Electronic Supplementary Material (ESI) for CrystEngComm

Zinc(II) and cadmium(II) coordination polymers mediated by rationally designed symmetrical/asymmetrical *V*-shaped heterocyclic aromatic ligands exhibiting different supramolecular architectures

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Supporting Information:

Table SI1. Intermolecular Hydrogen Bonding Parameters (Å, °) in Compounds Lsym, L1 and 1-4.

D–H···A	D–H	H···A	D···A	∠DHA	Symmetry code
Lsym					
C1–H1···N2	0.93	2.47	3.3637(19)	161	-1+*y*, *x*, -*z*
C5–H5···N2	0.93	2.55	3.4630(18)	166	-*x*+*y*, 1-*x*, 1/3+*z*
L1					
C4–H4···N2	0.93	2.43	3.315(10)	158	1+*x*, *y*, *z*
C5–H5···N2	0.93	2.58	3.396(9)	147	1-*x*, 1-*y*, -*z*
1					
C1–H1···O2	0.93	2.52	3.405(4)	159	*y*, -*x*+*y*, -*z*
C1–H1···O3	0.93	2.58	3.294(6)	134	*y*, -*x*+*y*, -*z*
C4–H4···O3	0.93	2.45	3.280(6)	149	1-*x*+*y*, 1-*x*, *z*
C11–H11···O2	0.93	2.51	3.376(5)	154	5/3-*x*, 4/3-*y*, 1/3-*z*
C12–H12···O4	0.93	2.37	3.267(5)	162	2/3-*x*+*y*, -2/3+*y*, -1/6+*z*
2					
C10–H10···N1	0.93	2.61	3.273(3)	128	*x*, -1+*y*, *z*
C2–H2···Cl1	0.93	2.79	3.584(2)	145	2-*x*, -1/2+*y*, 1/2-*z*
C5–H5···Cl1	0.93	2.73	3.585(2)	154	-1+*x*, *y*, *z*

C9–H9···Cl1	0.93	2.77	3.580(2)	146	-1+*x*, -1+*y*, *z*
3					
O2–H2A···O3	0.82	2.12	2.84(1)	147	*x*, 1/2-*y*, -1/2+*z*
O2–H2A···O5	0.82	2.52	3.260(3)	150	*x*, 1/2-*y*, -1/2+*z*
C2–H2···O5	0.93	2.53	3.368(3)	151	*x*, 1/2-*y*, -1/2+*z*
C4–H4···O2	0.93	2.42	3.351(3)	176	1-*x*, -*y*, 1-*z*
C7–H7···O5	0.93	2.51	3.186(3)	130	1+*x*, 1/2-*y*, -1/2+*z*
C10–H10···O4	0.93	2.55	3.290(3)	137	1+*x*, *y*, *z*
4					
C2–H2···O5	0.93	2.55	3.375(5)	148	*x*, 1/2-*y*, 1/2+*z*
C4–H4···O2	0.93	2.47	3.398(4)	174	1-*x*, -1/2+*y*, 1/2-*z*
C7–H7···O5	0.93	2.49	3.201(5)	133	-1+*x*, 1/2-*y*, 1/2+*z*
C10–H10···O4	0.93	2.49	3.270(5)	142	-1+*x*, *y*, *z*

