Electronic Supplementary Material (ESI) for CrystEngComm.

Halogen containing clusters N_2Br_2, N_2Br_4, S_2Br_4 and S_2Br_6 yield penannular inclusion compounds

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Electronic Supplementary Information

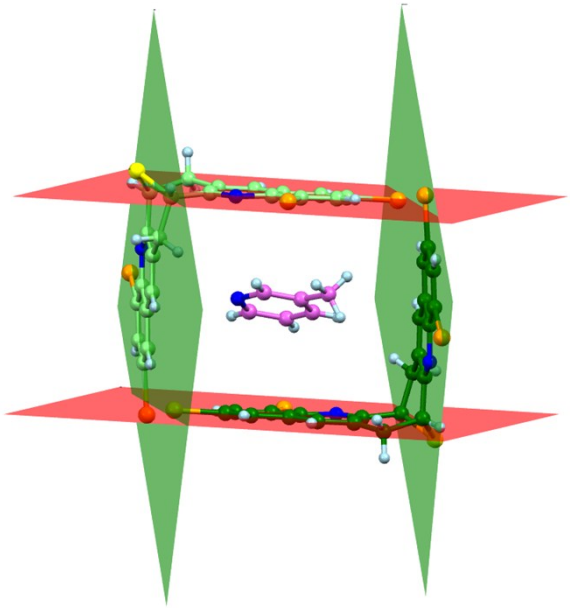

Fig. S1 Derivation of the molecular pen dimensions in Table 2, for the example of **11**, the (**7**)$_2$·(3-methylpyridine) compound.

