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.
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)