

Supplementary Materials: Steric Effects of Alkyl Substituents at *N*-Donor Bidentate Amines Directs the Nuclearity, Bonding and Bridging Modes in Isothiocyanato-Copper(II) Coordination Compounds

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Table S1. Selected bond lengths (Å) and angles (°) for compound 1.

Cu(1)-N(4)	1.952(4)	Cu(1)-N(3)	1.966(4)
Cu(1)-N(1)	2.024(4)	Cu(1)-N(2)	2.066(3)
C(6)-N(3)	1.167(6)	C(6)-S(1)	1.633(4)
C(7)-N(4)	1.150(6)	C(7)-S(2)	1.640(4)
Cu(1)-S(2')	2.8910(16)		
N(4)-Cu(1)-N(3)	89.43(16)	N(4)-Cu(1)-N(1)	172.27(19)
N(3)-Cu(1)-N(1)	93.99(16)	N(4)-Cu(1)-N(2)	90.02(14)
N(3)-Cu(1)-N(2)	171.9(2)	N(1)-Cu(1)-N(2)	85.62(14)
N(3)-C(6)-S(1)	178.6(5)	N(4)-C(7)-S(2)	179.4(4)

Symmetry code: ('): 3/2-x, 1-y, 1/2+z.

Table S2. Selected bond lengths (Å) and angles (°) for compound 2.

Cu(1)-N(3)	1.957(3)	Cu(1)-N(4')	1.992(3)
Cu(1)-N(1)	2.009(3)	Cu(1)-N(2)	2.094(3)
Cu(1)-S(2)	2.6421(11)	S(2)-C(10)	1.642(4)
S(3)-C(3)	1.637(4)	N(3)-C(3)	1.166(5)
C(10)-N(4')	1.152(5)		
N(3)-Cu(1)-N(4')	92.93(13)	N(3)-Cu(1)-N(1)	175.57(13)
N(4)-Cu(1)-N(1)	88.29(13)	N(3)-Cu(1)-N(2)	92.16(13)
N(4)-Cu(1)-N(2)	150.30(12)	N(1)-Cu(1)-N(2)	84.70(12)
N(3)-Cu(1)-S(2)	93.29(9)	N(4)-Cu(1)-S(2)	99.49(9)
N(1)-Cu(1)-S(2)	90.70(10)	N(2)-Cu(1)-S(2)	109.40(9)
C(10)-S(2)-Cu(1)	98.70(13)	C(3)-N(3)-Cu(1)	164.1(3)
N(3)-C(3)-S(3)	178.8(3)	N(4')-C(10)-S(2)	179.8(4)
C(10')-N(4')-Cu(1)	167.7(3)		

Symmetry code: ('): x, 1/2-y, -1/2+z.

Table S3. Selected bond lengths (Å) and angles (°) for compound 3.

Cu(1)-N(1)	1.955(6)	Cu(1)-N(3)	1.987(5)
Cu(1)-N(2)	2.024(5)	Cu(1)-N(4)	2.112(5)
Cu(1)-S(2)	2.6183(16)	S(1)-C(2)	1.642(8)
S(2)-C(1)	1.631(6)	N(1)-C(2)	1.165(8)
N(2')-C(1)	1.171(7)		
N(1)-Cu(1)-N(3)	170.08(19)	N(1)-Cu(1)-N(2)	87.2(2)
N(3)-Cu(1)-N(2)	85.7(2)	N(1)-Cu(1)-N(4)	90.5(2)
N(3)-Cu(1)-N(4)	93.3(2)	N(2)-Cu(1)-N(4)	157.0(2)
N(1)-Cu(1)-S(2)	95.51(14)	N(3)-Cu(1)-S(2)	92.63(14)

N(2)-Cu(1)-S(2)	100.56(14)	N(4)-Cu(1)-S(2)	102.41(16)
C(1)-S(2)-Cu(1)	99.4(2)	C(2)-N(1)-Cu(1)	164.9(5)
C(1'')-N(2)-Cu(1)	155.7(5)	N(2')-C(1)-S(2)	178.5(5)

Symmetry codes: ('): $x, -1/2 - y, z + 1/2$; (''): $x, 1/2 - y, z - 1/2$.

Table S4. Selected bond lengths (Å) and angles (°) for compound 4.

