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Table of Bond Distances in Angstroms for [Cu(2-BB)(MeOH)(ClO_4)](ClO_4) (I), [Cu(2-BB)(N_3)](ClO_4) (II) and [Cu(2-BB)(NO_2)](ClO_4)(MeCN) (III)

Atom 1	Atom 2	(I)	(II)	(III)
Cu	O1	2.333(7)		
Cu	O9	2.105(6)		
Cu	N1	1.954(7)	1.962(6)	1.965(6)
Cu	N3	1.958(7)	1.959(6)	1.964(7)
Cu	N5	2.021(8)	2.003(6)	2.017(7)
Cu	N6		1.946(6)	
Cu	O5			2.439(8)
Cu	O6			2.008(6)
Cl1	O1	1.453(7)	1.399(7)	1.37(1)
Cl1	O2	1.409(7)	1.367(8)	1.393(8)
Cl1	O3	1.403(9)	1.309(9)	1.43(1)
Cl1	O4	1.392(9)	1.37(1)	1.40(1)
Cl2	O5	1.431(8)		
Cl2	O6	1.35(1)		
Cl2	O7	1.32(1)		
Cl2	O8	1.42(1)		
O9	C21	1.42(1)		
N6	N7		1.150(8)	
N7	N8		1.172(9)	
O5	N6			1.23(1)
O6	N6			1.29(1)
N7	C22			1.30(2)
C21	C22			1.51(2)
N1	C1	1.30(1)	1.336(9)	1.34(1)
N1	C4	1.40(1)	1.38(1)	1.38(1)
N2	C1	1.35(1)	1.35(1)	1.38(1)
N2	C2	1.48(1)	1.48(1)	1.46(1)
N2	C3	1.36(1)	1.37(1)	1.36(1)
N3	C9	1.33(1)	1.32(1)	1.32(1)
N3	C12	1.39(1)	1.41(1)	1.42(1)
N4	C9	1.35(1)	1.36(1)	1.34(1)
N4	C10	1.47(1)	1.47(1)	1.47(1)
N4	C11	1.37(1)	1.39(1)	1.40(1)
N5	C17	1.45(1)	1.50(1)	1.51(1)
N5	C19A	1.40(2)	1.49(1)	1.53(1)
N5	C19B	1.33(2)		
C1	C18	1.51(1)	1.49(1)	1.45(1)
C3	C4	1.39(1)	1.42(1)	1.41(1)
C3	C5	1.38(1)	1.35(1)	1.41(1)
C4	C8	1.39(1)	1.39(1)	1.38(1)
C5	C6	1.39(2)	1.38(1)	1.36(2)
C6	C7	1.40(2)	1.42(1)	1.42(1)
C7	C8	1.37(1)	1.37(1)	1.40(1)
C9	C20	1.51(1)	1.48(1)	1.48(1)
C11	C12	1.40(1)	1.38(1)	1.40(1)
C11	C13	1.40(1)	1.41(1)	1.38(1)
C12	C16	1.37(1)	1.35(1)	1.37(1)
C13	C14	1.36(1)	1.35(1)	1.35(2)
C14	C15	1.39(2)	1.41(1)	1.42(1)
C15	C16	1.38(1)	1.40(1)	1.39(2)
C17	C18	1.49(2)	1.52(1)	1.52(1)
C19A	C20	1.41(2)	1.53(1)	1.54(2)
C19B	C20	1.53(2)		

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Table of Bond Angles in Degrees for [Cu(2-BB)(MeOH)(ClO_4)](ClO_4) (I), [Cu(2-BB)(N_3)](ClO_4) (II) and [Cu(2-BB)(NO_2)](ClO_4)(MeCN) (III)