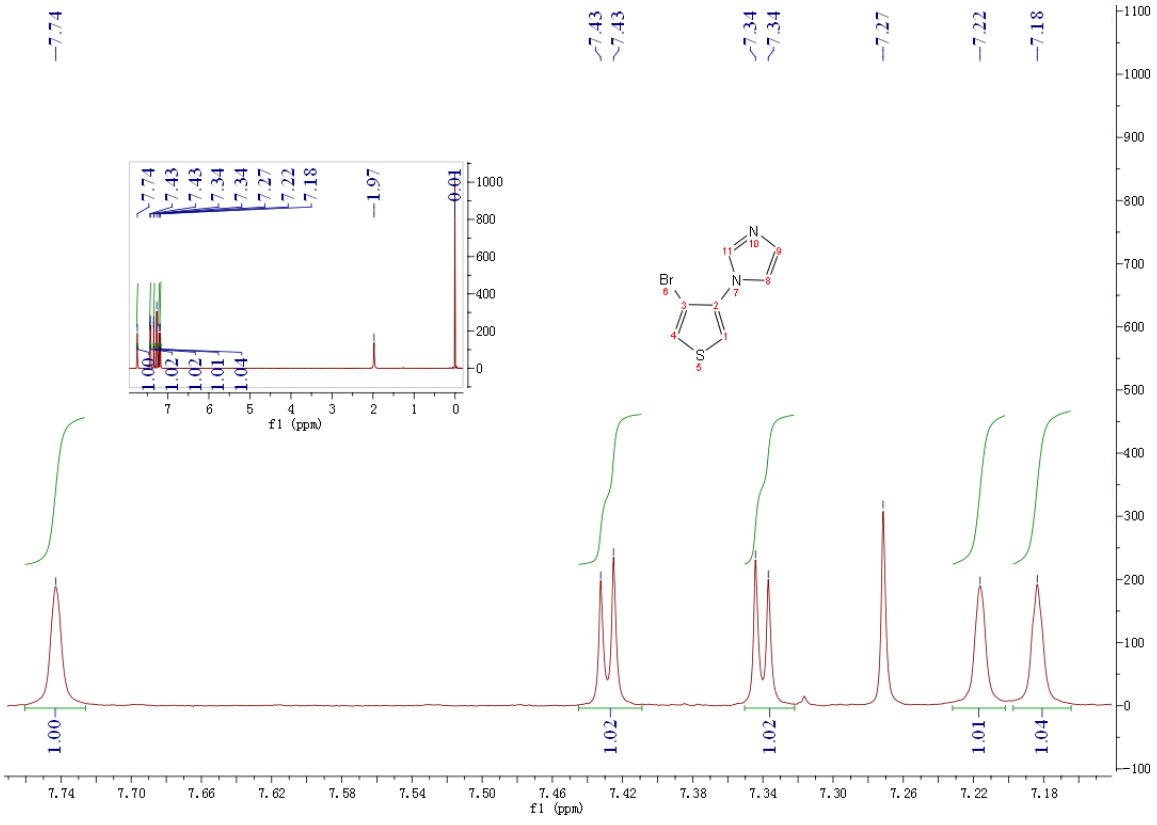

Fig. SI1. ^{1}H NMR spectrum of compound **L1**.