Cu(1)-N(1)	1.9487(13)	Cu(1)-N(2)	1.9712(12)
Cu(1)-N(3)	2.0312(12)	Cu(1)-N(4)	2.0386(12)
N(1)-C(1)	1.1565(19)	C(1)-S(1)	1.6417(14)
N(2)-C(2)	1.1615(19)	C(2)-S(2)	1.6305(14)
N(1)-Cu(1)-N(2)	92.77(5)	N(1)-Cu(1)-N(3)	173.67(5)
N(2)-Cu(1)-N(3)	90.08(5)	N(1)-Cu(1)-N(4)	95.60(5)
N(2)-Cu(1)-N(4)	143.78(5)	N(3)-Cu(1)-N(4)	85.38(5)
C(1)-N(1)-Cu(1)	173.82(11)	N(1)-C(1)-S(1)	179.19(13)
C(3)-N(2)-Cu(1)	163.99(11)	N(2)-C(2)-S(2)	178.87(13)

Table S5. Selected bond lengths (Å) and angles (°) for compound 5.

Cu(1)-N(1)	1.9378(17)	Cu(1)-N(3)	2.0102(16)
Cu(1)-N(2)	1.9303(17)	Cu(1)-N(2)	2.0037(15)
C(1)-N(1)	1.156(3)	C(1)-S(1)	1.637(2)
C(2)-N(2)	1.165(3)	C(2)-S(2)	1.618(2)
N(1)-Cu(1)-N(2)	97.93(7)	N(2)-Cu(1)-N(4)	97.07(7)
N(1)-Cu(1)-N(4)	140.11(7)	N(2)-Cu(1)-N(3)	138.29(7)
N(1)-Cu(1)-N(3)	104.91(7)	N(3)-Cu(1)-N(4)	87.32(6)
Cu(1)-N(1)-C(1)	161.73(16)	Cu(1)-N(2)-C(2)	160.43(17)
N(1)-C(1)-S(1)	179.07(18)	N(2)-C(2)-S(2)	179.6(2)

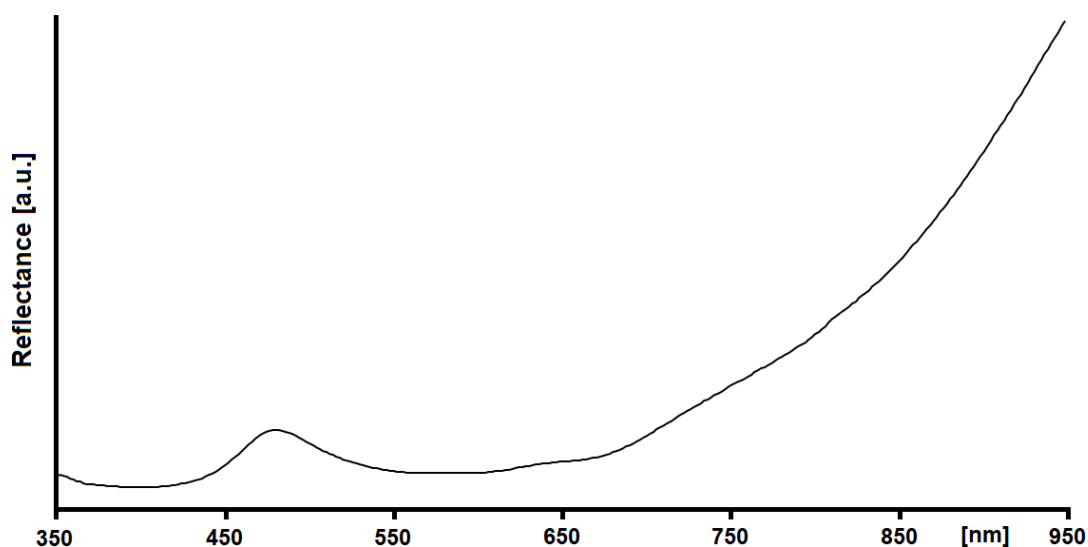


Figure S1. UV-Vis spectrum of solid sample of compound 1.

