$
P	$(Fo^2 + 2\ Fc^2) / 3$
Final R indices [I>2sigma(I)]	R1 = 0.0971, wR2 = 0.1832 *
R indices (all data)	R1 = 0.2313, wR2 = 0.2553 *
Largest diff. peak and hole	0.802 and -0.376 e.$Å^{-3}$

* $R1 = \Sigma \, || Fo| - |Fc|| \, / \, \Sigma \, |Fo|$; $wR2 = [\, \Sigma \, w(Fo^2 - Fc^2)^2 \, / \, \Sigma \, wFo^4]^{1/2}$

for $[H_2L2Cu(NCS)_2](ClO_4)_2 \cdot 3H_2O$.

	x/a	y/b	z/c	U(eq)
O(1)	3892(14)	-4180(11)	262(7)	85(4)
O(2)	13053(17)	10361(14)	7773(11)	151(7)
O(3)	5368(20)	-1897(13)	416(13)	193(9)
Cu	8561(2)	3313(2)	6276(1)	49(1)
S(1)	6845(6)	6609(4)	6447(3)	83(2)
N(8)	8128(14)	4777(11)	6305(8)	55(5)
C(28)	7624(22)	5510(17)	6332(11)	72(7)
S(2)	5445(5)	1335(4)	3966(3)	69(2)
N(9)	7133(17)	2349(12)	5361(8)	77(5)
C(29)	6426(16)	1901(14)	4806(11)	50(5)
Cl(1)	3620(7)	548(6)	1354(4)	93(2)
O(11)	4532(31)	790(25)	2000(14)	152(11)
O(12)	3212(35)	-679(22)	1252(22)	193(15)
O(13)	2300(42)	690(45)	1646(22)	255(21)
O(14)	3017(55)	928(37)	892(28)	271(22)
O(15)	4480(44)	242(41)	764(17)	270(19)
O(16)	4223(60)	1618(55)	1573(49)	393(43)
Cl(2)	2207(7)	3583(7)	8250(4)	108(2)
O(21)	3384(21)	3831(29)	8718(12)	274(16)
O(22)	2476(30)	3714(23)	7563(10)	263(14)
O(23)	1528(28)	4310(21)	8626(17)	276(14)
O(24)	1504(33)	2325(20)	8054(18)	295(16)
N(1)	9923(16)	7172(12)	9417(8)	63(4)
C(1)	10299(19)	8425(15)	9401(11)	73(6)
C(2)	11700(20)	8818(15)	9080(10)	70(6)
N(2)	11884(15)	8229(12)	8242(7)	55(4)
C(3)	10580(19)	7921(14)	7721(10)	64(6)
C(4)	10881(18)	7372(15)	6902(10)	64(6)
N(3)	11257(14)	6258(11)	6839(8)	52(4)
C(5)	12592(18)	6563(15)	7308(9)	61(6)
C(6)	12329(19)	7101(15)	8143(10)	63(6)
C(7)	11378(19)	5664(14)	6008(10)	68(6)
C(8)	11744(22)	4487(16)	5896(9)	58(6)
C(9)	13066(21)	4380(16)	5653(12)	72(6)
C(10)	13342(20)	3270(21)	5522(11)	80(7)
C(11)	12407(19)	2294(16)	5657(9)	50(5)
C(12)	11128(17)	2536(15)	5896(8)	38(4)
N(4)	10780(13)	3564(12)	6012(7)	43(4)
C(13)	12674(20)	1176(18)	5570(10)	71(6)
C(14)	11732(21)	295(17)	5770(11)	71(6)
C(15)	10420(19)	519(15)	6043(9)	49(5)
C(16)	10115(18)	1617(15)	6114(9)	43(5)
N(5)	8924(15)	1865(11)	6397(8)	47(4)

C(18)	8228(18)	-42(14)	6620(11)	58(5)
C(19)	9400(21)	-323(15)	6306(10)	60(6)
C(20)	6744(17)	1540(12)	6954(9)	48(5)
N(6)	7167(13)	2883(11)	7243(7)	47(4)
C(21)	8052(15)	3274(13)	7995(9)	43(5)
C(22)	8443(17)	4629(13)	8329(10)	52(5)
C(23)	6138(15)	4614(13)	7820(10)	51(5)
C(24)	5892(17)	3313(16)	7443(10)	62(6)
N(7)	7122(13)	4993(11)	8545(7)	43(4)
C(25)	7398(18)	6337(15)	8895(10)	65(6)
C(26)	8425(21)	6831(16)	9612(11)	80(7)
C(27)	10887(20)	7037(16)	10010(11)	88(7)

Cu-N(8)	1.897(14)
Cu-N(5)	1.932(13)
Cu-N(9)	2.017(14)
Cu-N(4)	2.187(13)
Cu-N(6)	2.312(13)
S(1)-C(28)	1.65(2)
N(8)-C(28)	1.10(2)
S(2)-C(29)	1.65(2)
N(9)-C(29)	1.12(2)
Cl(1)-O(16)	1.22(6)
Cl(1)-O(14)	1.26(4)
Cl(1)-O(11)	1.38(2)
Cl(1)-O(15)	1.38(3)
Cl(1)-O(12)	1.39(2)
Cl(1)-O(13)	1.43(4)
O(11)-O(16)	1.51(8)
O(13)-O(14)	1.60(6)
O(14)-O(16)	1.58(7)
O(14)-O(15)	1.81(5)
Cl(2)-O(23)	1.27(2)
Cl(2)-O(22)	1.31(2)
Cl(2)-O(21)	1.34(2)
Cl(2)-O(24)	1.43(2)
N(1)-C(1)	1.47(2)
N(1)-C(26)	1.49(2)
N(1)-C(27)	1.49(2)
C(1)-C(2)	1.51(2)
C(2)-N(2)	1.50(2)
N(2)-C(3)	1.48(2)
N(2)-C(6)	1.49(2)
C(3)-C(4)	1.49(2)
C(4)-N(3)	1.45(2)
N(3)-C(5)	1.46(2)
N(3)-C(7)	1.48(2)
C(5)-C(6)	1.51(2)
C(7)-C(8)	1.50(2)
C(8)-N(4)	1.33(2)
C(8)-C(9)	1.39(2)
C(9)-C(10)	1.38(3)
C(10)-C(11)	1.38(2)
C(11)-C(13)	1.40(2)
C(11)-C(12)	1.39(2)
C(12)-N(4)	1.32(2)
C(12)-C(16)	1.44(2)
C(13)-C(14)	1.36(2)
C(14)-C(15)	1.43(2)