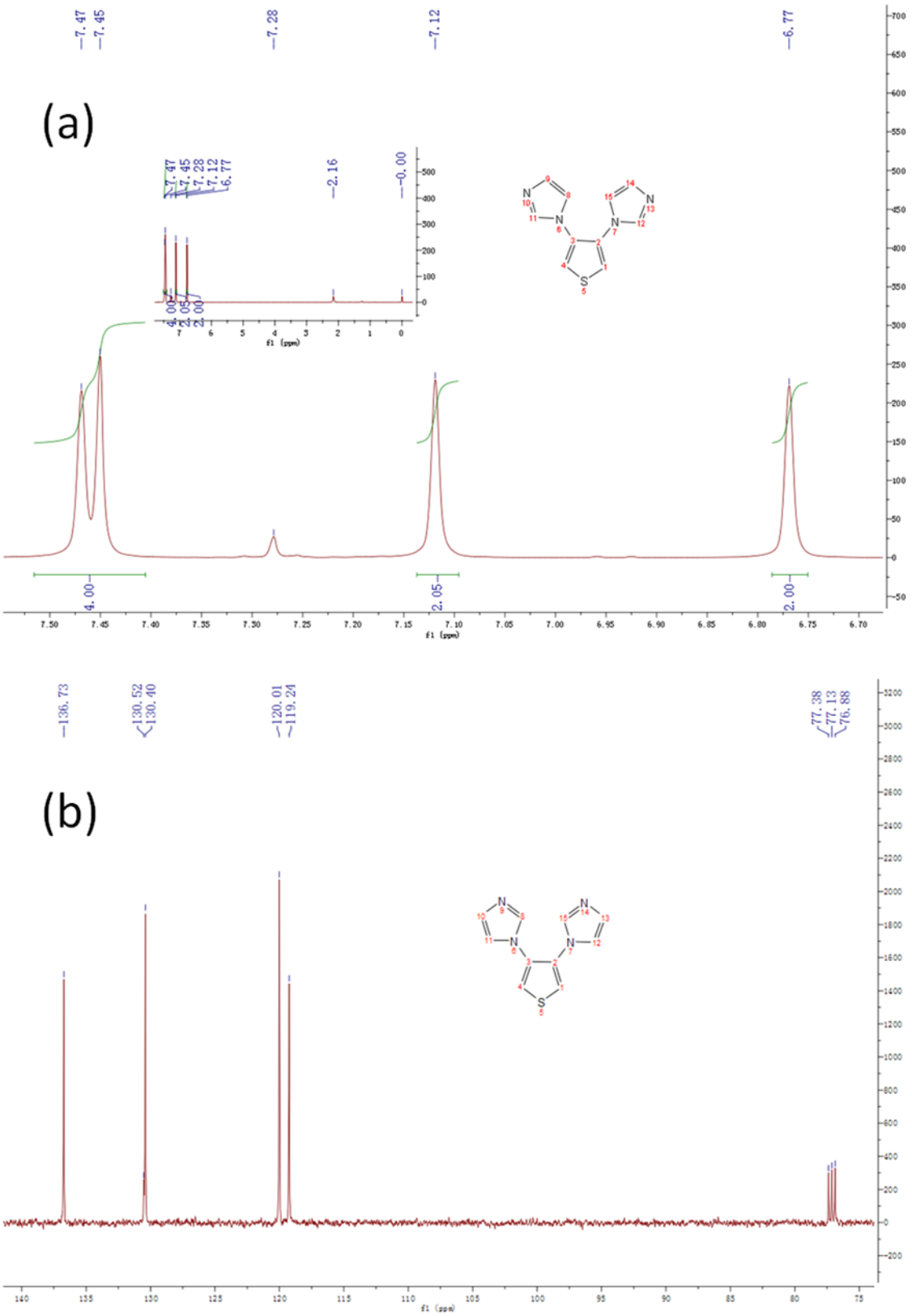

Fig. SI2. ^{1}H (**a**) and ^{13}C (**b**) NMR spectra of compound **Lsym**.

