Electronic Supplementary Material (ESI) for CrystEngComm

Electronic Supporting Information

A dual-synthon in pyridinium chloride: formation of ladder-like and columnar motifs through hydrogen bonds and cation-π interactions

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Contents

Table S1. Distances and angles of intermolecular hydrogen bonds in the crystal **1b**.

D-H···A[a] (Å)	D···A (Å)	H···A (Å)	∠DHA (deg)
N2^{i} - H2^{i} ···Cl^{i}	3.087(5)	2.218	169.48
C5-H1···Cl1	3.547(6)	2.726	145.1
C15-H15···Cl1	3.673(5)	2.804	152.52
N1-H1···Cl2	3.032(4)	2.201	157.04
C1^{ii} -H1^{ii} ···Cl2	3.488(6)	2.789	136.28
C19^{i} -H19^{i} ···Cl2	3.543(6)	2.637	159.82
C15^{i} -H15^{i} ···Cl1^{i}	3.673(5)	2.804	152.52
C1-H1···Cl2^{ii}	3.488(6)	2.789	136.28
N1^{ii} -H1^{ii} ···Cl2^{ii}	3.032(4)	2.201	157.04
N2- H1···Cl1^{i}	3.087(5)	2.218	169.48

[a] Symmetry transformations used to generate equivalent atoms:

(i) -X+1,-Y+1,-Z+2; (ii) -X+2,-Y+1,-Z+2

Table S2. Distances and angles of intermolecular hydrogen bonds in the crystal **1c**.

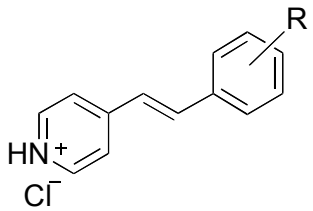
D-H···A[a] (Å)	D···A (Å)	H···A (Å)	∠DHA (deg)
N2^{i} -H2^{i}···Cl^{i}	3.027(5)	2.235	149.69
C5-H5 ···Cl^{i}	3.416(7)	2.778	125.43
C15^{i} -H15^{i} ···Cl1^{iii}	3.380(8)	2.643	134.82
N1-H1···Cl2^{iv}	3.076(5)	2.241	158.37
C12-H12···Cl2^{iv}	3.587(8)	2.673	161.71
N2^{i} -H2^{i} ···Cl1^{i}	3.027(5)	2.235	149.69
C15-H15···Cl^{i}	3.380(8)	2.643	134.82
N12-H12···Cl2^{v}	3.076(5)	2.241	158.37
C19^{i} -H19^{i} ···Cl2^{iv}	3.599(8)	2.864	134.94
C1-H1···Cl2^{v}	3.587(8)	2.673	161.71

[a] Symmetry transformations used to generate equivalent atoms:

(i) X+2,Y,Z; (ii) -X+3,-Y+1,-Z; (iii) -X+1,-Y,-Z; (iv) X+1,Y,Z; (v) -X+2,-Y+1,-Z

Table S3. Results of CSD search for styrylpyridinium chloride.

Refcode	R	H_2O(equiv)	Type	Column type
EQOSOT[1)]	H	3	close to III	head-to-tail
EQOTAG[1)]	4-CF3	3	close to III	head-to-tail
EQOTEK[1)]	3,5-diCl	0	IV	head-to-head
EQOTIO[1)]	perfluoro	0	close to IV	head-to-head
EQOTUA[1)]	4-F	3	close to III	head-to-tail
EQOVEM[1)]	4-Cl	2	close to III	head-to-tail
EQOVOW[1)]	4-Br	2	III	head-to-tail
EQOWAJ[1)]	4-I	2	III	head-to-tail
EQOWIR[1)]	4-MeO	2.67+(0.33HCl)	close to III	head-to-tail
UYAPIU[2)]	H	2	III	head-to-tail
YINTUL[3)]	Naphthyl	3	III	head-to-tail



References

1) B. Mondal, B. Captain and V. Ramamurthy, *Photochem. Photobiol. Sci*., 2011, **10**, 891.

2) S. Yamada, N. Uematsu and K. Yamashita, *J. Am. Chem. Soc*., 2007, **129**, 12100.

3) S. Yamada and Y. Nojiri, *Chem. Commun*., 2011, **47**, 9143.

