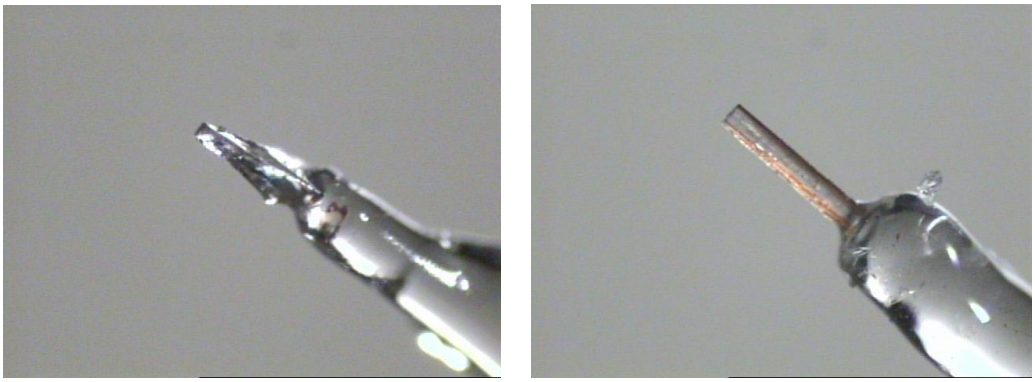
Electronic Supplementary Material for CrystEngComm

Electronic Supplementary Information‡

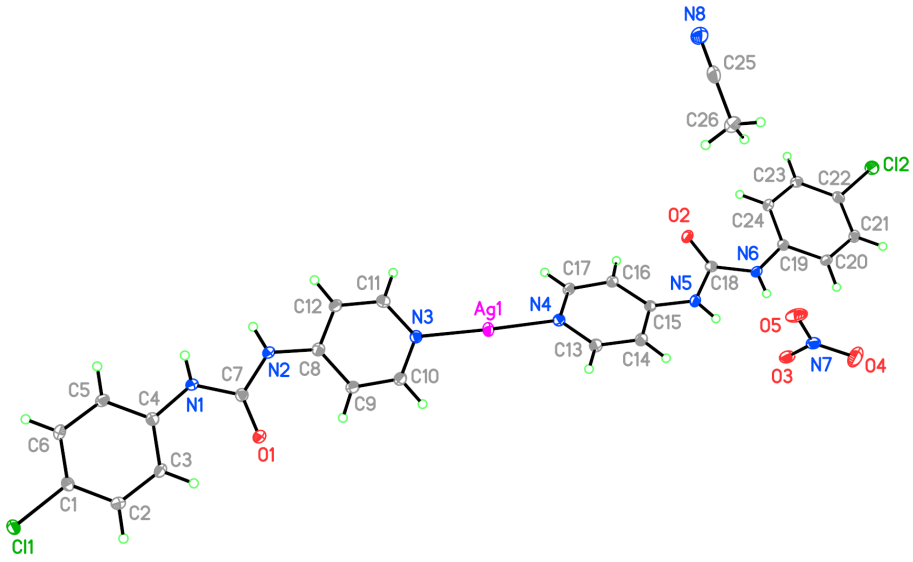
Silver complexes of *N*-4-halophenyl-*N*'-4-pyridyl urea. Isostructurality, urea···nitrate hydrogen bonding, and Ag···halogen interaction†‡

Sreekanth K. Chandran, Ranjit Thakuria, and Ashwini Nangia*
School of Chemistry, University of Hyderabad, Hyderabad 500 046, India.
E-mail: ashwini.nangia@gmail.com