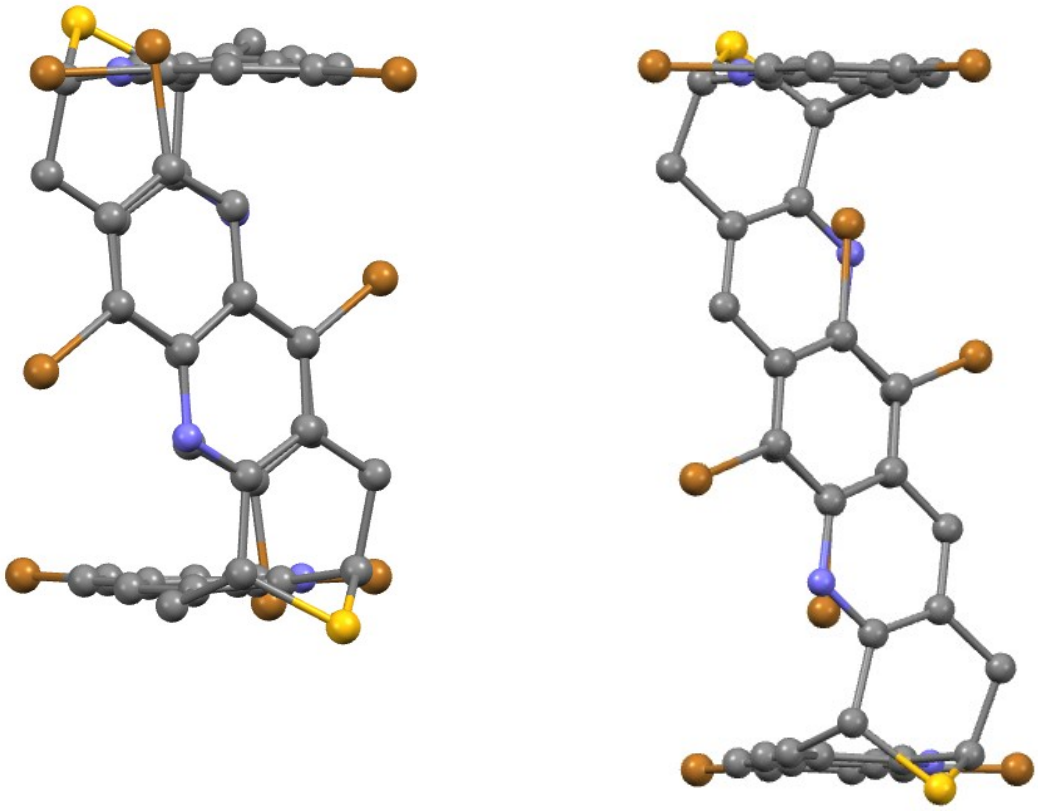

Fig. S2 Projection views of the long axis molecular pen aromatic wings for (left) **11**, the (3-methylpyridine compound), and (right) **13**, the (2-methylpyridine compound). These illustrate the dimensional increase in the cavity from 7.90 to 11.45 Å. In **11** both host aromatic rings are superposed, whereas in **13** only one ring is superposed on projection. All hydrogen atoms are omitted for clarity.

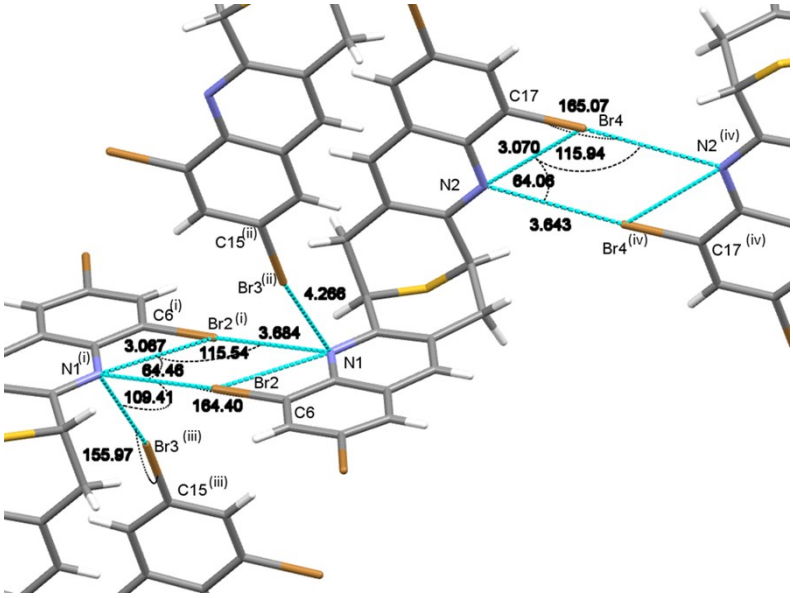

Fig. S3 The two types of centrosymmetric N/Br cluster present in **12**, the $(\mathbf{7})_2$·(4-methylpyridine) compound.

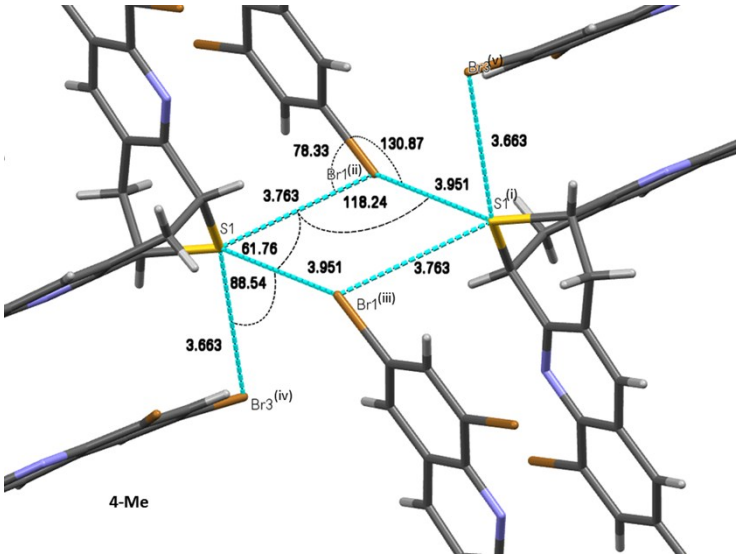

Fig. S4 The centrosymmetric S_2Br_4 cluster present in structure **12**, the 4-methylpyridine inclusion compound.