Atom 1	Atom 2	Atom 3	(I)	(II)	(III)
O1	Cu	O9	119.1(2)		
O1	Cu	N1	87.2(3)		
O1	Cu	N3	86.7(3)		
O1	Cu	N5	114.5(4)		
O9	Cu	N1	91.5(3)		
O9	Cu	N3	86.6(3)		
O9	Cu	N5	126.3(4)		
N1	Cu	N3	171.6(3)	150.5(3)	156.8(3)
N1	Cu	N5	94.5(3)	95.0(2)	93.4(3)
N3	Cu	N5	93.2(3)	91.1(3)	93.7(3)
N1	Cu	N6		94.0(3)	
N3	Cu	N6		98.5(3)	
N5	Cu	N6		142.5(3)	
O5	Cu	O6			55.5(3)
O5	Cu	N1			100.4(3)
O5	Cu	N3			100.6(3)
O5	Cu	N5			97.2(3)
O6	Cu	N1			91.0(3)
O6	Cu	N3			92.8(3)
O6	Cu	N5			152.6(3)
Cu	O1	C11	120.1(3)		
Cu	O9	C21	131.2(6)		
Cu	N1	C1	124.2(6)	125.7(6)	124.8(6)
Cu	N1	C4	128.5(5)	127.5(4)	127.3(6)
Cu	N3	C9	126.6(5)	125.7(5)	127.2(7)
Cu	N3	C12	125.6(5)	125.8(5)	126.6(6)
Cu	N5	C17	117.3(7)	111.7(5)	108.2(5)
Cu	N5	C19A	119.2(9)	106.2(4)	111.3(5)
Cu	N5	C19B	122(1)		
Cu	N6	N7		124.6(4)	
Cu	O5	N6			105.1(6)
Cu	O5	N6			85.9(6)
O1	Cl1	O2	107.8(5)	111.4(5)	112.7(6)
O1	Cl1	O3	108.0(4)	110.3(6)	101.9(8)
O1	Cl1	O4	109.7(4)	111.2(6)	118.3(7)
O2	Cl1	O3	110.4(5)	111.2(6)	111.4(5)
O2	Cl1	O4	111.2(5)	107.4(6)	110.0(6)
O3	Cl1	O4	109.7(6)	105.1(8)	101.5(7)
O5	Cl2	O6	111.3(7)		
O5	Cl2	O7	110.1(6)		
O5	Cl2	O8	108.2(5)		
O6	Cl2	O7	114.1(7)		
O6	Cl2	O8	104.8(7)		
O7	Cl2	O8	108.0(7)		
N6	N7	N8		176.3(9)	
O5	N6	O6			113.5(8)
N7	C22	C21			171.(2)
C1	N1	C4	106.5(7)	106.8(6)	107.9(6)
C1	N2	C2	126.6(7)	127.3(7)	124.9(8)
C1	N2	C3	108.0(7)	109.0(6)	108.5(7)
C2	N2	C3	125.4(8)	123.7(7)	126.6(8)
C9	N3	C12	106.8(7)	108.1(6)	105.7(7)
C9	N4	C10	127.4(7)	126.1(6)	126.5(8)
C9	N4	C11	107.9(7)	107.5(6)	108.1(7)
C10	N4	C11	124.6(8)	126.3(7)	125.4(8)
C17	N5	C19A	119(1)	111.1(6)	107.0(7)
C17	N5	C19B	118.(1)		
N1	C1	N2	111.7(7)	110.7(7)	109.3(8)
N1	C1	C18	123.8(8)	125.2(7)	128.0(7)

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Table of Bond Angles in Degrees for [Cu(2-BB)(MeOH)(ClO_4)](ClO_4) (I), [Cu(2-BB)(N_3)](ClO_4) (II) and [Cu(2-BB)(NO_2)](ClO_4)(MeCN) (III) (continued)