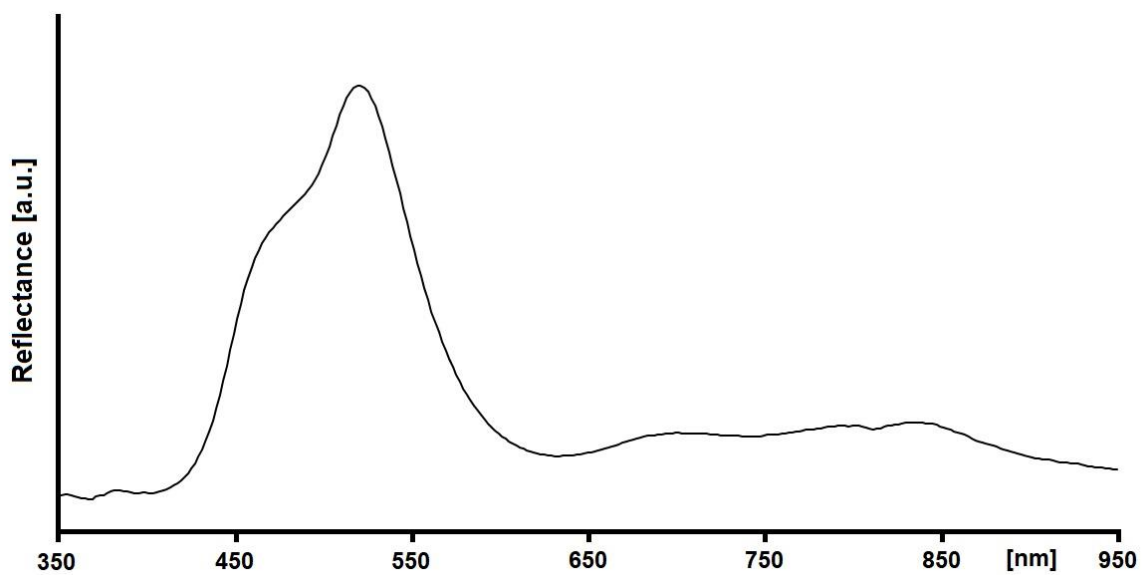


Figure S2. UV-Vis spectrum of solid sample of compound 2.

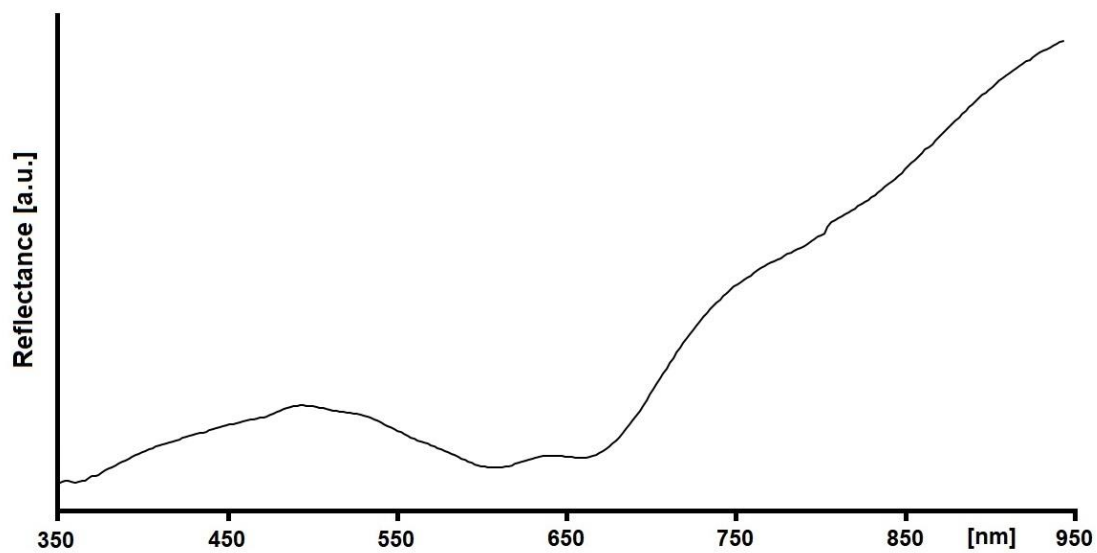


Figure S3. UV-Vis spectrum of solid sample of compound 3.