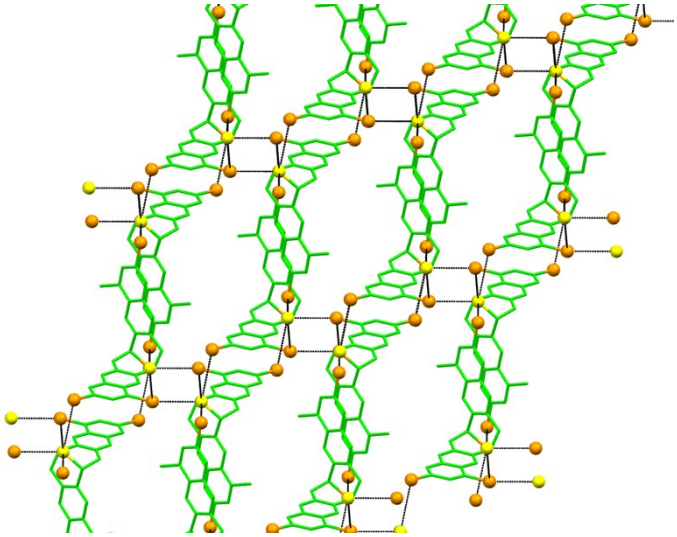

Fig. S5 The grid of S_2Br_6 clusters present in **14**, the $(\mathbf{7})_2$·(*tert*-butylcyclohexane) compound, and showing only the S···Br interactions.

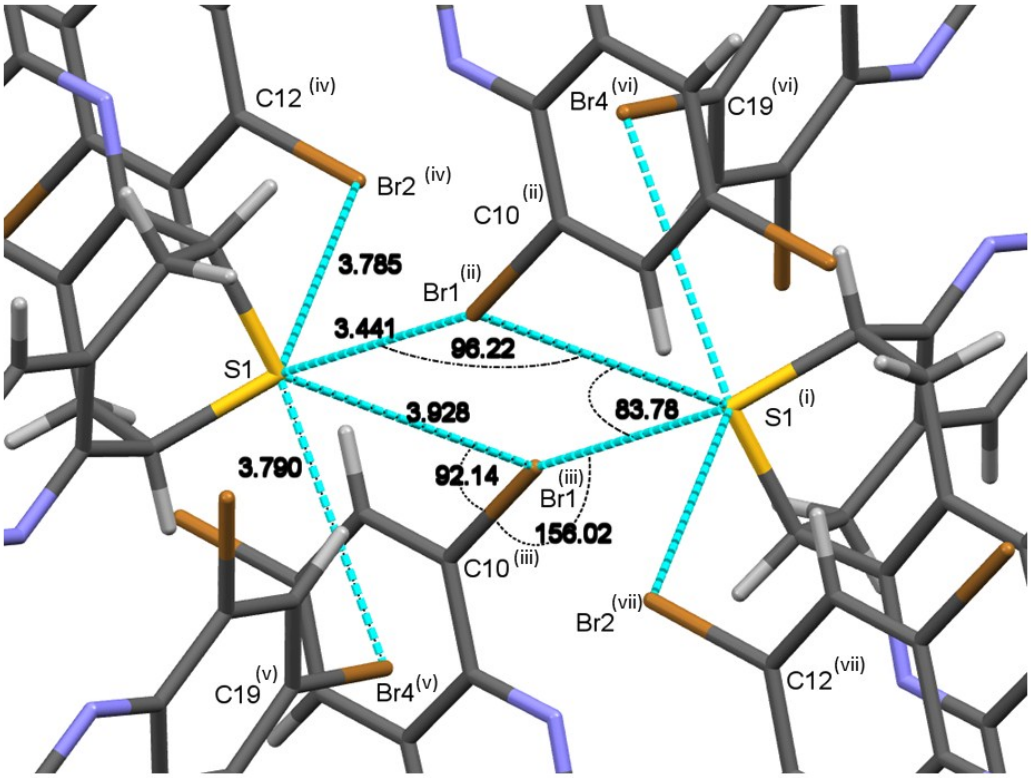

Fig. S6 The construction of one S_2Br_6 cluster in compound **14** showing only the S···Br interactions (blue).