Atom 1	Atom 2	Atom 3	(I)	(II)	(III)
N2	C1	C18	124.4(8)	124.1(6)	122.7(8)
N2	C3	C4	106.0(7)	104.9(7)	106.6(7)
N2	C3	C5	132.0(9)	131.6(7)	131.6(8)
C4	C3	C5	121.9(8)	123.4(7)	121.8(9)
N1	C4	C3	107.8(7)	108.6(6)	107.7(8)
N1	C4	C8	131.5(8)	132.5(7)	132.0(7)
C3	C4	C8	120.8(8)	118.8(7)	120.3(8)
C3	C5	C6	116.8(9)	117.6(7)	116.8(8)
C5	C6	C7	121.4(9)	120.1(9)	122.6(9)
C6	C7	C8	121.2(9)	121.4(8)	120(1)
C4	C8	C7	117.9(9)	118.5(7)	118.4(8)
N3	C9	N4	111.3(7)	110.6(6)	112.8(8)
N3	C9	C20	125.9(8)	127.4(7)	124.8(7)
N4	C9	C20	122.8(8)	122.0(7)	122.2(8)
N4	C11	C12	106.3(7)	107.3(7)	105.6(8)
N4	C11	C13	131.4(8)	132.0(8)	132.8(8)
C12	C11	C13	122.4(7)	120.7(7)	121.5(9)
N3	C12	C11	107.7(7)	106.5(7)	107.8(8)
N3	C12	C16	131.5(8)	130.9(8)	131.4(8)
C11	C12	C16	120.8(8)	122.6(7)	120.8(9)
C11	C13	C14	115.7(9)	116.7(8)	117.9(9)
C13	C14	C15	121.8(9)	122.9(8)	122.(1)
C14	C15	C16	122.8(8)	119.3(8)	120.(1)
C12	C16	C15	116.6(9)	117.8(8)	117.7(8)
N5	C17	C18	114.6(8)	110.5(7)	111.2(8)
C1	C18	C17	112.3(9)	113.6(6)	113.6(7)
N5	C19A	C20	125.(1)	111.1(7)	110.5(7)
N5	C19B	C20	121.(2)		
C9	C20	C19A	114.(1)	113.8(7)	115.1(8)
C9	C20	C19B	119(1)		

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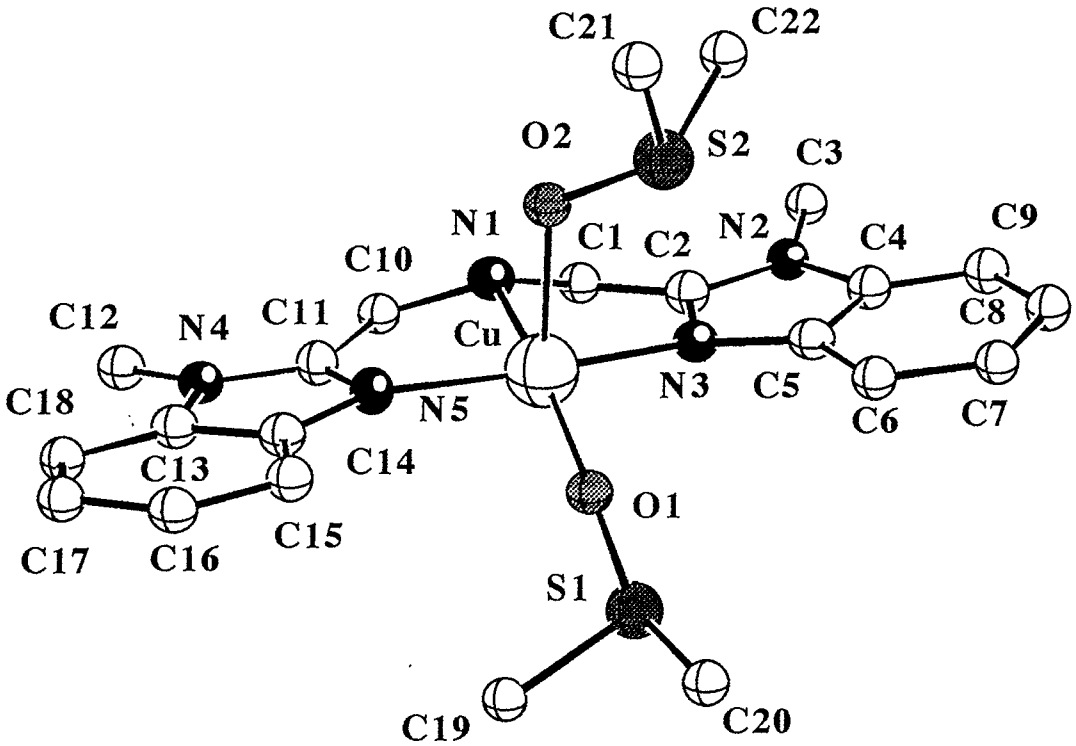
View of the $[Cu(1\text{-}BB)(O\text{-}DMSO)_2]^+$ cation in the crystal of $[Cu(1\text{-}BB)(O\text{-}DMSO)_2](BF_4)_2$(only S2 is shon for clarity)