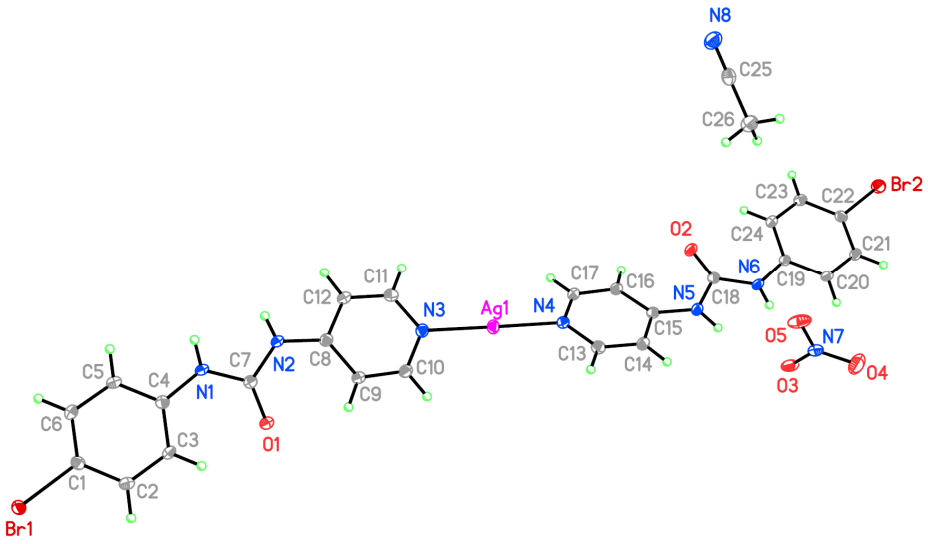


(a) (b)

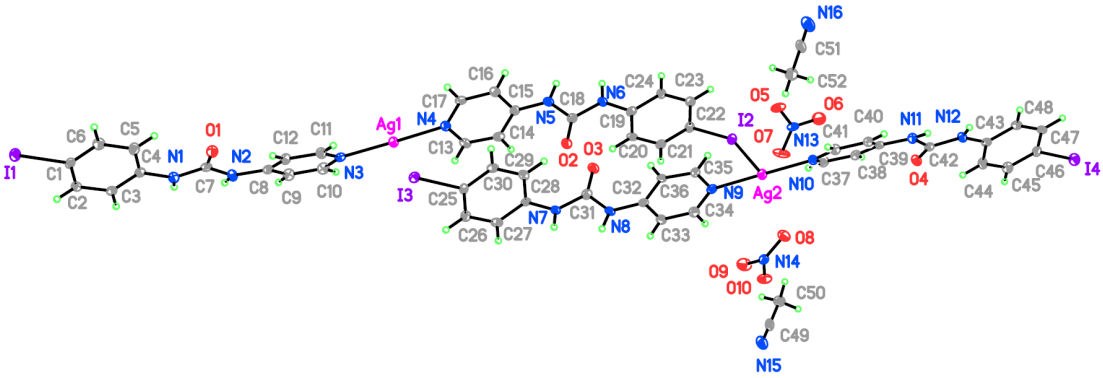
Fig. S1 Single crystal used for X-ray diffraction. (a) Colorless crystal of fluoro ligand **4** and (b) pale brown crystal of fluoro ligand **5**.



