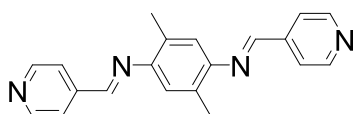
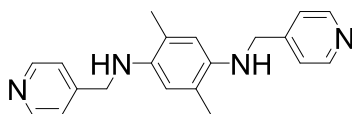


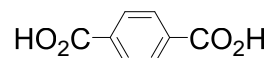
Compound Diagrams and naming scheme



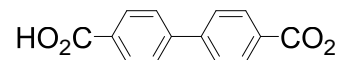
L1_imine



L1



H2bdc



H2bpdc

[Co₂(L1)(bdc)₂].n(DMF) compound 1

Bulk de-solvated compound 1 designated 1a

Different polymorphs and solvates of compound 1 designated (ace - acetone, EtOH = ethanol):

α-1(L); β-1(S); γ-1(L); δ-1(L); ε-1(L); β-1(S)^{ace}; γ-1(L)^{EtOH}; ζ-1(S)^{EtOH}

[Co₂(L1)₂(bdc)₂].H₂O compound 2

[Co₂(L1)₂(bpdc)₂].n(DMF) compound 3

[Co₂(L1)₂(bpdc)₂] compound 3a

[Co₂(L1)₂(bpdc)₂].1.5(EtOH) compound 3

Spectroscopy, CHN and Thermal Analysis (spec.zip)

Nuclear Magnetic Resonance spectra and fid of (¹H and ¹³C) of **L1_imine** and **L1**.

Mass spectra of **L1_imine** and **L1** as pdf

Infrared spectra of **L1_imine**; **L1**, **compounds 1a** and **3a** as pdf

Thermogravimetric Analysis (TGA) of **compounds 1** and **1a** and **3** and **3a** as pdf

CHN microanalysis of **L1_imine**; **L1**, **compounds 1a**, **2**, **3a** as name_CHN.jpg

Single crystal X-ray Structures (sXRD.zip)

All structures:

name.cif (crystallographic information file with embedded calculated and observed structure factors and SHELX instruction file)

name.hkl (data file)

Powder X-Ray Diffraction (pXRD.zip)

For **1a** and **3a**

name_Cu.xls data collected on Bruker Phaser D2 diffractometer using Cu- $K\alpha$ radiation in 2theta vs Intensity format

name_synchrotron.dat data collected at SPring-8 BL02B2 synchrotron Japan at room temperature, $\lambda = 1.000414(2)$ Å as text list of 2theta vs Intensity

Gas and vapour sorption (sorption.zip)

For compounds **1a** (mixed phases) and **3a**

gas = EtOH, N₂, CO₂, CH₄, H₂

Filename key (excel or txt format): compound name_gas_temp