C(15)-C(19)	1.42(2)
C(16)-N(5)	1.34(2)
N(5)-C(17)	1.30(2)
C(17)-C(18)	1.43(2)
C(17)-C(20)	1.51(2)
C(18)-C(19)	1.35(2)
C(20)-N(6)	1.49(2)
N(6)-C(24)	1.47(2)
N(6)-C(21)	1.49(2)
C(21)-C(22)	1.51(2)
C(22)-N(7)	1.48(2)
C(23)-C(24)	1.47(2)
C(23)-N(7)	1.50(2)
N(7)-C(25)	1.51(2)
C(25)-C(26)	1.51(2)

N(8)-Cu-N(5)	171.8(6)
N(8)-Cu-N(9)	92.8(6)
N(5)-Cu-N(9)	91.4(5)
N(8)-Cu-N(4)	105.3(6)
N(5)-Cu-N(4)	79.1(6)
N(9)-Cu-N(4)	115.0(6)
N(8)-Cu-N(6)	97.6(5)
N(5)-Cu-N(6)	74.9(6)
N(9)-Cu-N(6)	97.5(6)
N(4)-Cu-N(6)	138.6(5)
C(28)-N(8)-Cu	167(2)
N(8)-C(28)-S(1)	175(2)
C(29)-N(9)-Cu	172(2)
N(9)-C(29)-S(2)	176(2)
O(16)-Cl(1)-O(14)	79(4)
O(16)-Cl(1)-O(11)	71(4)
O(14)-Cl(1)-O(11)	149(2)
O(16)-Cl(1)-O(15)	96(4)
O(14)-Cl(1)-O(15)	86(3)
O(11)-Cl(1)-O(15)	101(2)
O(16)-Cl(1)-O(12)	164(4)
O(14)-Cl(1)-O(12)	117(3)
O(11)-Cl(1)-O(12)	94(2)
O(15)-Cl(1)-O(12)	84(2)
O(16)-Cl(1)-O(13)	95(4)
O(14)-Cl(1)-O(13)	73(3)
O(11)-Cl(1)-O(13)	106(2)
O(15)-Cl(1)-O(13)	153(2)
O(12)-Cl(1)-O(13)	92(2)
Cl(1)-O(11)-O(16)	50(2)
Cl(1)-O(13)-O(14)	49(2)

Cl(1)-O(14)-O(13)	58(2)
O(16)-O(14)-O(13)	76(4)
Cl(1)-O(14)-O(15)	50(2)
O(16)-O(14)-O(15)	69(3)
O(13)-O(14)-O(15)	107(3)
Cl(1)-O(15)-O(14)	44(2)
Cl(1)-O(16)-O(11)	60(3)
Cl(1)-O(16)-O(14)	52(3)
O(11)-O(16)-O(14)	111(4)
O(23)-Cl(2)-O(22)	112(2)
O(23)-Cl(2)-O(21)	104(2)
O(22)-Cl(2)-O(21)	113(2)
O(23)-Cl(2)-O(24)	117(2)
O(22)-Cl(2)-O(24)	102(2)
O(21)-Cl(2)-O(24)	110(2)
C(1)-N(1)-C(26)	109.6(14)
C(1)-N(1)-C(27)	109.7(14)
C(26)-N(1)-C(27)	109.7(14)
N(1)-C(1)-C(2)	115(2)
N(2)-C(2)-C(1)	119.1(14)
C(3)-N(2)-C(6)	107.6(12)
C(3)-N(2)-C(2)	113.2(14)
C(6)-N(2)-C(2)	111.4(13)
N(2)-C(3)-C(4)	109(2)
N(3)-C(4)-C(3)	109.6(14)
C(4)-N(3)-C(5)	107.5(13)
C(4)-N(3)-C(7)	108.2(14)
C(5)-N(3)-C(7)	112.0(13)
N(3)-C(5)-C(6)	107.5(14)
N(2)-C(6)-C(5)	110.6(14)
N(3)-C(7)-C(8)	111.3(14)
N(4)-C(8)-C(9)	122(2)
N(4)-C(8)-C(7)	119(2)
C(9)-C(8)-C(7)	119(2)
C(10)-C(9)-C(8)	118(2)
C(11)-C(10)-C(9)	123(2)
C(10)-C(11)-C(13)	125(2)
C(10)-C(11)-C(12)	112(2)
C(13)-C(11)-C(12)	122(2)
N(4)-C(12)-C(11)	127(2)
N(4)-C(12)-C(16)	115(2)
C(11)-C(12)-C(16)	117(2)
C(12)-N(4)-C(8)	118(2)
C(12)-N(4)-Cu	109.4(10)
C(8)-N(4)-Cu	132.7(13)
C(14)-C(13)-C(11)	121(2)
C(13)-C(14)-C(15)	118(2)

C(16)-C(15)-C(14)	122(2)
C(19)-C(15)-C(14)	122(2)
N(5)-C(16)-C(15)	123(2)
N(5)-C(16)-C(12)	118(2)
C(15)-C(16)-C(12)	119(2)
C(17)-N(5)-C(16)	121(2)
C(17)-N(5)-Cu	123.1(13)
C(16)-N(5)-Cu	115.6(12)
N(5)-C(17)-C(18)	121(2)
N(5)-C(17)-C(20)	114(2)
C(18)-C(17)-C(20)	125(2)
C(19)-C(18)-C(17)	118(2)
C(18)-C(19)-C(15)	121(2)
N(6)-C(20)-C(17)	108.9(12)
C(24)-N(6)-C(21)	104.8(12)
C(24)-N(6)-C(20)	108.9(12)
C(21)-N(6)-C(20)	108.8(11)
C(24)-N(6)-Cu	123.4(10)
C(21)-N(6)-Cu	110.0(9)
C(20)-N(6)-Cu	100.5(9)
N(6)-C(21)-C(22)	110.6(12)
N(7)-C(22)-C(21)	107.7(12)
C(24)-C(23)-N(7)	109.6(13)
C(23)-C(24)-N(6)	116.0(13)
C(22)-N(7)-C(23)	108.4(12)
C(22)-N(7)-C(25)	112.0(12)
C(23)-N(7)-C(25)	108.0(12)
C(26)-C(25)-N(7)	112.8(14)
N(1)-C(26)-C(25)	112(2)

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[H_2L2Cu(NCS)_2](ClO_4)_2 \cdot 3H_2O$.