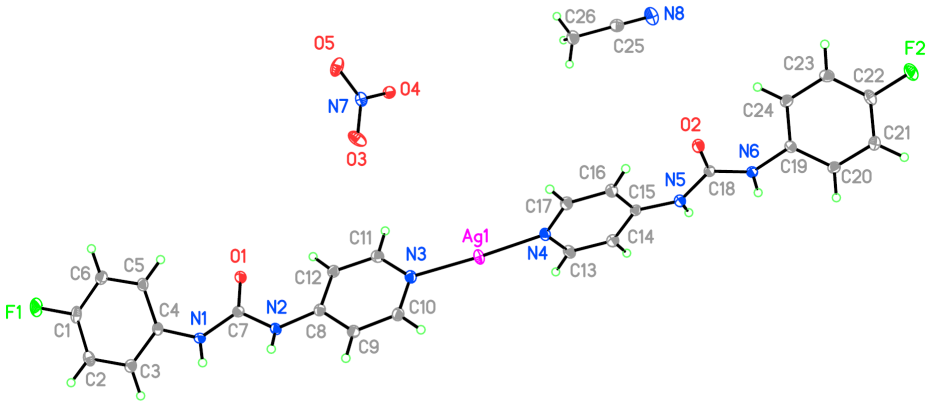
Crystal structure **1**



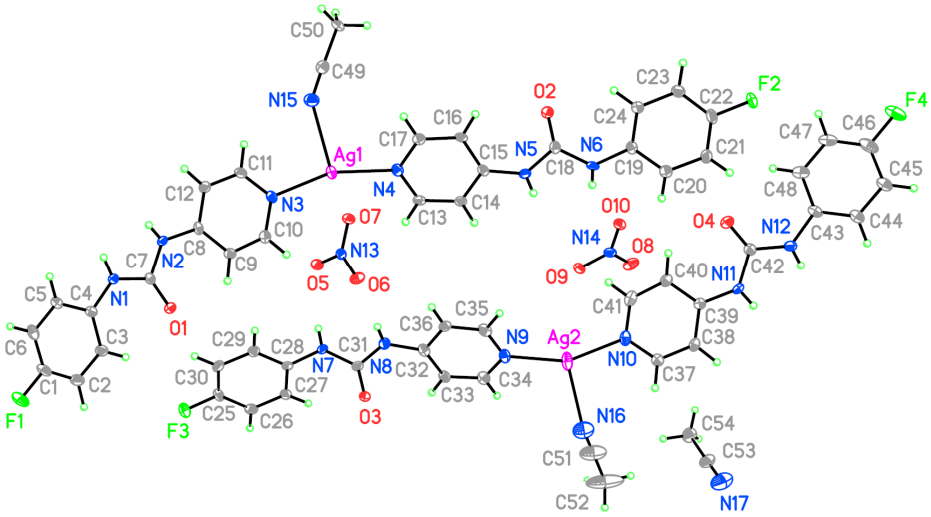
Crystal structure **2**



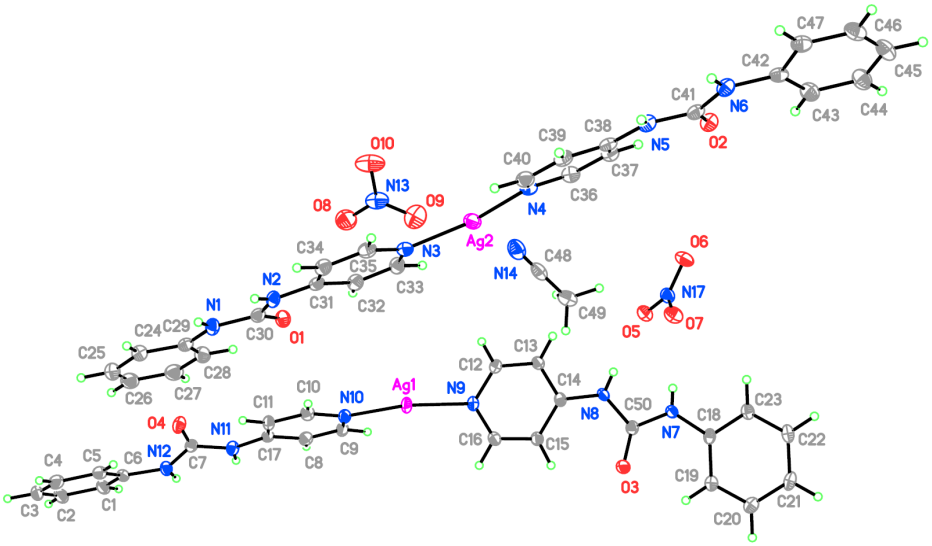
Crystal structure **3**



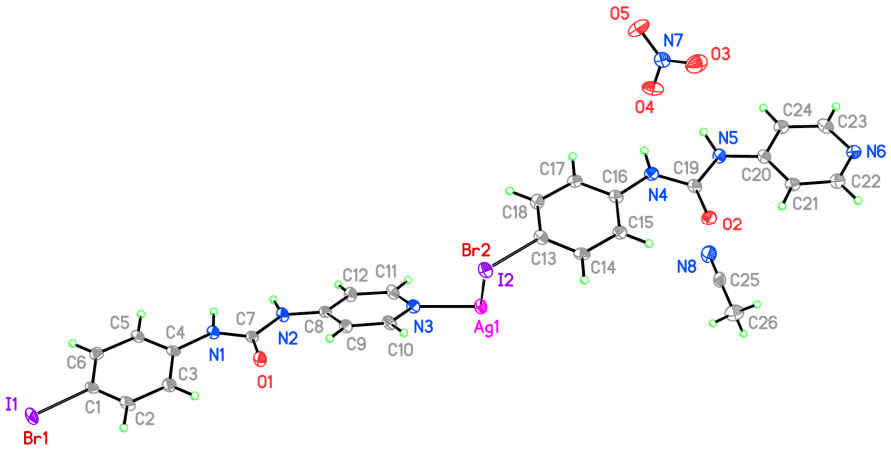
Crystal structure **4**



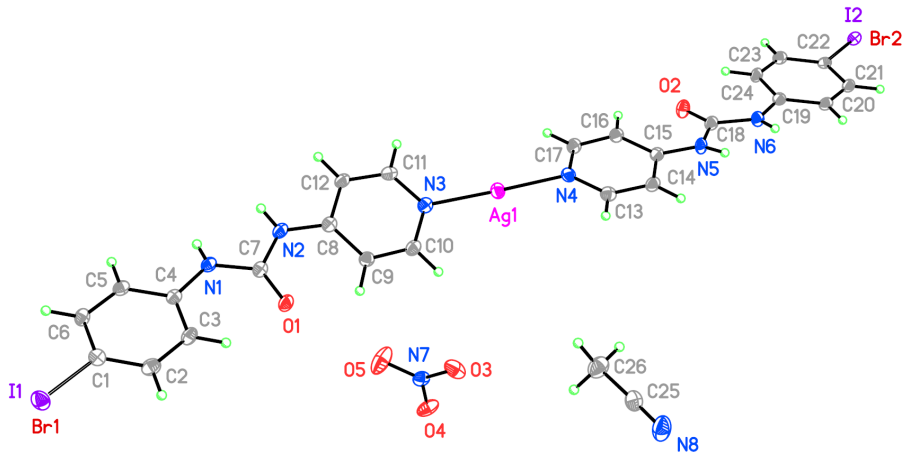
Crystal structure **5**



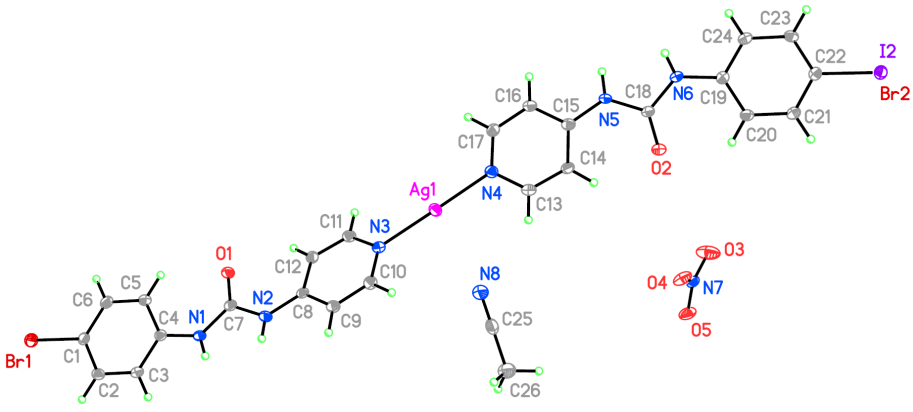
Crystal structure **6**



Crystal structure **7**



Crystal structure **8**



Crystal structure **9**

Fig. S2 ORTEP of crystal structures **1–9** are drawn at 35% probability of thermal ellipsoids for heavy atoms.

CSD results

The Cambridge Structural Database (CSD V5.29, November 2007 release) was searched for crystal structures with 3D coordinates, no errors, and Ag···X–C contact in the distance range 2.5–3.5Å. The *R*-factor was limited to <0.10 for chloro and bromo structures. Only one crystal structure with iodo group was retrieved with $R = 0.105$. The charge on Ag metal atom is +1.

List of CSD refcodes containing Ag^{+}···Cl–C interaction.

