Electronic supplementary information

Directed Synthesis of μ-1,3,5 bridged Dicyanamides by Thermal Decomposition of μ-1,5 bridged Precursors

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- Thermal ellipsoid plot of **1-Co**, **2-Fe** and **2-Co**.

  (Fig. S1-S3)

- DTG, TG, DTA and MS trend scan curves for **1-Fe**, **1-Co** and **1-Ni**.

  (Fig. S4-S6)

- Experimental and calculated XRPD pattern for **1-Mn**, **1-Fe**, **1-Co**, **1-Ni**, **2-Mn**, **2-Fe** and **2-Co**.

  (Fig. S7-S13)

- IR spectroscopic data for **1-Mn**, **1-Fe**, **1-Co**, **1-Ni**, **2-Mn**, **2-Fe** and **2-Co**.

  (Fig. S14-S20)

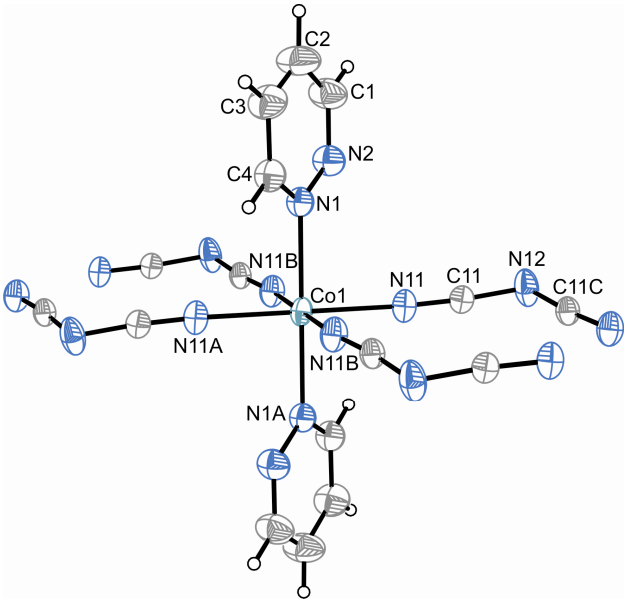

Fig. S1. Thermal ellipsoid plot of the crystal structure of **1-Co** with view of the coordination sphere of the metal cation with labeling and displacement ellipsoids drawn at the 50% probability level. Symmetry codes: A = -x, -y, -z + 1; B = -x, y, -z + 1; C = x, -y + 1, z.

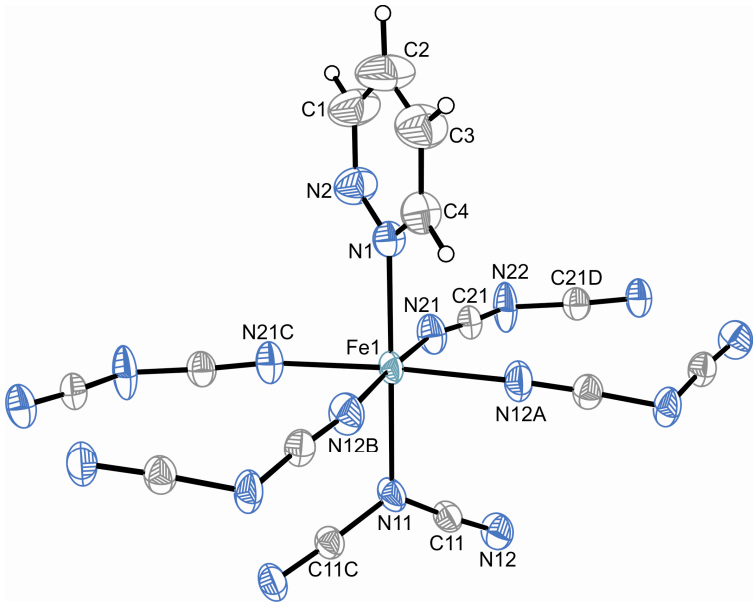

Fig. S2. Thermal ellipsoid plot of the crystal structure of **2-Fe** with view of the coordination sphere of the metal cation with labeling and displacement ellipsoids drawn at the 50% probability level. Symmetry codes: A = -x + 1/2, -y + 1, z + 1/2; B = -x + 1/2, y + 1/2, z + 1/2; C = x, -y + 3/2, z; D = x, -y + 1/2, z.