	U11	U22	U33	U23	U13	U12
O(1)	108(11)	89(9)	58(8)	34(7)	15(8)	13(8)
O(2)	106(13)	136(14)	194(18)	67(13)	13(12)	-21(11)
O(3)	211(19)	76(11)	284(23)	56(13)	119(18)	20(12)
Cu	56(2)	40(1)	53(1)	15(1)	2(1)	16(1)
S(1)	92(4)	54(3)	114(5)	33(3)	11(4)	31(3)
N(8)	69(10)	35(9)	61(10)	10(8)	3(8)	17(8)
C(28)	94(16)	65(14)	54(13)	28(12)	11(12)	1(13)
S(2)	60(3)	79(4)	59(4)	13(3)	-4(3)	11(3)
N(9)	105(13)	58(10)	55(11)	9(9)	-41(10)	7(9)
C(29)	33(10)	47(11)	77(14)	18(10)	37(10)	21(9)
Cl(1)	102(5)	84(4)	76(5)	12(4)	4(4)	10(4)
O(11)	189(25)	166(24)	80(16)	56(16)	-72(18)	-14(20)
O(12)	190(30)	65(17)	273(41)	27(21)	9(28)	-29(19)
O(13)	184(34)	414(60)	162(34)	51(37)	18(29)	114(38)
O(14)	367(50)	222(35)	279(44)	99(35)	-109(44)	147(37)
O(15)	396(41)	407(50)	92(22)	60(26)	167(27)	272(40)
O(16)	223(57)	291(65)	548(117)	29(70)	-100(65)	-28(50)
Cl(2)	77(4)	161(6)	91(5)	48(4)	-5(4)	28(4)
O(21)	96(15)	562(45)	115(17)	49(22)	6(13)	61(21)
O(22)	398(36)	287(26)	60(12)	82(15)	-49(17)	-23(25)
O(23)	320(26)	244(21)	302(34)	6(21)	61(25)	230(20)
O(24)	379(37)	114(17)	339(35)	63(21)	-73(30)	-22(21)
N(1)	94(12)	49(9)	55(10)	20(8)	22(9)	30(9)
C(1)	78(14)	58(13)	74(15)	-8(11)	19(12)	33(11)
C(2)	87(15)	57(12)	50(13)	-5(10)	-24(12)	13(11)
N(2)	78(11)	58(9)	35(9)	22(8)	-1(8)	18(8)
C(3)	85(14)	33(10)	69(14)	11(10)	-6(12)	12(10)
C(4)	64(13)	67(12)	72(14)	40(11)	8(11)	15(11)
N(3)	46(9)	47(9)	59(10)	14(8)	-3(8)	5(7)
C(5)	60(13)	66(12)	57(13)	22(11)	17(11)	13(10)
C(6)	64(13)	63(13)	60(14)	28(11)	-10(11)	0(11)
C(7)	66(14)	59(12)	71(15)	45(11)	-1(11)	-26(11)
C(8)	100(16)	54(12)	26(11)	13(9)	5(11)	28(12)
C(9)	63(14)	55(12)	99(16)	42(12)	-5(13)	-6(11)
C(10)	56(13)	127(18)	67(14)	54(14)	31(11)	15(14)
C(11)	66(13)	58(12)	29(11)	10(9)	-2(10)	27(11)
C(12)	47(11)	66(12)	11(9)	8(8)	15(8)	34(10)
N(4)	44(9)	41(9)	35(9)	9(7)	5(7)	-1(8)
C(13)	90(15)	89(15)	55(14)	22(12)	27(12)	60(13)
C(14)	85(15)	85(14)	55(14)	14(11)	-7(12)	51(12)
C(15)	72(13)	60(12)	27(11)	14(9)	-2(10)	37(11)
C(16)	52(12)	55(12)	24(10)	15(9)	-2(9)	14(10)
N(5)	50(9)	32(8)	52(10)	-1(7)	-8(8)	14(8)
C(17)	75(14)	16(10)	57(13)	-3(9)	-7(11)	-4(10)
C(18)	55(12)	36(10)	98(15)	47(10)	2(11)	6(9)
C(19)	88(15)	51(12)	43(12)	14(10)	-16(11)	21(12)
C(20)	62(12)	28(10)	56(12)	20(9)	-4(10)	6(9)
N(6)	49(9)	47(9)	50(9)	19(7)	5(8)	16(7)
C(21)	27(9)	53(11)	58(12)	34(9)	4(9)	8(8)
C(22)	56(12)	37(11)	44(11)	3(9)	-10(10)	-12(9)
C(23)	27(10)	46(11)	73(13)	8(10)	3(10)	8(9)

N(7)	39(9)	28(8)	46(9)	-4(7)	-9(7)	1(7)
C(25)	53(12)	85(14)	58(14)	20(12)	16(11)	21(11)
C(26)	123(18)	65(13)	61(15)	13(11)	43(14)	46(13)
C(27)	112(17)	83(14)	78(15)	38(13)	-3(14)	26(13)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[H_2\mathbf{L2}Cu(NCS)_2](ClO_4)_2 \cdot 3H_2O$.