Refcode	Distance (Å)
ALISIX	3.16
ALISIX	3.25
ALISIX	3.39
BEGJON	3.31
CABJUL	3.26
ESEDUB	3.03
ETOQAF	3.29
FASTIC	3.09
FASTIC	3.01
FIZCEX	3.42
FOCGIO	3.34
FOCGIO	3.49
GEHFUV	3.18
HIFKUD	3.45
LARJEU	3.05
MIRGEZ	3.24
RIDPAW	3.32
VARVIT	3.35
YECTOQ	3.17
YEPFUV	3.13
YIDXAL	3.30
YOPCIP	3.34

There is only one crystal structure with Ag^{+}···Br–C interaction of 3.36 Å (refcode EBITUF) and one crystal structure with Ag^{+}···I–C interaction of 3.37 Å (FIGGIL).

CHN analysis on selected complexes

2 $C_{26}H_{23}AgBr_2N_8O_5$: Calcd. C 39.27, H 2.92, N 14.09. Found 39.36, H 2.90, N 13.87 (%).

3 $C_{26}H_{23}AgI_2N_8O_5$: Calcd. C 35.12, H 2.61, N 12.60. Found C 35.11, H 2.67, N 12.76 (%).

7 $C_{26}H_{23}AgBr_{1.09}I_{0.91}N_8O_5$: Calcd. C 37.27, H 2.77, N 13.37. Found C 36.49, H 2.74, N 13.13 (%).

9 $C_{26}H_{23}AgBr_{1.94}I_{0.06}N_8O_5$: Calcd. C 39.13, H 2.91, N 14.04. Found C 39.06, H 2.82, N 13.92 (%).

Elemental analyses were carried out on Thermo Finnigan Flash EA 1112 instrument.