

Supporting Information

Table 1 Hydrogen bond lengths (Å) and bond angles (°) for **1** and **2**

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠D–H···A
1				
N1–H1A···N7 #1	0.9000	2.5800	3.4177	155
N1–H1A···N8 #1	0.9000	2.3800	3.1576	145.00
N1–H1B···N11 #2	0.9000	2.2100	3.0565	156.00
N2–H2A···N11	0.9000	2.2500	3.1113	159.00
N2–H2B···N8 #3	0.9000	2.3100	3.0989	146.00
N9–H9A···N4 #4	0.9000	2.4900	3.2995	150.00
N9–H9B···N4 #4	0.9000	2.4300	3.2006	144.00
N10–H10A···N13 #5	0.9000	2.3000	3.1284	153.00
N10–H10A···N5	0.9000	2.4000	3.2402	155.00
2				
N1–H1A···O1 #5	0.9100	2.1200	2.9812	156.00
N1–H1B···O1 #1	0.8700	2.3400	3.1305	152.00
N2–H1B···N3 #6	0.8900	2.4800	3.2513	144.00
N2–H1B···O2 #7	0.8900	2.2400	2.8462	125.00
C1–H1A···N5 #8	0.9900	2.4500	3.3325	148.00

Symmetry transformations: #1 $1/2-x, 1/2-y, -z$; #2 $x, -1+y, z$; #3 $1/2-x, 3/2-y, -z$; #4 $x, 1+y, z$;

#5 $1/2-x, -1/2+y, 1/2-z$; #6 $-x, 1-y, -z$; #7 $1/2+x, 1/2+y, z$; #8 $1/2+x, 1/2-y, 1/2+z$

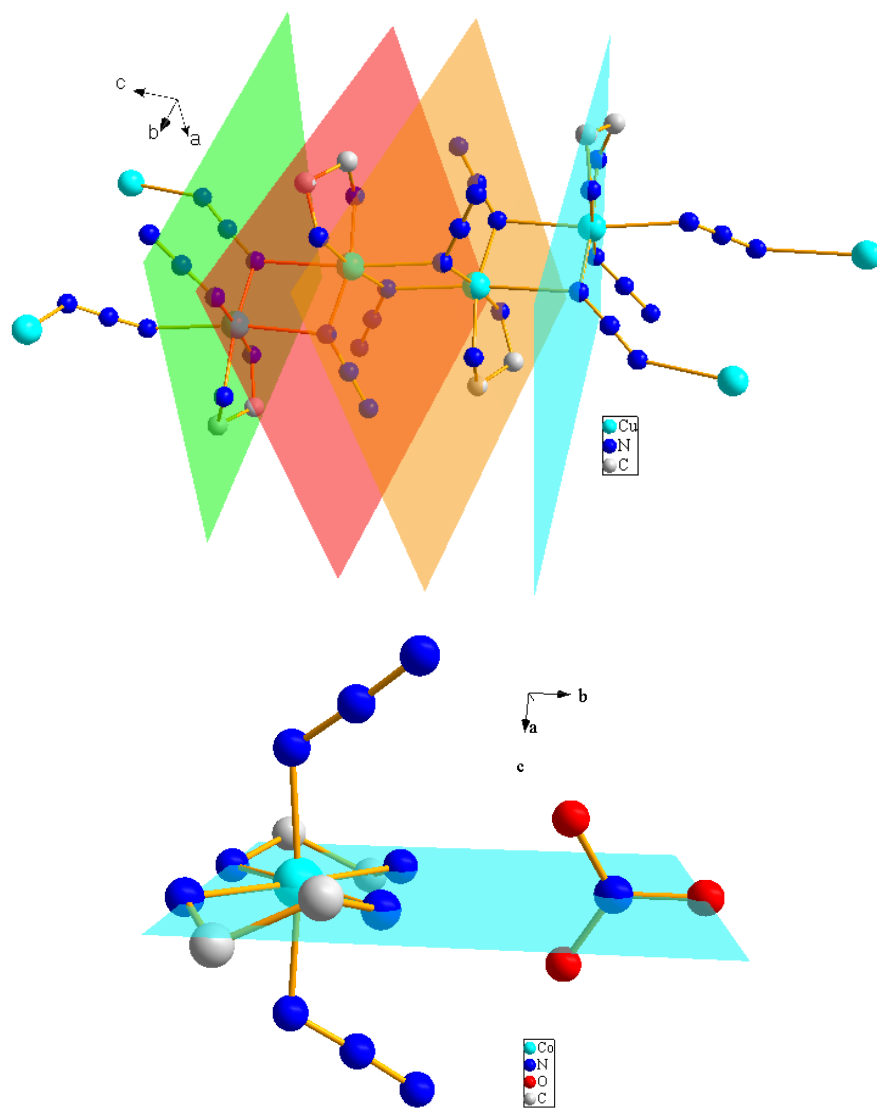


Figure 1 The octahedral coordination structures and the coplanar structures of metal cations in compound 1 and 2