	x/a	y/b	z/c	U(eq)
H(1A)	10323(19)	8949(15)	9927(11)	34(7)
H(1B)	9558(19)	8533(15)	9089(11)	34(7)
H(2A)	11891(20)	9677(15)	9158(10)	34(7)
H(2B)	12428(20)	8702(15)	9396(10)	34(7)
H(3A)	10273(19)	8641(14)	7759(10)	34(7)
H(3B)	9826(19)	7357(14)	7875(10)	34(7)
H(4A)	10050(18)	7212(15)	6552(10)	34(7)
H(4B)	11655(18)	7927(15)	6753(10)	34(7)
H(5A)	13311(18)	7138(15)	7141(9)	34(7)
H(5B)	12919(18)	5847(15)	7251(9)	34(7)
H(6A)	11595(19)	6526(15)	8301(10)	34(7)
H(6B)	13189(19)	7275(15)	8475(10)	34(7)
H(7A)	12106(19)	6192(14)	5812(10)	34(7)
H(7B)	10486(19)	5522(14)	5713(10)	34(7)
H(9)	13740	5032	5582	50
H(10)	14203	3175	5333	50
H(13)	13512	1034	5371	50
H(14)	11931	-436	5732	50
H(18)	7576	-581	6809	50
H(19)	9540	-1076	6262	50
H(20A)	5988(17)	1266(12)	6540(9)	34(7)
H(20B)	6399(17)	1217(12)	7373(9)	34(7)
H(21A)	8908(15)	3001(13)	7912(9)	34(7)
H(21B)	7530(15)	2914(13)	8361(9)	34(7)
H(22A)	9110(17)	4884(13)	8785(10)	34(7)
H(22B)	8882(17)	4999(13)	7947(10)	34(7)
H(23A)	5243(15)	4801(13)	7954(10)	34(7)
H(23B)	6552(15)	5052(13)	7465(10)	34(7)
H(24A)	5279(17)	3091(16)	6969(10)	34(7)
H(24B)	5384(17)	2892(16)	7786(10)	34(7)
H(25A)	7774(18)	6726(15)	8509(10)	34(7)
H(25B)	6507(18)	6531(15)	9030(10)	34(7)
H(26A)	8198(21)	7533(16)	9959(11)	34(7)
H(26B)	8322(21)	6230(16)	9883(11)	34(7)
H(27A)	11849(22)	7252(64)	9879(25)	45(24)
H(27B)	10638(54)	6217(22)	10018(32)	45(24)
H(27C)	10793(60)	7557(52)	10513(12)	45(24)

$[H_2L2Cu(NCS)_2](ClO_4)_2 \cdot 3H_2O$
(Nardelli, Musatti, Domiano & Andreetti Ric.Sci.(1965),15(II-A),807).
Equation of the plane: m1*X+m2*Y+m3*Z=d

Plane 1
m1 = -0.41912(0.00401)
m2 = -0.27576(0.00503)
m3 = -0.86504(0.00228)
D = -12.89380(0.02143)

Atom	d	s	d/s	(d/s)**2
N8 *	0.2274	0.0140	16.214	262.909
N4 *	-0.2315	0.0124	-18.704	349.853
N5 *	0.3475	0.0134	25.843	667.880
N6 *	-0.2608	0.0129	-20.213	408.564
Cu	0.3747	0.0023	164.201	26961.961

Weighted least-squares lines through the starred atoms
(Schoemaker,Waser,Marsh & Bergman,Acta Cryst.(1959).12,600)
m1,m2,m3 are the direction cosines referred to the X,Y,Z orthogonal axes.
X0,Y0,Z0 are the coordinates of the centroid of the set of atoms.
Equation of the line: (X-X0)/m1=(Y-Y0)/m2=(Z-Z0)/m3

Line 1
m1 = -0.54493(0.00660) X0 = 6.77464(0.01183)
m2 = -0.31098(0.00755) Y0 = 0.14615(0.01083)
m3 = -0.77868(0.00490) Z0 = 9.99187(0.01033)

Atom	d	s	d/s	(d/s)**2
Cu *	0.0000	0.0032	0.004	0.000
N9 *	0.0000	0.0220	0.001	0.000

Angles formed by lines and normals to planes

Line	plane	angle (e.s.d.)
1	1	8.98(0.40)

Empirical formula	$C_{27}H_{44}Cl_3Cu_2N_7O_{16}$
Formula weight	956.12
Temperature	298 K
Wavelength	1.54178 Å
Crystal system	monoclinic
Space group	P $2_1/a$
Unit cell dimensions	a = 19.573(2) Å
	b = 9.320(10) Å
	c = 21.552(2) Å
	β = 108.556(9) deg.
Volume	3727(4) $Å^3$
Z	4
Density (calculated)	1.704 Mg/m^3
Absorption coefficient	4.099 mm^{-1}
F(000)	1968
Crystal size	0.2 x 0.05 x 0.05 mm
Theta range for data collection	4.33 to 49.96 deg.
Index ranges	$-19 \le h \le 19, 0 \le k \le 9, -21 \le l \le 41$
Scan rate	variable
Scan mode	θ - 2θ
Scan width	0.80 + 0.15 tg θ
Reflections collected	3952
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3816 / 0 / 512
Goodness-of-fit on F^2	1.026
Unique obs. reflections [I > 2sigma(I)]	2246
Transmission factors	0.81 - 0.42
w	$1 / [\sigma^2(Fo^2) + (0.1492\ P)^2 + 15.25\ P]^{½}$
P	$Fo^2 / 3 + 2\ Fc^2 / 3$
Final R indices [I>2sigma(I)]	R1 = 0.0835, wR2 = 0.2221*
R indices (all data)	R1 = 0.1583, wR2 = 0.2759*
Largest diff. peak and hole	1.905 and -0.786 $e.Å^{-3}$

* $R1 = ||Fo| - |Fc|| / |Fo|$; $wR2 = [\ w(Fo^2 - Fc^2)^2 / wFo^4]^{½}$

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Cu_2L2(\mu\text{-}OH)(H_2O)(ClO_4)](ClO_4)_2 \cdot 2H_2O$.