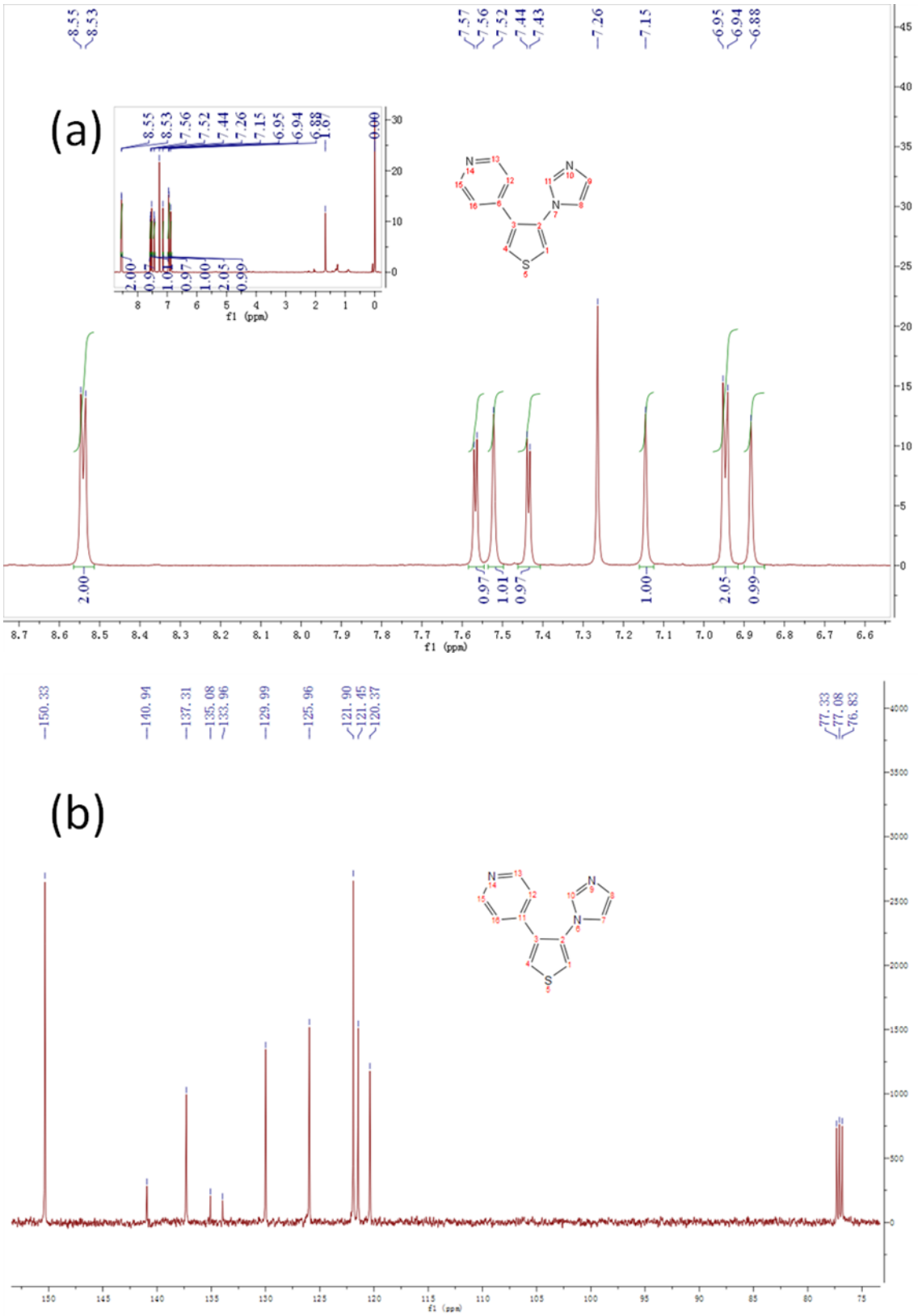

Fig. SI3. ^{1}H (**a**) and ^{13}C (**b**) NMR spectra of compound **Lasym**.

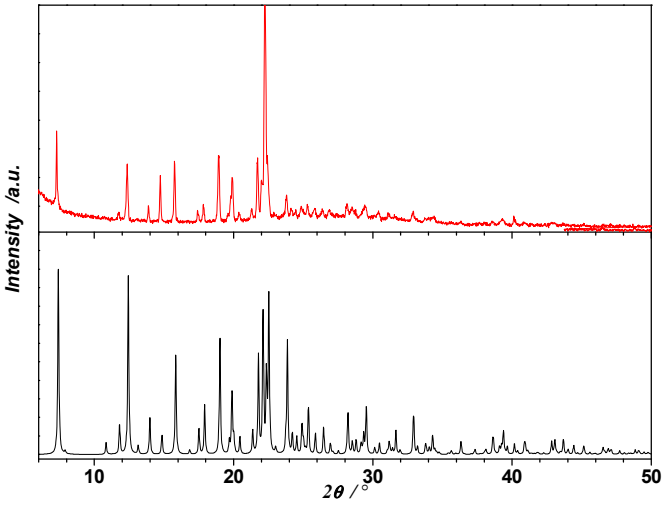

Fig. SI4. Diagrams of the simulative (black line) and experimental (red line) powder X-ray diffraction patterns for **1**.

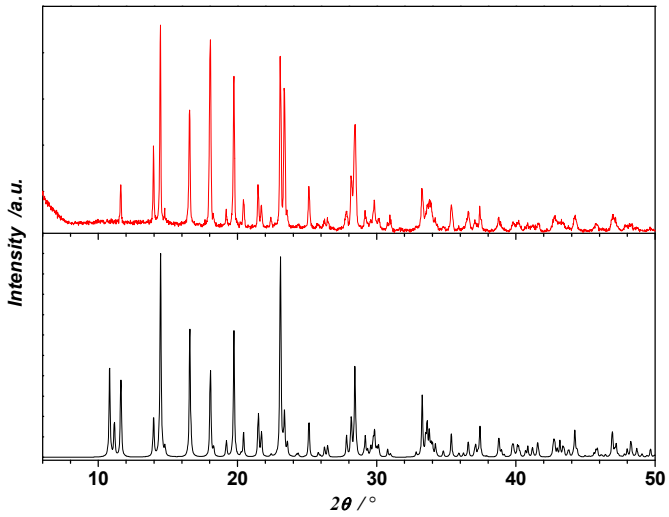

Fig. SI5. Diagrams of the simulative (black line) and experimental (red line) powder X-ray diffraction patterns for **2**.

