Supplementary Material (ESI) for Chemical Communications

An Incommensurate Thiourea Inclusion Compound

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Details of Structure Determination of BIB/Thiourea

Single-crystal XRD data were recorded at 110 K using graphite monochromated MoKα radiation on a Bruker-Nonius Kappa CCD diffractometer with an Oxford Cryosystems cooling apparatus. The data collection was based on a 3-dimensional reciprocal lattice corresponding to the "h" diffraction data. The thiourea host structure was solved from these data by direct methods and refined using SHELX-97 (G.M. Sheldrick, *Acta Crystallogr*. *Sect*. *A*, 2008, **64**, 112). The strategy to introduce guest electron density into the tunnels was the same as reported previously.[3b] Non-hydrogen atoms of thiourea were refined with anisotropic displacement parameters and hydrogen atoms were inserted in idealized positions and a riding model was used (with U_{iso} equal to 1.2 times U_{eq} for the parent atom).

Details of Solid-State ^{13}C NMR Experiments

The solid-state ^{13}C CPMAS NMR spectrum of BIB/thiourea was recorded at 20 °C on a Chemagnetics Infinity Plus spectrometer operating at 75.48 MHz using ramped ^{1}H→^{13}C CP (MAS frequency, 8 kHz; ^{1}H TPPM decoupling, 83 kHz; recycle delay, 3 s; 16384 scans). The dipolar dephasing experiment used the same conditions, but with a dephasing delay of 100 μs.