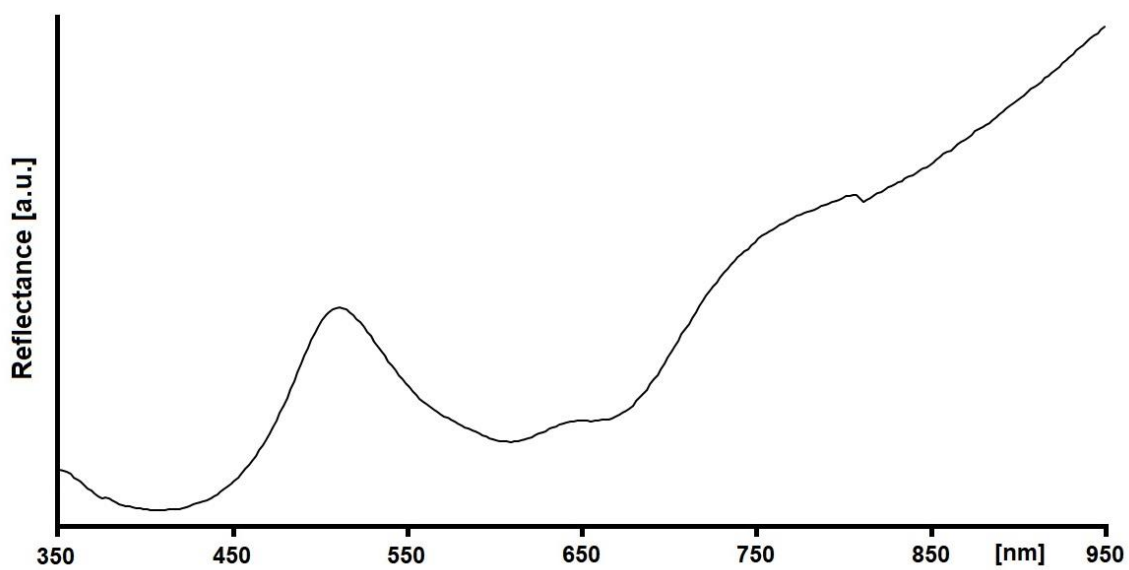


Figure S4. UV-Vis spectrum of solid sample of compound 4.

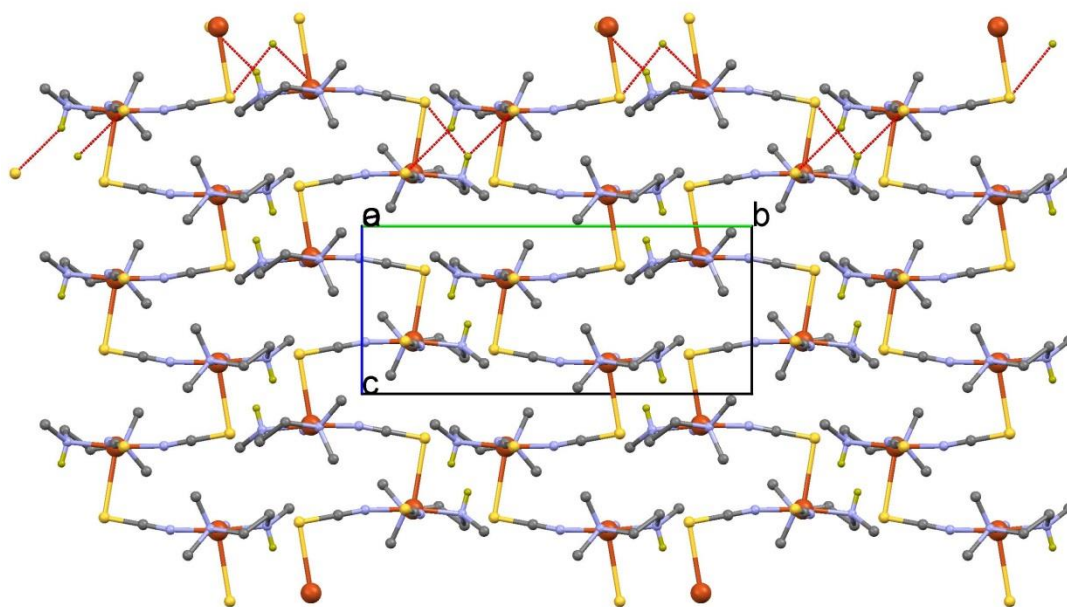


Figure S5. Packing plot of compound 1.