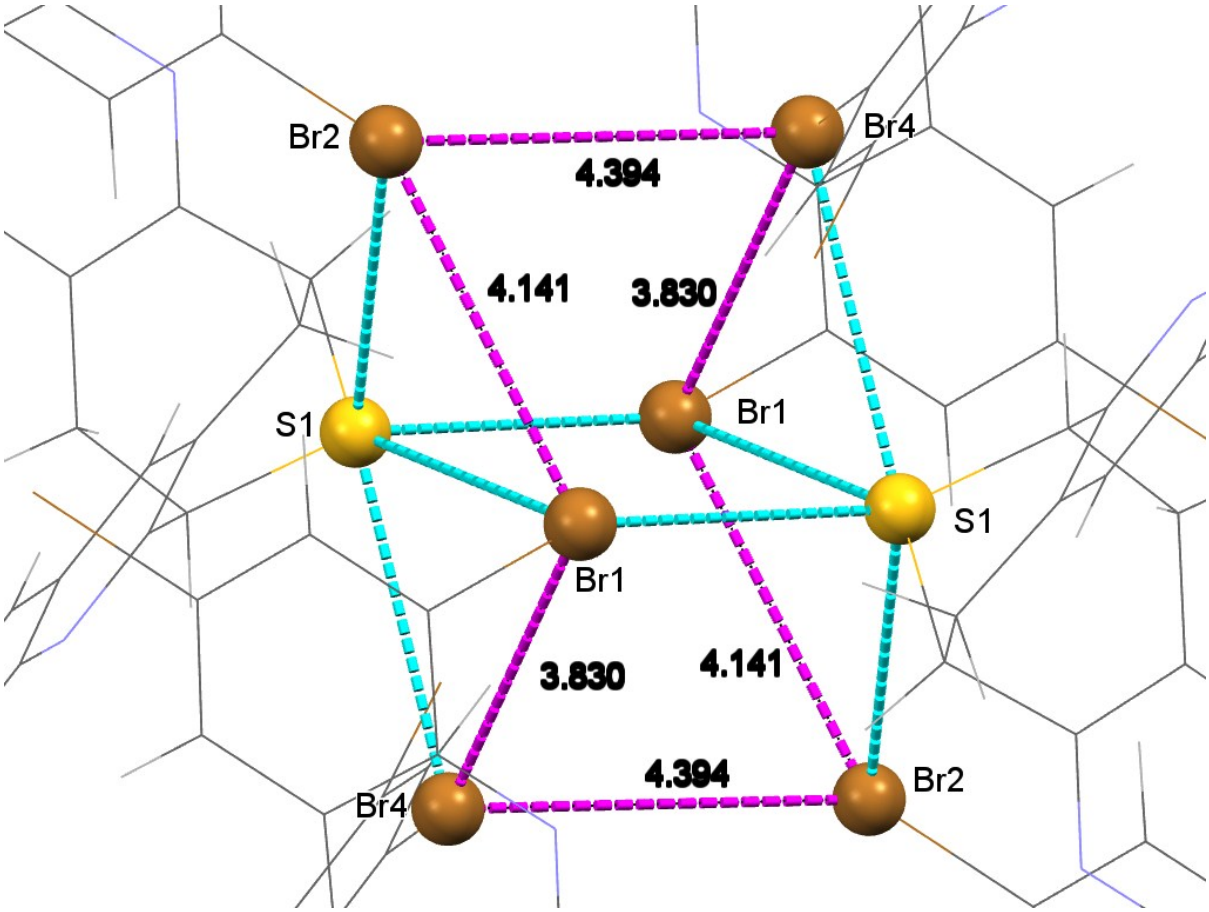

Fig. S7 The net construction of one S_2Br_6 cluster in compound **14** after the Br/Br contacts (magenta) have been added.