	x /a	y/b	z/c	U(eq)
Cl(1)	2673(2)	-1762(4)	6123(2)	58(1)
O(11)	2591(5)	-2893(12)	5680(5)	74(3)
O(12)	2096(6)	-1794(14)	6407(6)	93(4)
O(13)	3339(6)	-1900(15)	6621(6)	104(4)
O(14)	2601(7)	-432(13)	5784(7)	106(4)
Cl(2)	737(2)	4349(5)	7122(2)	71(1)
O(21)	664(8)	2848(12)	7063(6)	97(4)
O(22)	1442(9)	4694(17)	7499(10)	166(8)
O(23)	700(15)	4959(18)	6534(8)	195(10)
O(24)	475(19)	4723(47)	7630(20)	130(20)
O(24')	161(19)	5017(49)	7198(33)	178(30)
Cl(3)	1371(3)	1301(7)	10107(2)	94(2)
O(31)	1564(9)	2532(18)	9824(7)	131(5)
O(32)	909(8)	1685(17)	10464(7)	122(5)
O(33)	1996(8)	715(20)	10532(9)	156(7)
O(34)	1032(9)	332(20)	9617(8)	139(6)
O(3)	-24(11)	2475(19)	1378(9)	167(7)
O(4)	8617(10)	4009(23)	1148(9)	176(7)
Cu(1)	3334(1)	1347(2)	8147(1)	60(1)
O(1)	2623(4)	1175(11)	7331(4)	56(3)
O(2)	3929(7)	-545(17)	7906(7)	103(5)
Cu(2)	1721(1)	575(2)	6846(1)	56(1)
N(1)	4064(7)	1640(17)	9034(6)	77(4)
C(1)	4154(10)	3213(22)	9079(8)	88(6)
C(2)	4364(9)	3700(20)	8494(8)	84(5)
N(2)	3814(6)	3257(13)	7869(6)	63(3)
C(3)	3240(9)	4361(19)	7632(8)	75(5)
C(4)	2933(8)	4463(17)	6893(7)	66(4)
N(3)	2958(6)	3052(13)	6605(6)	57(3)
C(5)	3716(8)	2563(19)	6732(8)	72(5)
C(6)	4189(9)	3099(21)	7371(8)	81(5)
C(7)	2569(8)	2983(17)	5896(8)	64(4)
C(8)	1760(8)	2989(18)	5710(7)	60(4)
C(9)	1370(10)	3866(16)	5209(8)	65(4)
C(10)	643(10)	3759(17)	4923(7)	68(4)
C(11)	276(7)	2733(16)	5156(6)	50(4)
C(12)	684(7)	1879(15)	5691(6)	46(3)
N(4)	1424(5)	2014(12)	5964(5)	46(3)
C(13)	-474(9)	2410(22)	4884(7)	71(5)
C(14)	-798(7)	1412(21)	5107(8)	63(5)
C(15)	-389(7)	533(16)	5657(7)	52(4)
C(16)	350(7)	774(15)	5925(6)	43(3)
N(5)	753(5)	12(12)	6443(5)	44(3)
C(17)	485(8)	-1038(16)	6693(7)	52(4)
C(18)	-249(9)	-1428(16)	6444(8)	60(4)
C(19)	-676(7)	-628(20)	5919(8)	63(5)
C(20)	1021(8)	-1798(17)	7251(7)	63(4)
N(6)	1604(6)	-784(12)	7602(5)	53(3)
C(21)	2259(8)	-1577(16)	7978(8)	65(4)
C(22)	2600(10)	-938(21)	8655(8)	86(6)
N(7)	2636(6)	628(18)	8652(6)	71(4)
C(23)	1907(8)	1302(17)	8369(7)	63(4)
C(24)	1346(7)	149(17)	8053(7)	61(4)
C(25)	3003(17)	1586(41)	9328(15)	59(9)
C(25')	2962(20)	834(48)	9314(18)	72(11)

C(27)	4767(10)	937(21)	9153(9)	105(7)

Table S9. Bond lengths [Å] and angles [°] for $[Cu_2L2(\mu\text{-}OH)(H_2O)(ClO_4)](ClO_4)_2 \cdot 2H_2O$..

Cl(1)-O(11)	1.396(11)
Cl(1)-O(13)	1.406(11)
Cl(1)-O(14)	1.423(13)
Cl(1)-O(12)	1.447(11)
Cl(2)-O(24')	1.34(4)
Cl(2)-O(23)	1.37(2)
Cl(2)-O(24)	1.39(3)
Cl(2)-O(22)	1.40(2)
Cl(2)-O(21)	1.408(11)
O(24)-O(24')	0.98(7)
Cl(3)-O(33)	1.38(2)
Cl(3)-O(34)	1.39(2)
Cl(3)-O(31)	1.41(2)
Cl(3)-O(32)	1.409(13)
Cu(1)-O(1)	1.871(8)
Cu(1)-N(1)	2.007(12)
Cu(1)-N(7)	2.108(12)
Cu(1)-N(2)	2.184(12)
Cu(1)-O(2)	2.262(14)
O(1)-Cu(2)	1.830(8)
Cu(2)-N(5)	1.889(10)
Cu(2)-N(6)	2.132(11)
Cu(2)-N(4)	2.246(11)
N(1)-C(26)	1.45(2)
N(1)-C(27)	1.47(2)
N(1)-C(1)	1.48(2)
C(1)-C(2)	1.51(2)
C(2)-N(2)	1.49(2)
N(2)-C(6)	1.49(2)
N(2)-C(3)	1.49(2)
C(3)-C(4)	1.52(2)
C(4)-N(3)	1.46(2)
N(3)-C(7)	1.48(2)
N(3)-C(5)	1.49(2)
C(5)-C(6)	1.48(2)
C(7)-C(8)	1.50(2)
C(8)-N(4)	1.34(2)
C(8)-C(9)	1.38(2)
C(9)-C(10)	1.36(2)
C(10)-C(11)	1.38(2)
C(11)-C(12)	1.42(2)
C(11)-C(13)	1.43(2)
C(12)-N(4)	1.39(2)
C(12)-C(16)	1.40(2)
C(13)-C(14)	1.30(2)
C(14)-C(15)	1.45(2)
C(15)-C(16)	1.39(2)
C(15)-C(19)	1.42(2)
C(16)-N(5)	1.35(2)
N(5)-C(17)	1.31(2)
C(17)-C(18)	1.41(2)
C(17)-C(20)	1.50(2)
C(18)-C(19)	1.39(2)
C(20)-N(6)	1.49(2)
N(6)-C(21)	1.48(2)
N(6)-C(24)	1.51(2)
C(21)-C(22)	1.52(2)
C(22)-N(7)	1.46(2)
N(7)-C(25')	1.38(4)
N(7)-C(23)	1.50(2)