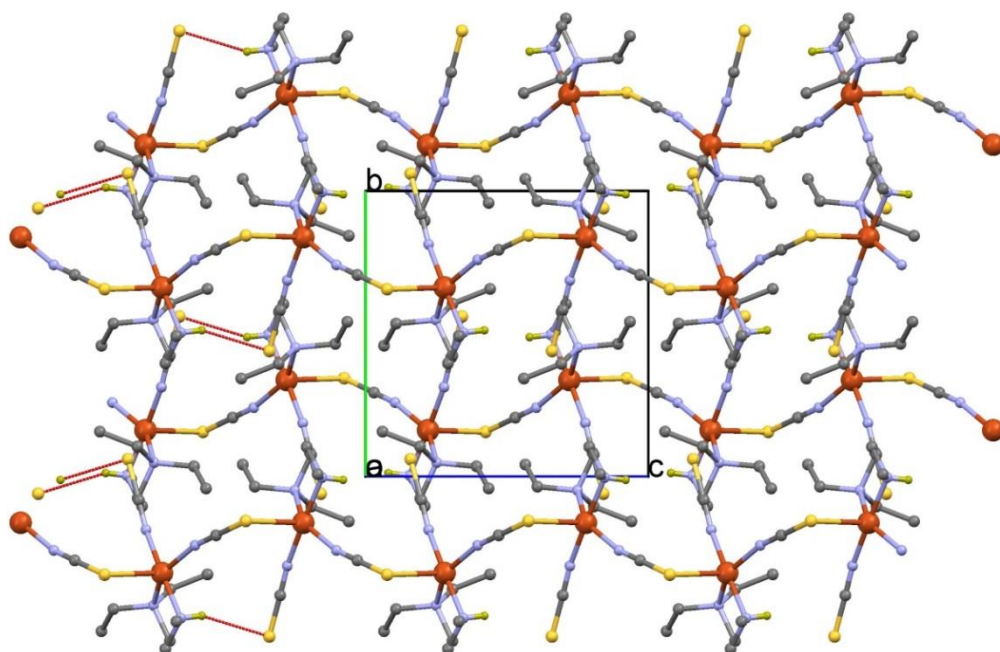


Figure S6. Packing plot of compound 2.

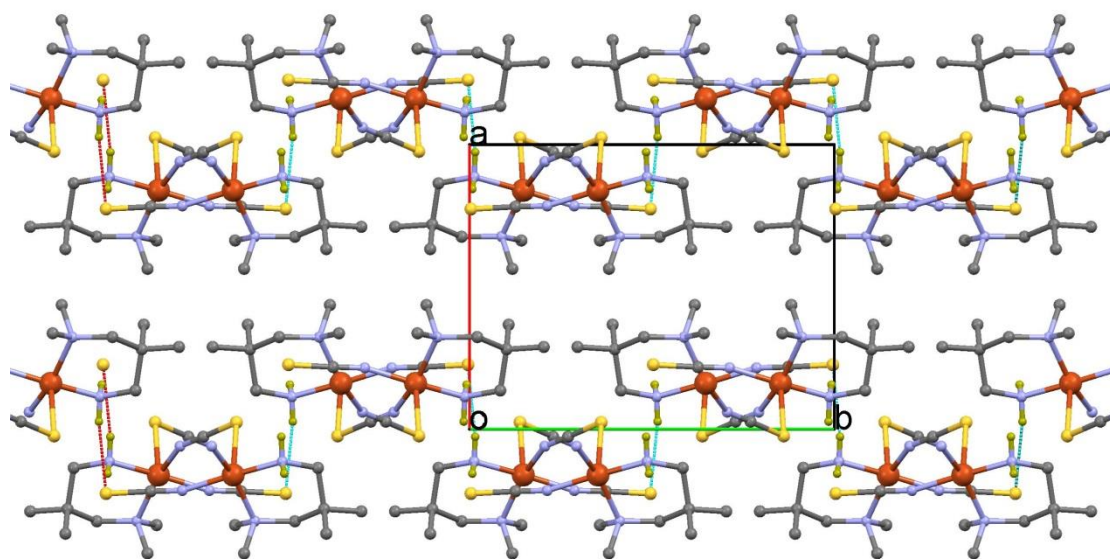


Figure S7. Packing plot of compound 3.