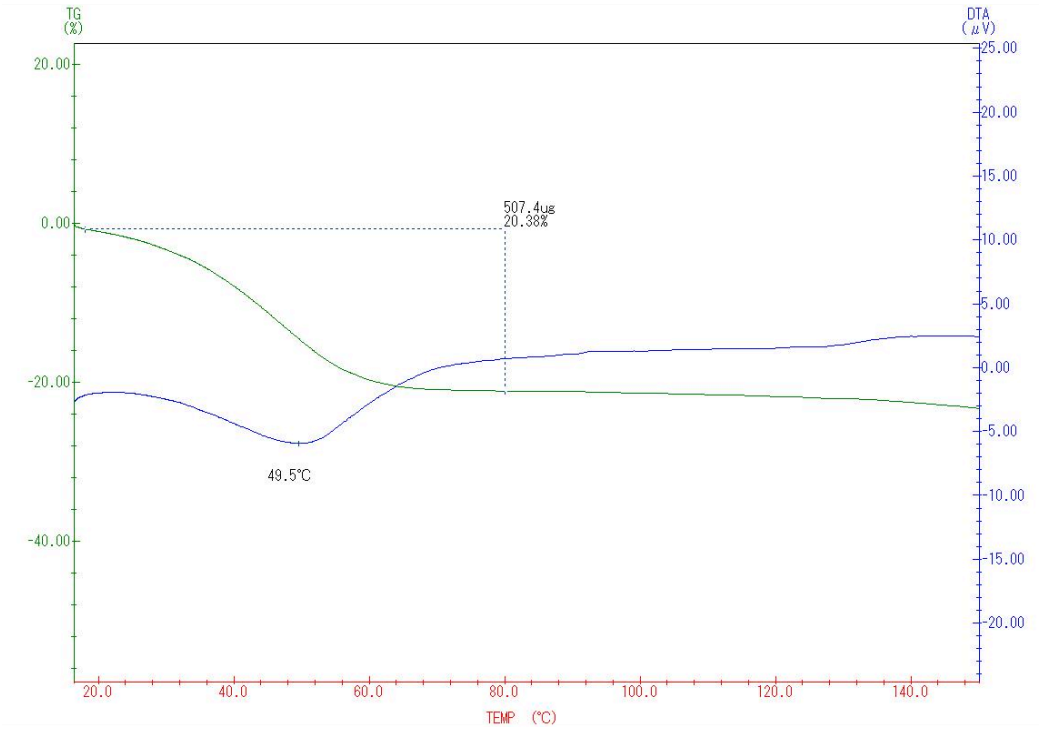


Fig. S1. Thermogravimetric analysis of **1b**.