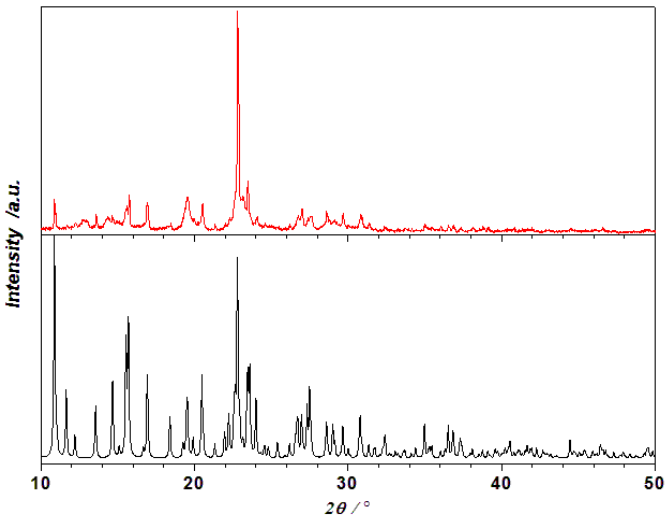

Fig. SI6. Diagrams of the simulative (black line) and experimental (red line) powder X-ray diffraction patterns for **3**.

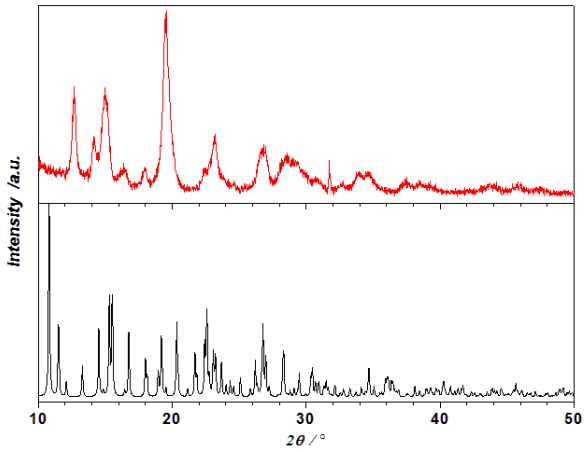

Fig. SI7. Diagrams of the simulative (black line) and experimental (red line) powder X-ray diffraction patterns for **4**.

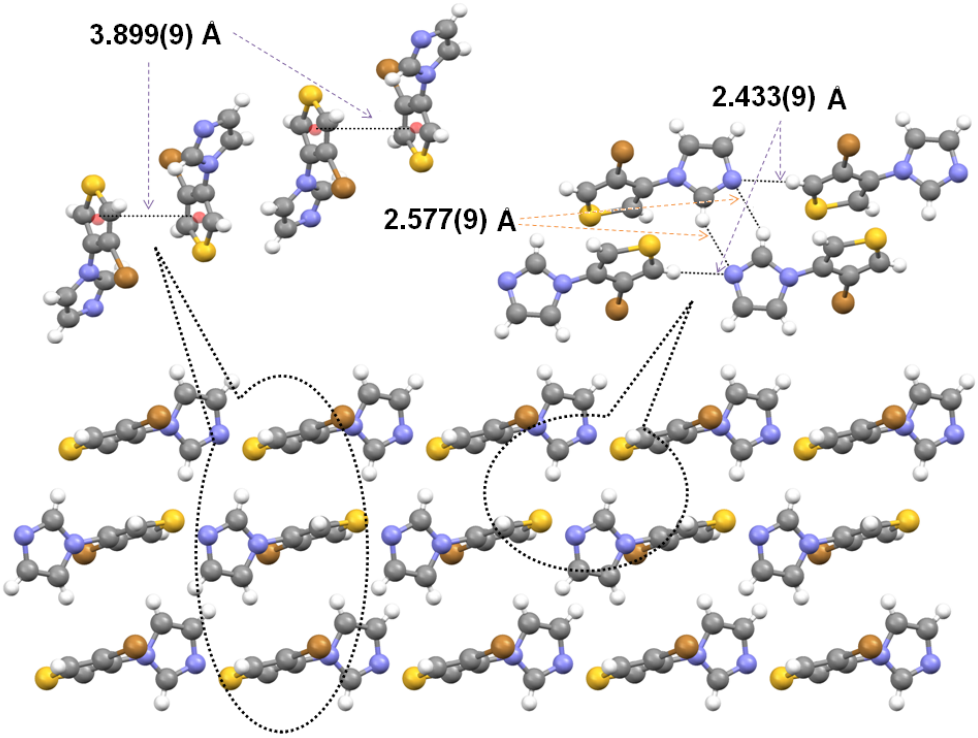

Fig. SI8. View of the hydrogen bonding and π-π stacking interactions in **L1**.