

Supporting information

Table S1. Relative contributions of the various intermolecular interactions to the total Hirshfeld surface of crystals **1-3**, respectively.

	1	2	3
Cu...H/H... Cu	1.4	2.4	2.4
N...C/ C...N	1.3	0.1	0.1
N...H/H...N	7.1	8.0	8.0
C...C	14.3	7.3	7.3
C...H/H...C	26.5	27.1	26.8
H...H	48.4	55	55.4

Table S2. Selected bond angles of crystals **1, 2, 3**

angles	1	angles	2	angles	3
N1-Cu1-N1	177.4	N1-Cu1-N1	177.4	N1-Cu1-N1	177.2
Cu1-N1-C1	125.64	Cu1-N1-C1	126.6	Cu1-N1-C4	126.9
C4-N1-C1	107.88	C4-N1-C1	106.4	C4-N1-C1	106.1
C6-C5-C4	108.60	C4-C3-C2	107.0	C3-C2-C1	106.9
C10-C8-C2	118.90	C7-C6-C11	119.2	C7-C6-C11	121.6
C2-C8-C7	121.22	C7-C6-C5	121.2	C11-C6-C5	119.5
C9-C11-C10	118.63	C9-C11-C10	120.2	C9-C8-C7	119.5
N1-C1-C7	127.34	N1-C1-C5	126.0	N1-C4-C5	125.2
C4-C1-C7	124.81	C2-C1-C5	123.8	C3-C4-C5	124.8
C5-C6-C7	125.81	C3-C4-C5	124.8	C2-C1-C5	123.3

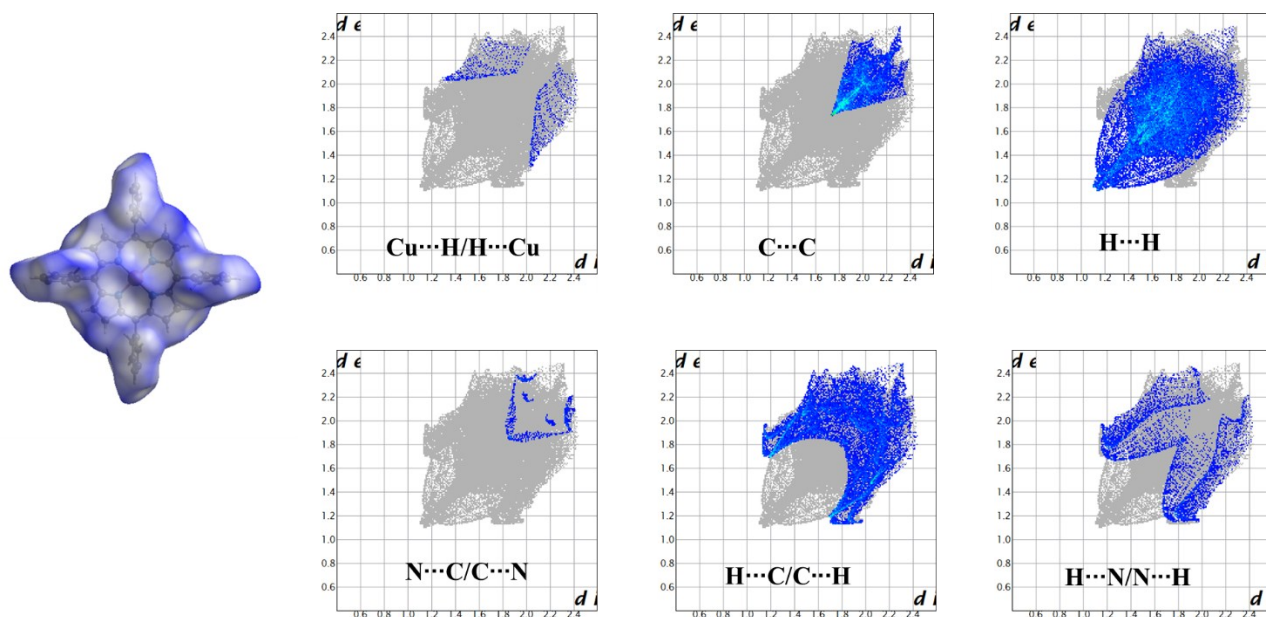


Figure S1. 3D d_{norm} Hirshfeld surface (left) and 2D fingerprint plots (right) of crystal **1**.

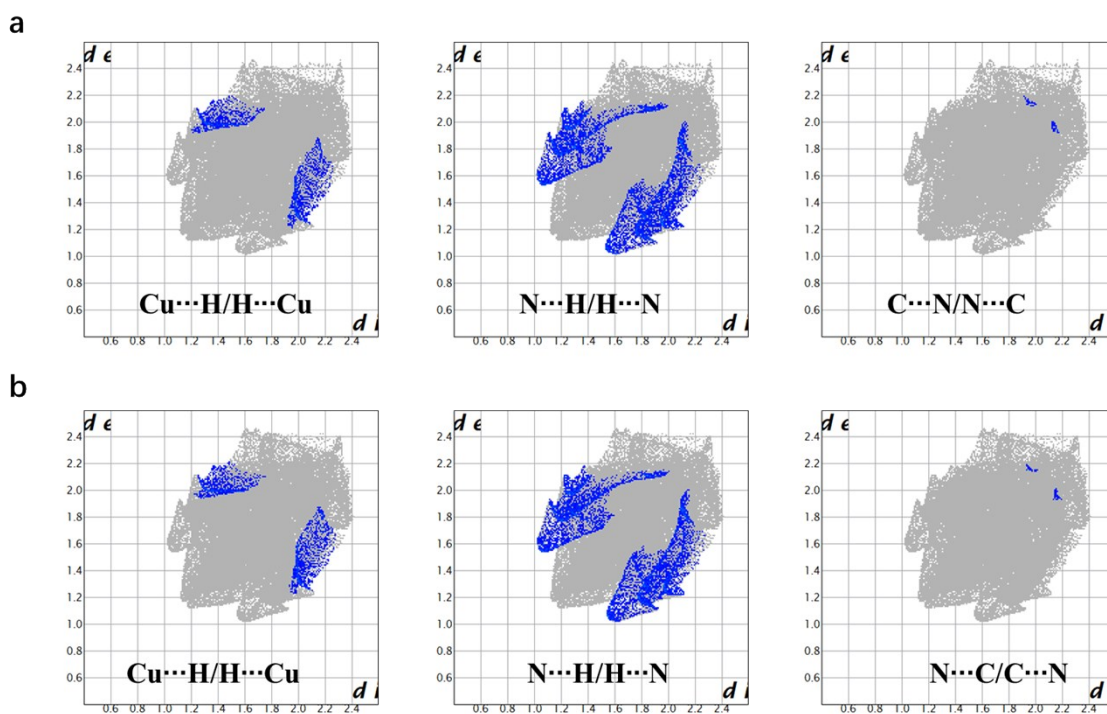


Figure S2. 2D fingerprint plots (right) resolved into Cu–H, N...H/H...N and C...N/N...C interaction for crystals **2** (upper **a**) and **3** (lower **b**), respectively; the full fingerprint appears beneath each decomposed plot as a grey shadow.