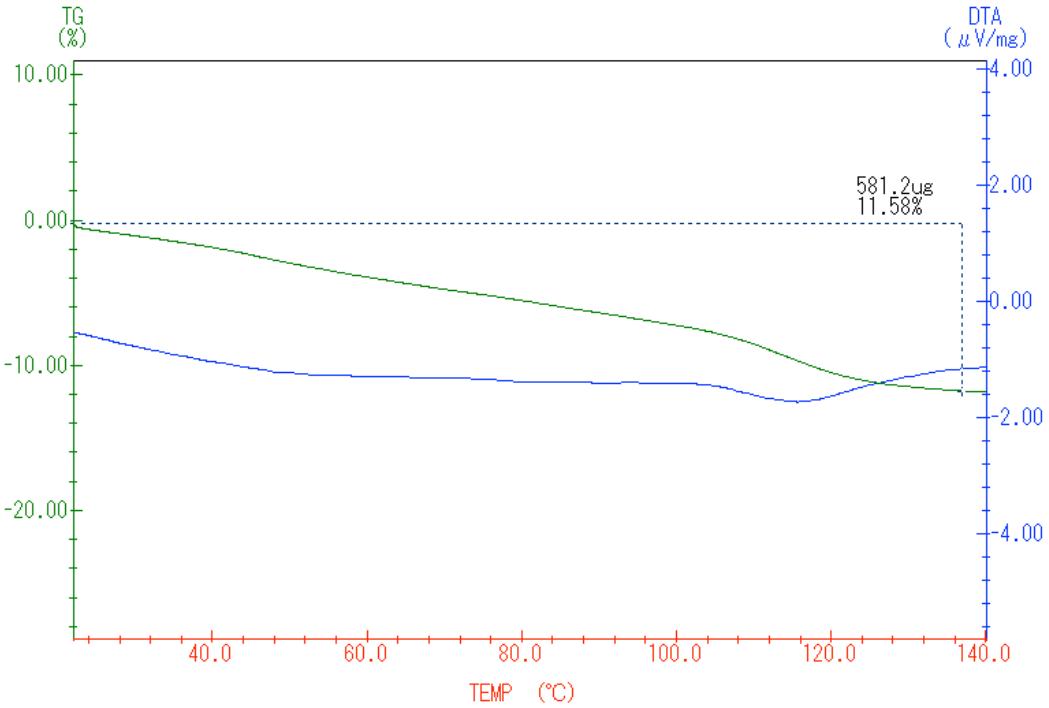


Fig. S2. Thermogravimetric analysis of **1c**.