C(23)-C(24)	1.53(2)
C(25)-C(25')	0.70(4)
C(25)-C(26)	1.45(4)
C(25')-C(26)	1.48(4)
O(11)-Cl(1)-O(13)	109.3(7)
O(11)-Cl(1)-O(14)	109.6(8)
O(13)-Cl(1)-O(14)	112.8(9)
O(11)-Cl(1)-O(12)	109.8(7)
O(13)-Cl(1)-O(12)	109.5(8)
O(14)-Cl(1)-O(12)	105.8(8)
O(24')-Cl(2)-O(23)	97(3)
O(24')-Cl(2)-O(24)	42(3)
O(23)-Cl(2)-O(24)	134(2)
O(24')-Cl(2)-O(22)	122(2)
O(23)-Cl(2)-O(22)	101.2(14)
O(24)-Cl(2)-O(22)	92(2)
O(24')-Cl(2)-O(21)	114(2)
O(23)-Cl(2)-O(21)	110.7(9)
O(24)-Cl(2)-O(21)	106(2)
O(22)-Cl(2)-O(21)	109.5(9)
O(24')-O(24)-Cl(2)	66(4)
O(24)-O(24')-Cl(2)	72(3)
O(33)-Cl(3)-O(34)	110.7(12)
O(33)-Cl(3)-O(31)	107.9(11)
O(34)-Cl(3)-O(31)	109.4(10)
O(33)-Cl(3)-O(32)	108.9(10)
O(34)-Cl(3)-O(32)	110.2(10)
O(31)-Cl(3)-O(32)	109.7(10)
O(1)-Cu(1)-N(1)	176.4(5)
O(1)-Cu(1)-N(7)	92.7(4)
N(1)-Cu(1)-N(7)	86.2(5)
O(1)-Cu(1)-N(2)	93.9(4)
N(1)-Cu(1)-N(2)	85.0(6)
N(7)-Cu(1)-N(2)	143.8(6)
O(1)-Cu(1)-O(2)	90.0(5)
N(1)-Cu(1)-O(2)	93.6(6)
N(7)-Cu(1)-O(2)	109.6(6)
N(2)-Cu(1)-O(2)	105.9(5)
Cu(2)-O(1)-Cu(1)	149.0(5)
O(1)-Cu(2)-N(5)	172.5(4)
O(1)-Cu(2)-N(6)	93.7(4)
N(5)-Cu(2)-N(6)	81.4(5)
O(1)-Cu(2)-N(4)	104.1(4)
N(5)-Cu(2)-N(4)	79.9(5)
N(6)-Cu(2)-N(4)	160.0(4)
C(26)-N(1)-C(27)	108(2)
C(26)-N(1)-C(1)	111(2)
C(27)-N(1)-C(1)	110.3(14)
C(26)-N(1)-Cu(1)	107.1(11)
C(27)-N(1)-Cu(1)	116.6(11)
C(1)-N(1)-Cu(1)	103.4(10)
N(1)-C(1)-C(2)	108(2)
N(2)-C(2)-C(1)	111.1(13)
C(6)-N(2)-C(3)	108.2(12)
C(6)-N(2)-C(2)	107.4(12)
C(3)-N(2)-C(2)	111.5(13)
C(6)-N(2)-Cu(1)	118.2(10)
C(3)-N(2)-Cu(1)	108.3(9)
C(2)-N(2)-Cu(1)	103.2(10)
N(2)-C(3)-C(4)	114.0(13)
N(3)-C(4)-C(3)	109.6(13)

C(4)-N(3)-C(5)	111.2(12)
C(7)-N(3)-C(5)	109.5(11)
C(6)-C(5)-N(3)	111.1(13)
C(5)-C(6)-N(2)	113.4(13)
N(3)-C(7)-C(8)	115.4(12)
N(4)-C(8)-C(9)	120.3(14)
N(4)-C(8)-C(7)	120.1(13)
C(9)-C(8)-C(7)	119(2)
C(10)-C(9)-C(8)	123(2)
C(9)-C(10)-C(11)	118.4(14)
C(10)-C(11)-C(12)	117.3(13)
C(10)-C(11)-C(13)	126(2)
C(12)-C(11)-C(13)	117.0(14)
N(4)-C(12)-C(16)	117.3(12)
N(4)-C(12)-C(11)	122.5(13)
C(16)-C(12)-C(11)	120.0(13)
C(8)-N(4)-C(12)	118.1(12)
C(8)-N(4)-Cu(2)	136.4(9)
C(12)-N(4)-Cu(2)	105.0(9)
C(14)-C(13)-C(11)	123.8(14)
C(13)-C(14)-C(15)	119.9(13)
C(16)-C(15)-C(19)	116.6(14)
C(16)-C(15)-C(14)	118.5(14)
C(19)-C(15)-C(14)	124.8(14)
N(5)-C(16)-C(15)	121.1(13)
N(5)-C(16)-C(12)	118.0(12)
C(15)-C(16)-C(12)	120.8(13)
C(17)-N(5)-C(16)	122.0(11)
C(17)-N(5)-Cu(2)	119.6(10)
C(16)-N(5)-Cu(2)	118.2(9)
N(5)-C(17)-C(18)	122.1(13)
N(5)-C(17)-C(20)	114.5(13)
C(18)-C(17)-C(20)	123(2)
C(19)-C(18)-C(17)	116.5(14)
C(18)-C(19)-C(15)	121.5(13)
N(6)-C(20)-C(17)	109.6(12)
C(21)-N(6)-C(20)	110.6(11)
C(21)-N(6)-C(24)	110.1(11)
C(20)-N(6)-C(24)	109.6(10)
C(21)-N(6)-Cu(2)	115.5(9)
C(20)-N(6)-Cu(2)	103.9(8)
C(24)-N(6)-Cu(2)	106.8(9)
N(6)-C(21)-C(22)	111.8(13)
N(7)-C(22)-C(21)	113.2(13)
C(25')-N(7)-C(22)	98(2)
C(25')-N(7)-C(23)	116(2)
C(22)-N(7)-C(23)	112.3(12)
C(25')-N(7)-C(25)	25(2)
C(22)-N(7)-C(25)	123(2)
C(23)-N(7)-C(25)	103(2)
C(25')-N(7)-Cu(1)	109(2)
C(22)-N(7)-Cu(1)	111.1(10)
C(23)-N(7)-Cu(1)	110.2(10)
C(25)-N(7)-Cu(1)	96.4(13)
N(7)-C(23)-C(24)	110.0(13)
N(6)-C(24)-C(23)	110.6(10)
C(25')-C(25)-C(26)	78(5)
C(25')-C(25)-N(7)	54(4)
C(26)-C(25)-N(7)	101(2)
C(25)-C(25')-N(7)	101(5)
C(25)-C(25')-C(26)	74(5)
N(7)-C(25')-C(26)	115(3)

C(25)-C(26)-C(25')	28(2)
N(1)-C(26)-C(25')	120(2)

Table S10. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Cu_2\mathbf{L2}(\mu\text{-}OH)(H_2O)(ClO_4)](ClO_4)_2 \cdot 2H_2O$..

