

Table S1 Hydrogen-bond geometry (Å, °) for (IA)

Cg1 is the centroid of the C16-C19, C23, and C24 ring. Cg2 is the centroid of the N4, C19-C23 ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2...C11 ⁱ	0.93	2.74	3.665(2)	171
C9—H9...C11 ⁱⁱ	0.93	2.80	3.561(3)	140
C5—H5...Cg1 ⁱⁱⁱ	0.93	2.86	3.537(2)	131
C8—H8...Cg1 ^{iv}	0.93	2.92	3.612(3)	132
C8—H8...Cg2 ^{iv}	0.93	2.97	3.628(3)	129

Symmetry codes: (i) $3/2-x, -1/2+y, 1/2+z$; (ii) $x, 1+y, z$; (iii) $-1/2+x, 3/2-y, z$; (iv) $3/2-x, 1/2+y, -1/2+z$.

Table S2 Hydrogen-bond geometry (Å, °) for (IIA)

Cg1 is the centroid of the C4—C7, C11, and C12 ring. Cg2 is the centroid of the N1, C1-C4, and C12 ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C6—H6A...C11 ⁱ	0.93	2.80	3.6743(18)	158
C5—H5A...C11 ⁱⁱ	0.93	2.85	3.6375(17)	144
C2—H2A...Cg1 ⁱⁱⁱ	0.93	2.99	3.768(2)	142
C8—H8A...Cg2 ^{iv}	0.93	2.90	3.608(2)	134

Symmetry codes: (i) $1/2+x, 3/2-y, -z$; (ii) $1/2+x, 1/2+y, 1/2-z$; (iii) $x, 2-y, -1/2+z$; (iv) $3/2-x, 3/2-y, -1/2+z$.

Figure S1 Supramolecular structure of (IA): structure of the chain parallel to the *b*-axis (a) and the packing diagram viewed parallel to the *b*-axis (b). (Blue dashed lines represent for C-H... π interactions and green dash lines for C-H...Cl hydrogen bonds. All H atoms except those related to hydrogen-bonding interactions have been omitted for clarity. Symmetry codes: (i) $3/2-x, -1/2+y, 1/2+z$; (ii) $x, 1+y, z$; (iii) $-1/2+x, 3/2-y, z$; (iv) $3/2-x, 1/2+y, -1/2+z$.)

Figure S2 Supramolecular structure of (IIA): structure of a layer parallel to the *ac*-plane (a) and the interactions between two neighbouring layers (blue and pink) viewed parallel to the *b* axis. (Green dash lines represent for C-H...Cl hydrogen bonds and blue dash lines represent for C-H... π stacking. All H atoms except those related to hydrogen-bonding interactions have been omitted for clarity. Symmetry codes: (i) $1/2+x, 3/2-y, -z$; (ii) $1/2+x, 1/2+y, 1/2-z$; (iii) $x, 2-y, -1/2+z$; (iv) $3/2-x, 1/2+y, -1/2+z$.)

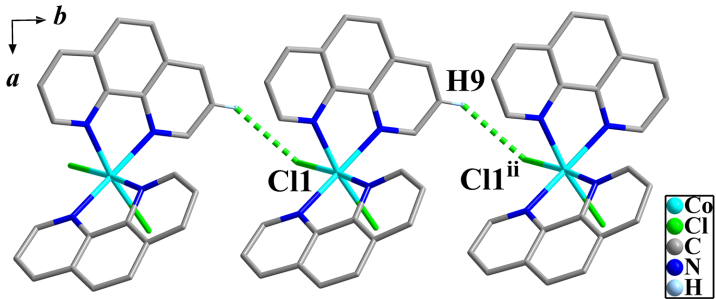


Fig. 1a

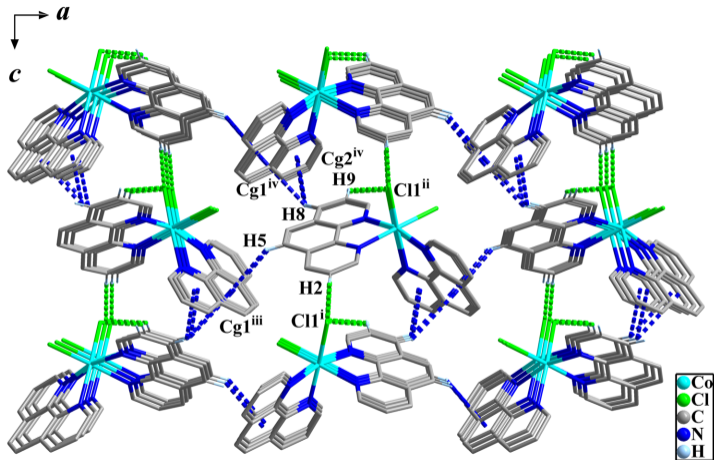


Fig. 1b

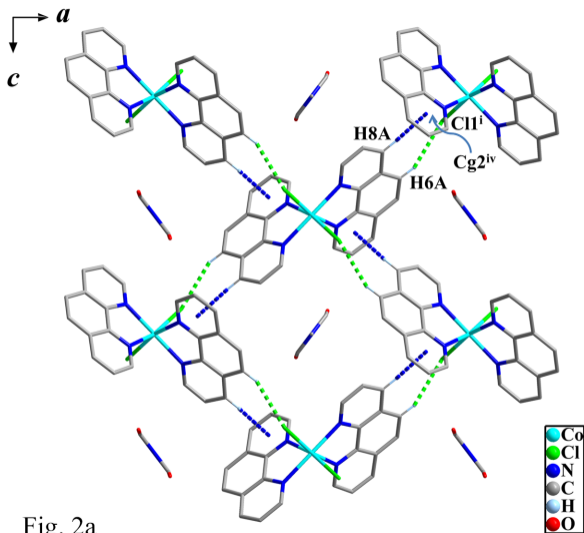


Fig. 2a

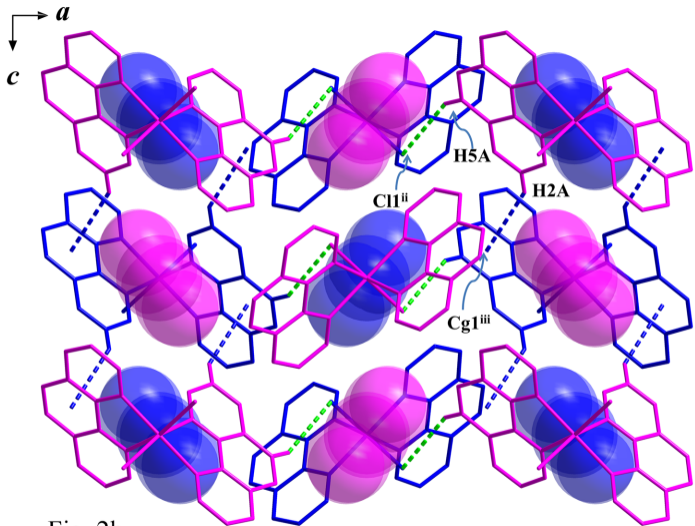


Fig. 2b