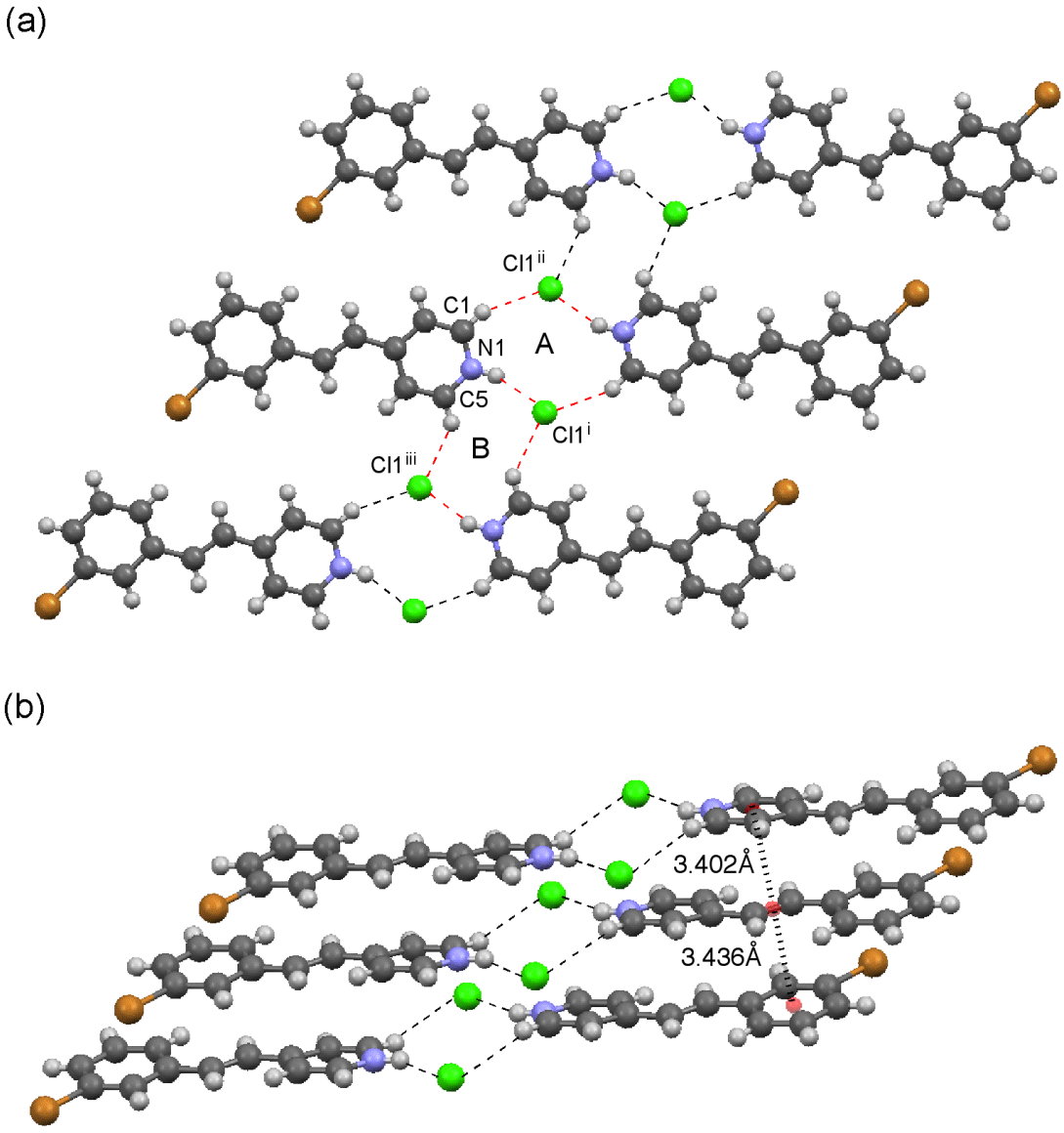


Fig. S3 Crystal structure of **2**. (a) Top view of the packing structure. The 2D sheet motif contains dual-synthons, A and B. (b) Side view of the column with a head-to-head arrangement