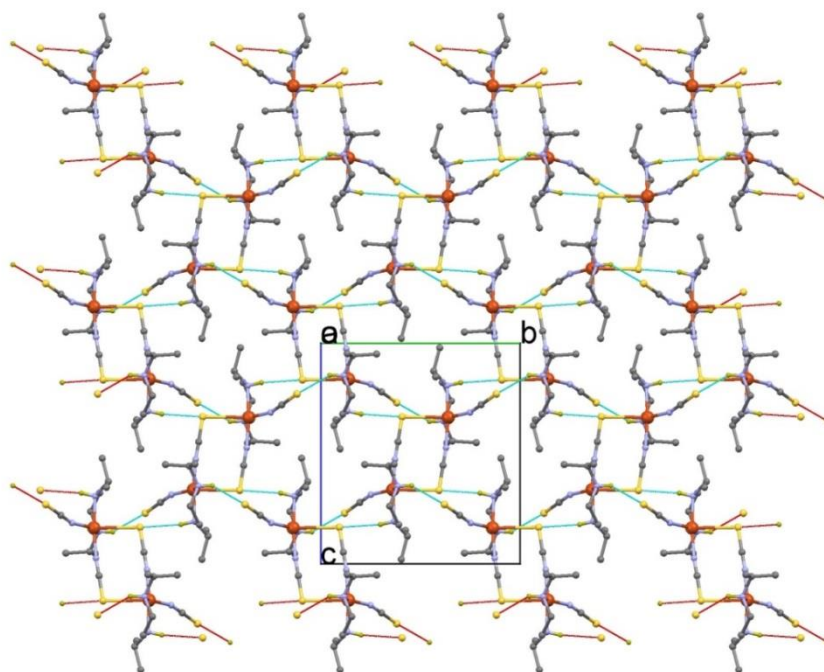


Figure S8. Packing plot of compound 4.

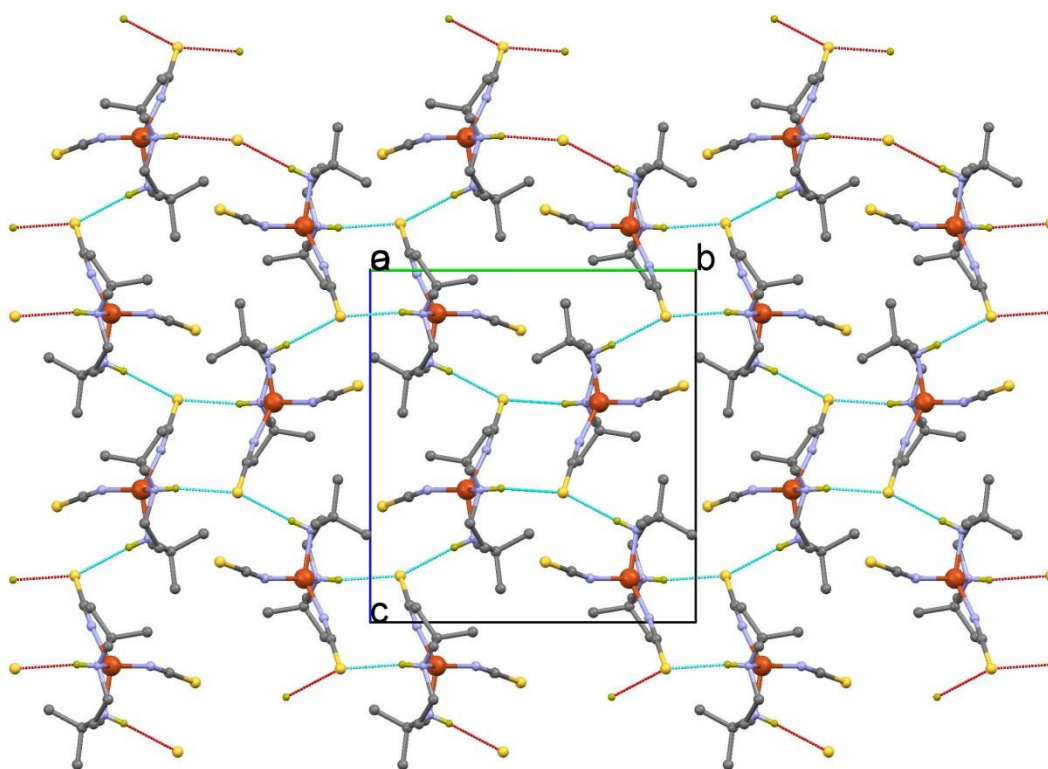


Figure S9. Packing plot of compound 5.