Supplementary Material for Chemical Communications

A Unique New Multiband Molecular Conductor: $[BDTA][Ni(dmit)_2]_2$

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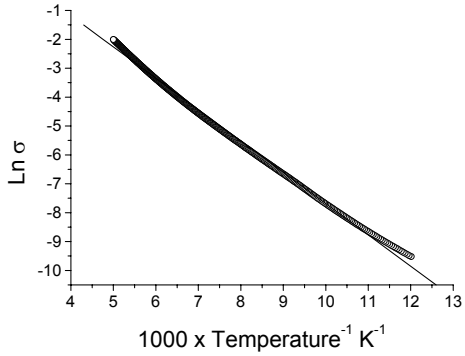
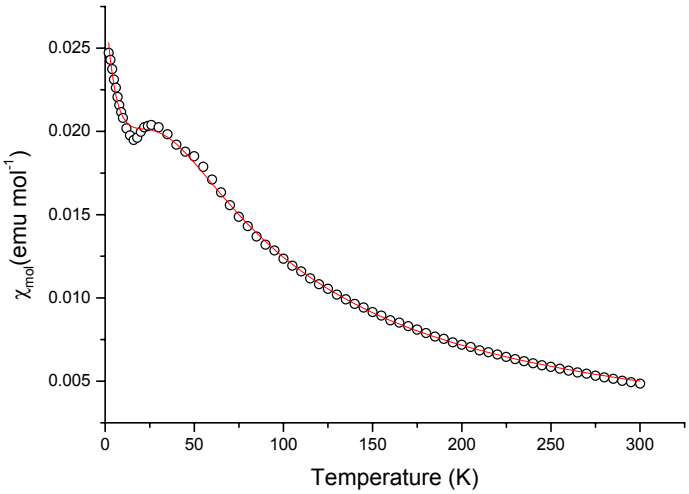
Supplementary Information:
Experimental conductivity and magnetic data. Calculated HOMO and LUMO

Conductivity Data over the temperature range 80 – 200 K measured on a compressed pellet using a four-probe d.c. method.



Magnetic Susceptibility Data and fit to a combination of a Curie model and a 1-D antiferromagnetic Heisenberg spin ½ chain (solid red line).
Magnetic susceptibility measurements were performed on a microcrystalline sample of $[BDTA][Ni(dmit)_2]_2$ from 300K-2K in a field of 0.1 T using a Quantum design $MPMS_2$ SQUID magnetometer with MPMS MultiVu Application software to process the data. The sample was found to have linear field dependence between 0 and 5 T.



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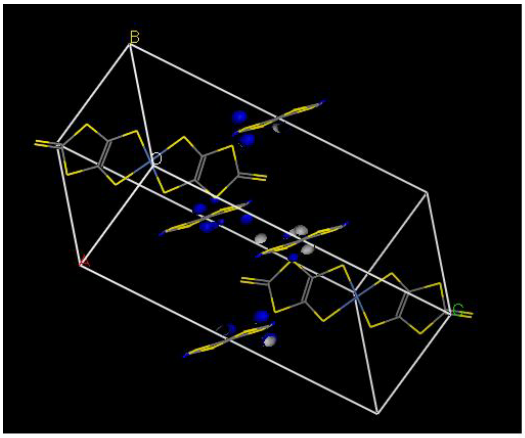
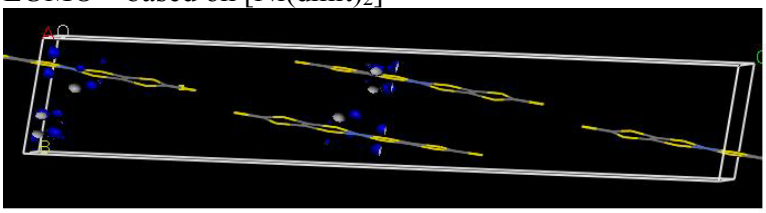
Frontier Orbitals from the DFT plane wave calculation

HOMO – based on BDTA



LUMO – based on $[Ni(dmit)_2]$



Least Squares Plane Functions

$[Ni(dmit)_2]$, (-0.7478, -6.2837, 2.4806)
BDTA, (3.5955, -6.4802, 11.1236)

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