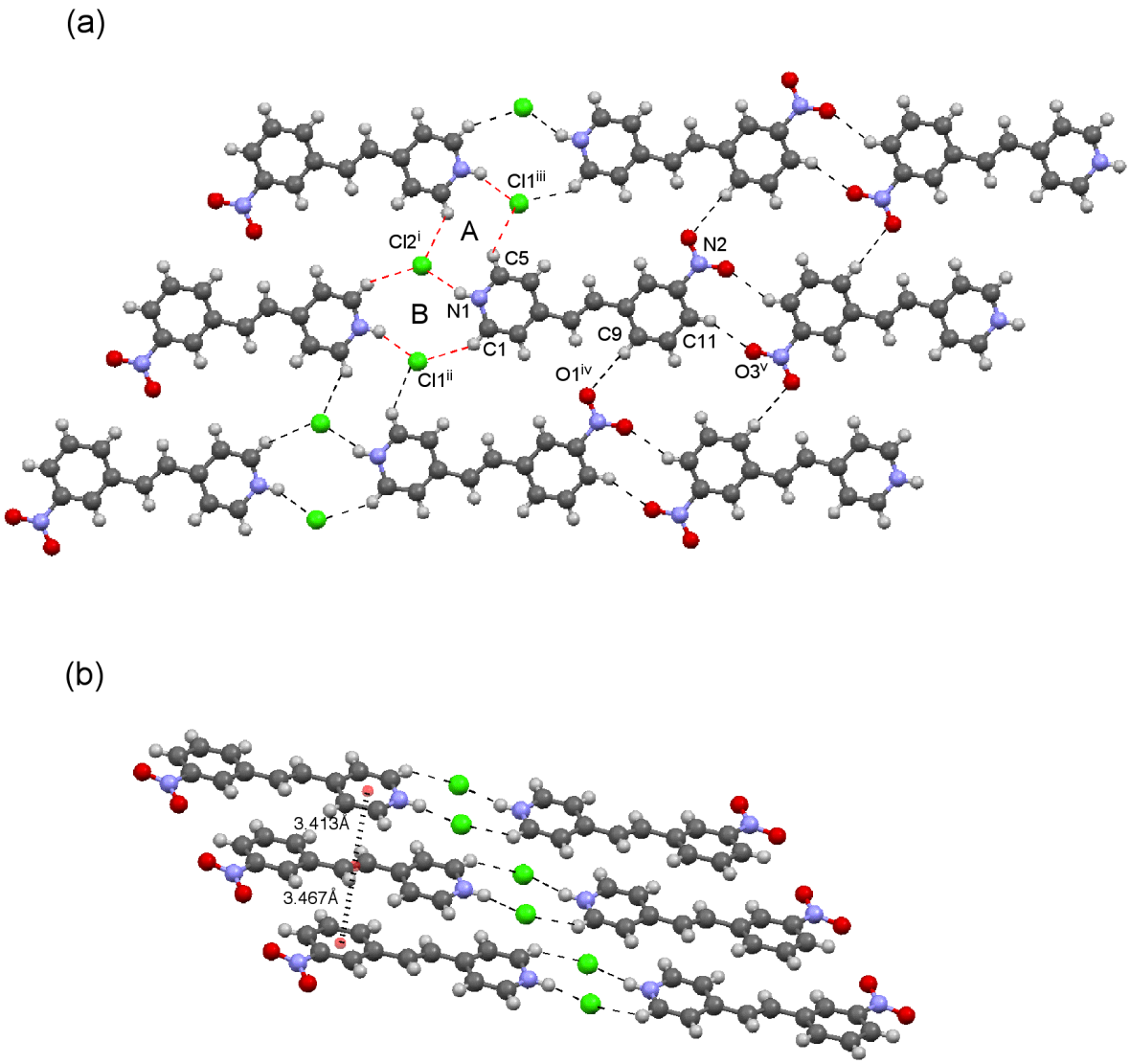


Fig. S4 Crystal structure of **3**. (a) Top view of the packing structure. The 2D sheet motif contains dual-synthons A and B. (b) Side view of the column with a head-to-tail arrangement.

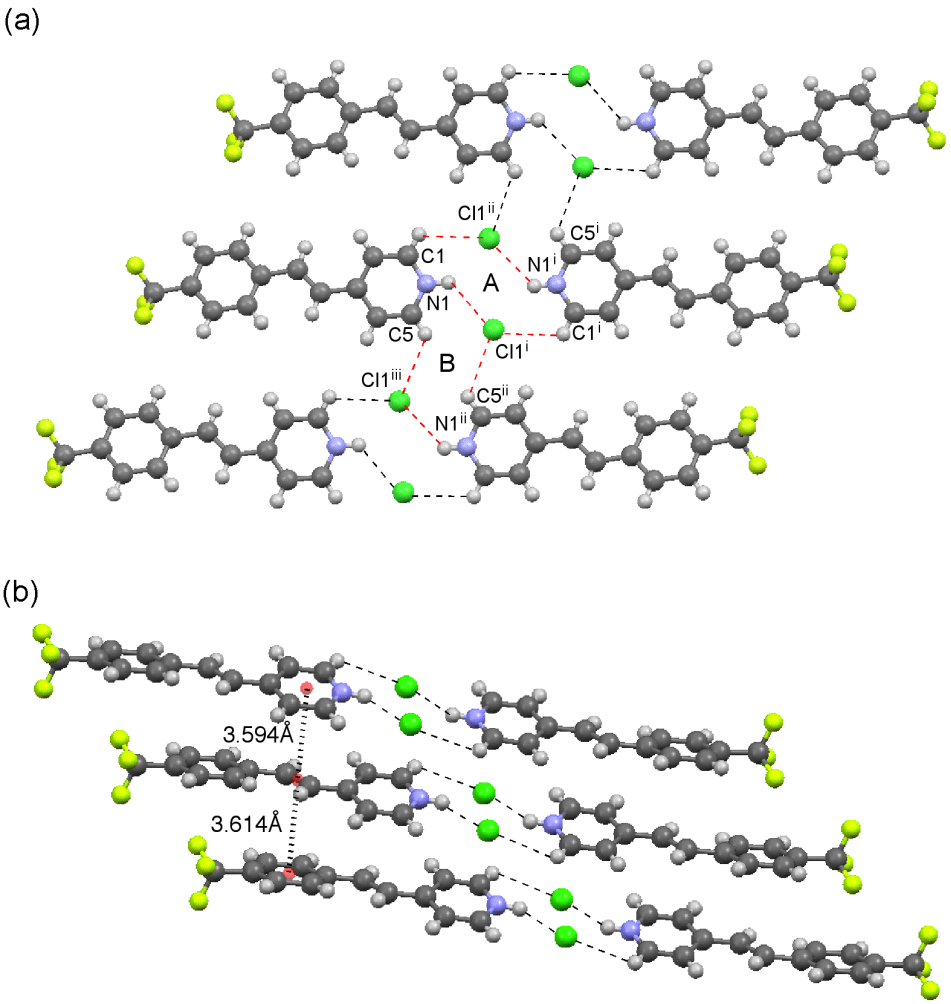


Fig. S5 Crystal structure of **4**. (a) Top view of the packing structure. The 2D sheet motif contains dual-synthons A and B. (b) Side view of the column with a head-to-tail arrangement.

