Calculation details:

Electronic structure calculation was based on density function theory (DFT),[1] in which wave functions were explained in a plane wave basis set and the spin polarized version of the PW-91 GGA was employed for the exchange-correlation functional in the CASTEP code.[2]

1 J. P. Perew, K. Burke, M. Ernzerhof, *Phy. Rev. Lett.* 1996, **77**, 3865.

2 M. Segall, P. Lindan, M. Probert, C. Pickard et al, Materials Studio CASTEP version 4.1,2006.

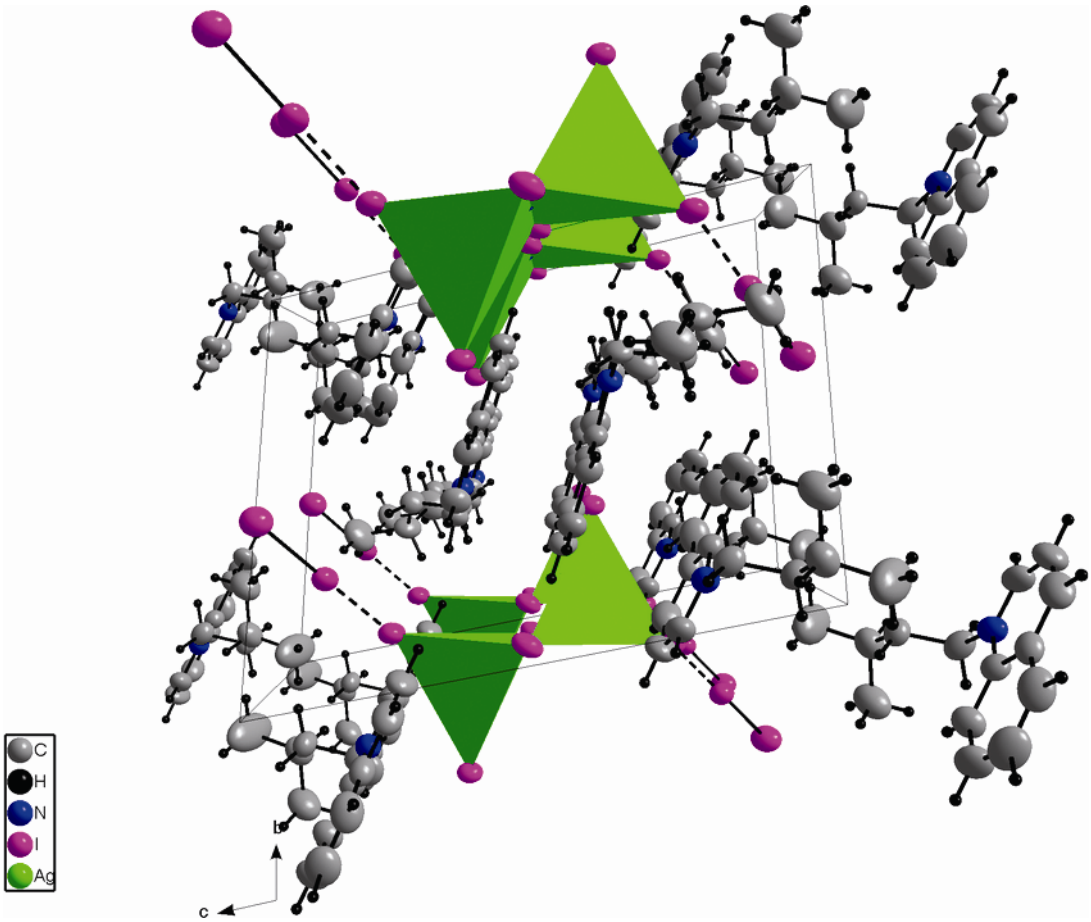

Fig. S1 Packing diagram of **1**

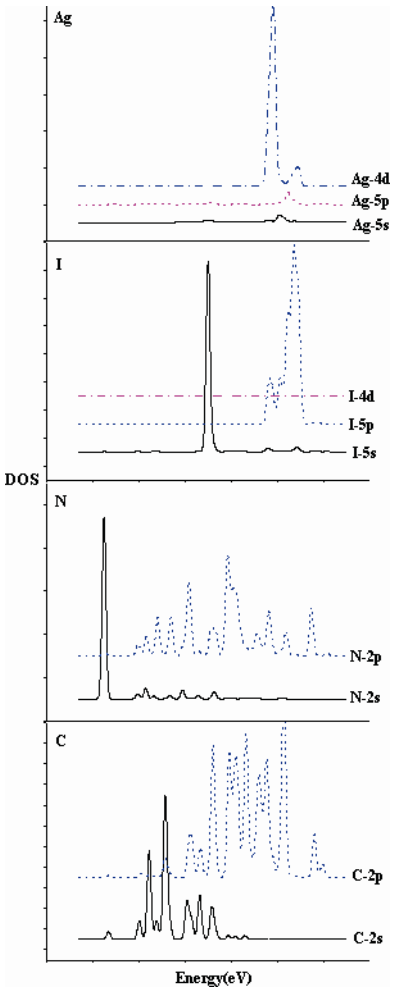

Fig. S2 PDOS of compound **1**

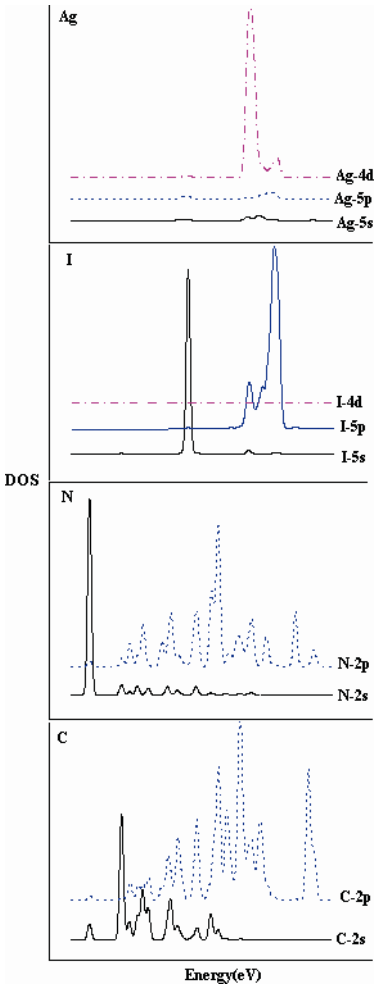

Fig. S3 PDOS of compound **2**