	U11	U22	U33	U23	U13	U12
Cl(1)	49(2)	66(3)	61(2)	-6(2)	20(2)	9(2)
O(11)	70(7)	80(8)	67(7)	-15(6)	14(5)	9(6)
O(12)	79(8)	122(11)	90(8)	-12(7)	44(7)	-4(7)
O(13)	60(7)	128(11)	104(9)	-43(8)	-2(7)	32(7)
O(14)	133(11)	64(9)	132(11)	9(8)	59(9)	6(7)
Cl(2)	73(3)	64(3)	80(3)	-4(2)	29(2)	-1(2)
O(21)	156(12)	46(8)	107(9)	-14(7)	67(9)	-6(7)
O(22)	109(12)	101(13)	259(22)	2(13)	19(14)	15(10)
O(23)	374(32)	85(12)	98(12)	3(10)	34(15)	-16(15)
O(24)	113(29)	144(36)	195(36)	-143(33)	136(30)	-79(27)
O(24')	59(22)	64(20)	405(90)	-49(38)	67(33)	-17(18)
Cl(3)	92(3)	111(4)	77(3)	6(3)	26(3)	3(3)
O(31)	172(15)	135(14)	101(10)	16(10)	64(10)	13(12)
O(32)	122(11)	166(15)	104(10)	-13(10)	72(9)	6(10)
O(33)	91(10)	171(16)	177(16)	28(13)	0(10)	15(11)
O(34)	144(13)	174(16)	107(11)	-26(11)	49(10)	-17(12)
O(3)	195(18)	132(15)	154(15)	18(12)	26(13)	-15(13)
O(4)	166(16)	222(21)	138(14)	-20(14)	46(12)	14(15)
Cu(1)	51(1)	76(2)	49(1)	3(1)	9(1)	-5(1)
O(1)	48(5)	78(7)	35(5)	-4(5)	6(4)	-6(5)
O(2)	87(9)	137(13)	75(10)	-7(9)	14(8)	35(8)
Cu(2)	48(1)	64(2)	55(1)	1(1)	14(1)	-2(1)
N(1)	64(9)	94(13)	63(9)	-13(8)	6(7)	-7(8)
C(1)	85(13)	99(17)	61(12)	-17(10)	-6(10)	11(11)
C(2)	59(10)	88(13)	87(13)	-12(11)	-4(10)	-21(9)
N(2)	55(7)	62(9)	76(9)	7(7)	27(7)	8(7)
C(3)	75(11)	83(12)	69(11)	-1(10)	25(9)	7(10)
C(4)	69(10)	62(12)	70(11)	4(9)	28(8)	7(9)
N(3)	62(8)	57(8)	63(8)	12(7)	33(7)	5(6)
C(5)	59(10)	83(13)	84(12)	13(10)	39(9)	9(9)
C(6)	57(10)	99(14)	87(13)	5(11)	23(10)	-3(9)
C(7)	58(10)	64(11)	83(12)	-8(9)	41(9)	-16(8)
C(8)	63(10)	65(11)	59(10)	3(9)	27(8)	8(9)
C(9)	92(13)	46(10)	65(10)	10(8)	35(10)	0(9)
C(10)	88(13)	56(10)	51(9)	6(8)	10(9)	10(9)
C(11)	55(10)	56(10)	46(8)	-9(8)	25(8)	4(8)
C(12)	54(9)	44(9)	38(8)	-4(7)	11(7)	9(7)
N(4)	43(7)	39(7)	59(7)	-10(6)	21(6)	2(6)
C(13)	69(12)	103(15)	40(9)	0(9)	17(8)	33(11)
C(14)	29(8)	105(14)	53(10)	-31(10)	9(8)	11(9)
C(15)	47(9)	51(9)	61(10)	-18(8)	23(8)	-3(8)
C(16)	47(9)	39(9)	44(8)	-12(7)	16(7)	3(7)
N(5)	42(6)	47(7)	50(7)	-10(6)	22(6)	-6(6)
C(17)	51(10)	53(10)	57(9)	-4(8)	25(8)	11(8)
C(18)	65(11)	54(11)	77(11)	-16(9)	46(10)	-5(8)
C(19)	33(8)	85(13)	79(11)	-43(11)	26(8)	1(9)
C(20)	56(9)	62(10)	72(10)	-1(9)	21(8)	-8(8)
N(6)	48(7)	51(8)	61(7)	10(6)	19(6)	-10(6)
C(21)	53(9)	60(11)	76(11)	4(9)	13(8)	5(8)
C(22)	79(12)	100(17)	80(13)	35(11)	28(10)	0(11)
N(7)	50(8)	113(13)	48(7)	-3(8)	12(6)	-11(8)
C(23)	74(11)	70(11)	53(9)	-12(8)	34(8)	-10(9)
C(24)	48(9)	86(12)	56(9)	-12(8)	28(7)	-6(8)

C(27)	56(15)	96(18)	89(14)	12(11)	-18(11)	17(12)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for $[Cu_2$**L2**$(\mu\text{-}OH)(H_2O)(ClO_4)](ClO_4)_2 \cdot 2H_2O$..