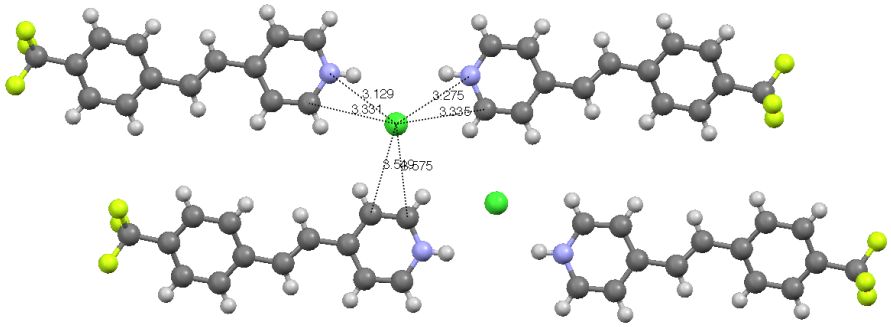


Fig. S6 Hydrogen bonds of a chloride ion of **4**

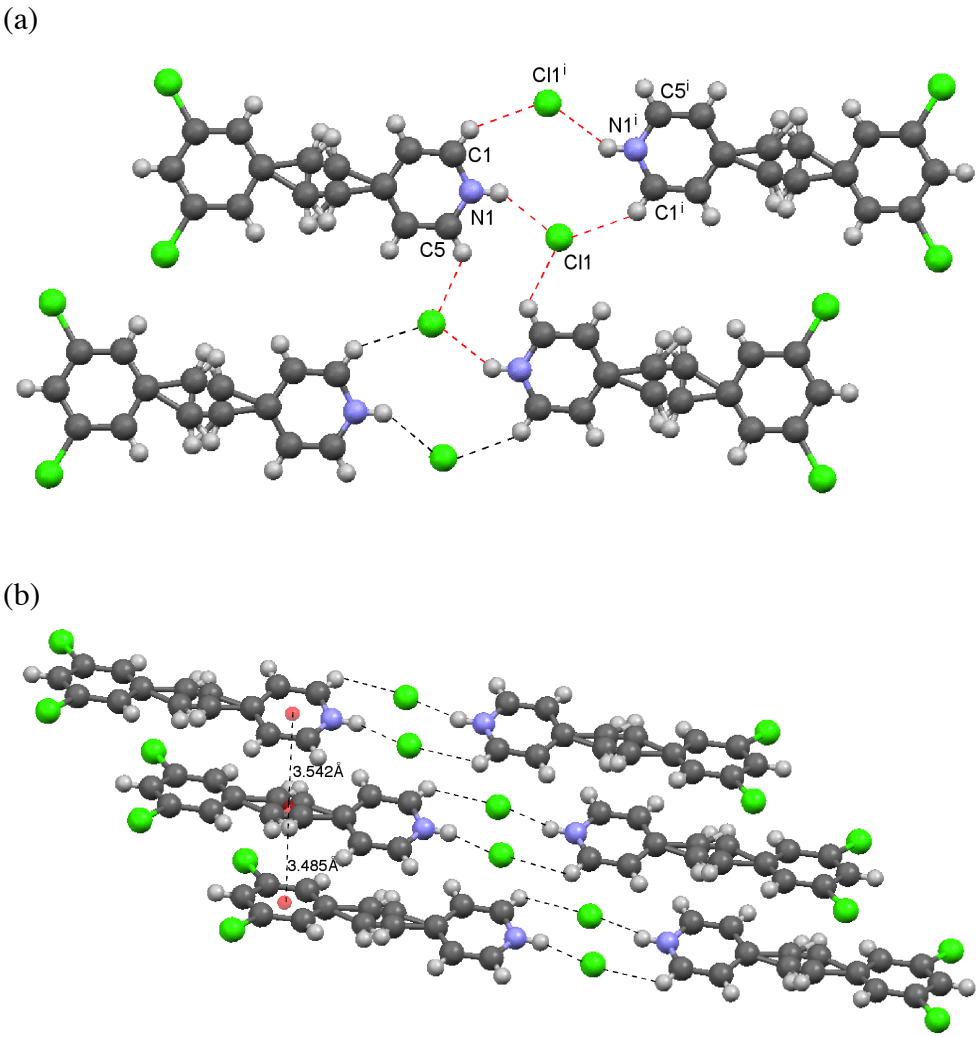


Fig. S7 Crystal structure of **5**. (a) Top view of the packing structure. The 2D sheet motif contains dual-synthons A and B. (b) Side view of the column with a head-to-tail arrangement.