	x/a	y/b	z/c	U(eq)
HO2	3807(69)	-636(145)	7527(61)	41(43)
H(1A)	4526(10)	3472(22)	9482(8)	82(10)
H(1B)	3707(10)	3668(22)	9075(8)	82(10)
H(2A)	4412(9)	4737(20)	8503(8)	82(10)
H(2B)	4827(9)	3288(20)	8518(8)	82(10)
H(3A)	3436(9)	5288(19)	7804(8)	82(10)
H(3B)	2851(9)	4142(19)	7806(8)	82(10)
H(4A)	2439(8)	4799(17)	6768(7)	82(10)
H(4B)	3211(8)	5144(17)	6731(7)	82(10)
H(5A)	3730(8)	1523(19)	6730(8)	82(10)
H(5B)	3892(8)	2909(19)	6387(8)	82(10)
H(6A)	4384(9)	4024(21)	7306(8)	82(10)
H(6B)	4591(9)	2443(21)	7537(8)	82(10)
H(7A)	2716(8)	2119(17)	5722(8)	82(10)
H(7B)	2716(8)	3795(17)	5687(8)	82(10)
H(9)	1616	4569	5057	50
H(10)	400	4361	4580	50
H(13)	-747	2945	4527	50
H(14)	-1290	1262	4915	50
H(18)	-437	-2182	6622	50
H(19)	-1161	-860	5737	50
H(20A)	783(8)	-2165(17)	7550(7)	82(10)
H(20B)	1226(8)	-2604(17)	7086(7)	82(10)
H(21A)	2605(8)	-1555(16)	7741(8)	82(10)
H(21B)	2134(8)	-2571(16)	8021(8)	82(10)
H(22A)	2324(10)	-1235(21)	8935(8)	82(10)
H(22B)	3084(10)	-1318(21)	8839(8)	82(10)
H(23A)	1921(8)	2009(17)	8043(7)	82(10)
H(23B)	1774(8)	1786(17)	8712(7)	82(10)
H(24A)	1259(7)	-438(17)	8392(7)	82(10)
H(24B)	895(7)	605(17)	7808(7)	82(10)
H(25A)	2781	2023	9372	82(10)
H(25B)	2829	421	9600	82(10)
H(25C)	2775	935	9639	82(10)
H(25D)	2865	2372	9289	82(10)
H(26A)	3878	1797	9886	82(10)
H(26B)	3909	213	9662	82(10)
H(26C)	3798	99	9562	82(10)
H(26D)	3934	1585	9918	82(10)
H(27A)	4947(34)	1139(117)	8796(33)	140(47)
H(27B)	4712(17)	-81(26)	9187(64)	140(47)
H(27C)	5100(22)	1293(106)	9553(35)	140(47)

$OH)(H_2O)(ClO_4)](ClO_4)_2 \cdot 2H_2O$.

(Nardelli, Musatti, Domiano & Andreetti Ric.Sci.(1965),15(II-A),807).

Equation of the plane: m1*X+m2*Y+m3*Z=d

Plane 1

m1 = 0.63247(0.00379)
m2 = -0.76355(0.00319)
m3 = -0.13029(0.00517)
D = -2.85880(0.08369)

Atom	d	s	d/s	(d/s)**2
N7 *	-0.3814	0.0151	-25.296	639.891
N1 *	0.3983	0.0152	26.256	689.372
N2 *	-0.2457	0.0124	-19.750	390.069
O1 *	0.1372	0.0095	14.511	210.573
Cu1	0.3243	0.0023	143.920	20712.904

Plane 2

m1 = 0.51898(0.00338)
m2 = -0.72736(0.00248)
m3 = -0.44900(0.00326)
D = -7.48524(0.04316)

Atom	d	s	d/s	(d/s)**2
O1 *	0.0178	0.0092	1.937	3.753
N4 *	-0.0284	0.0109	-2.612	6.824
N5 *	0.0385	0.0114	3.377	11.407
N6 *	-0.0335	0.0112	-2.986	8.914
Cu2	0.1257	0.0021	58.487	3420.732

Plane 3

m1 = 0.55992(0.00221)
m2 = 0.54328(0.00307)
m3 = -0.62556(0.00095)
D = -9.20435(0.01704)

Atom	d	s	d/s	(d/s)**2
O2 *	0.0930	0.0148	6.277	39.403
Cu1 *	-0.0021	0.0021	-1.011	1.023
Cu2 *	0.0018	0.0021	0.895	0.800
O12 *	-0.0572	0.0124	-4.623	21.372
O13	0.8973	0.0126	71.412	5099.605
O1	0.4887	0.0088	55.569	3087.937

Weighted least-squares lines through the starred atoms
(Schoemaker,Waser,Marsh & Bergman,Acta Cryst.(1959).12,600)
m1,m2,m3 are the direction cosines referred to the X,Y,Z orthogonal axes.
X0,Y0,Z0 are the coordinates of the centroid of the set of atoms.
Equation of the line: (X-X0)/m1=(Y-Y0)/m2=(Z-Z0)/m3

Line 1

m1 = 0.58760(0.00548) X0 = 1.60186(0.01024)
m2 = -0.77923(0.00420) Y0 = 0.37383(0.01140)
m3 = -0.21800(0.00635) Z0 = 16.39943(0.01020)

Atom	d	s	d/s	(d/s)**2
Cu1 *	0.0000	0.0029	0.002	0.000
O2 *	0.0000	0.0207	0.000	0.000

Line 2

m1 = 0.39887(0.00447) X0 = -0.81047(0.00887)
m2 = -0.84976(0.00259) Y0 = -0.56810(0.00951)
m3 = -0.34469(0.00438) Z0 = 13.53908(0.00834)

Atom	d	s	d/s	(d/s)**2
Cu2 *	0.0000	0.0028	0.004	0.000

Dihedral angles formed by LSQ-planes

Plane	- plane	angle (e.s.d.)
1	2	19.59(0.33)
1	3	88.81(0.29)
2	3	79.85(0.23)

Angles formed by LSQ-lines

Line	- line	angle (e.s.d.)
1	2	13.67(0.41)

Angles formed by lines and normals to planes

Line	- plane	angle (e.s.d.)
1	1	5.72(0.46)
1	2	14.16(0.41)
1	3	87.59(0.32)
2	1	18.91(0.36)
2	2	11.52(0.29)
2	3	91.30(0.27)