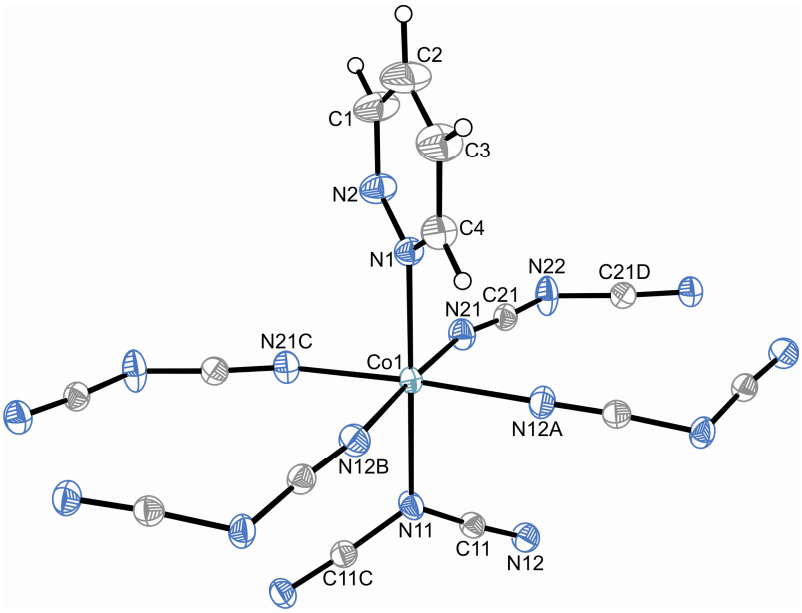

Fig. S3. Thermal ellipsoid plot of the crystal structure of **2-Co** with view of the coordination sphere of the metal cation with labeling and displacement ellipsoids drawn at the 50% probability level. Symmetry codes: A = -x + 1/2, -y + 1, z + 1/2; B = -x + 1/2, y + 1/2, z + 1/2; C = x, -y + 3/2, z; D = x, -y + 1/2, z.

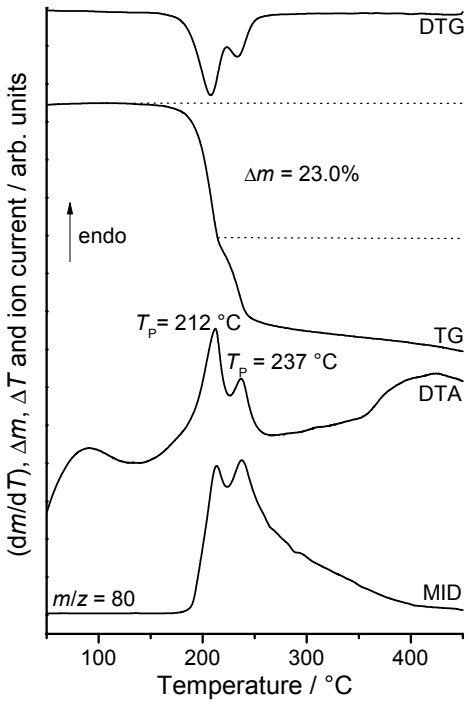

Fig. S4. DTG, TG, DTA and MS trend scan curves for **1-Fe**. Heating rate = 4 °C/min; *m*/*z* = 80 (pydz); given are the mass changes (%) and the peak temperatures T_P (°C).

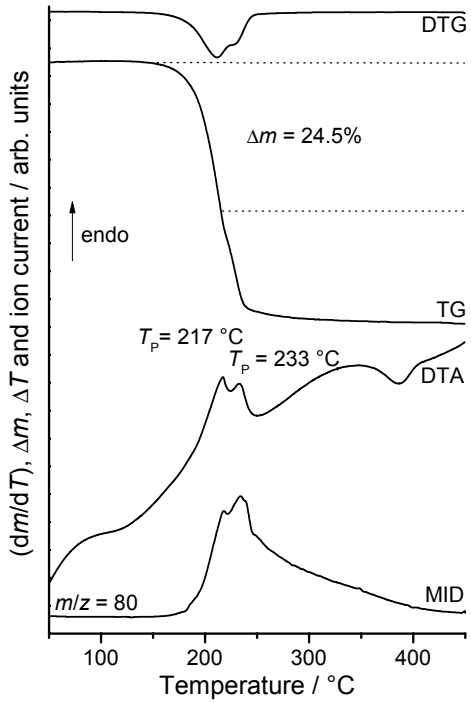

Fig. S5. DTG, TG, DTA and MS trend scan curves for **1-Co**. Heating rate = 4 °C/min; *m*/*z* = 80 (pydz); given are the mass changes (%) and the peak temperatures T_P (°C).

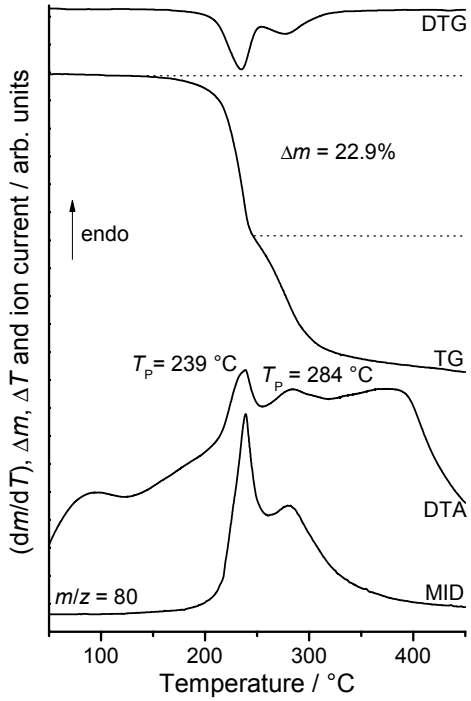

Fig. S6. DTG, TG, DTA and MS trend scan curves for **1-Ni**. Heating rate = 4 °C/min; *m*/*z* = 80 (pydz); given are the mass changes (%) and the peak temperatures T_P (°C).

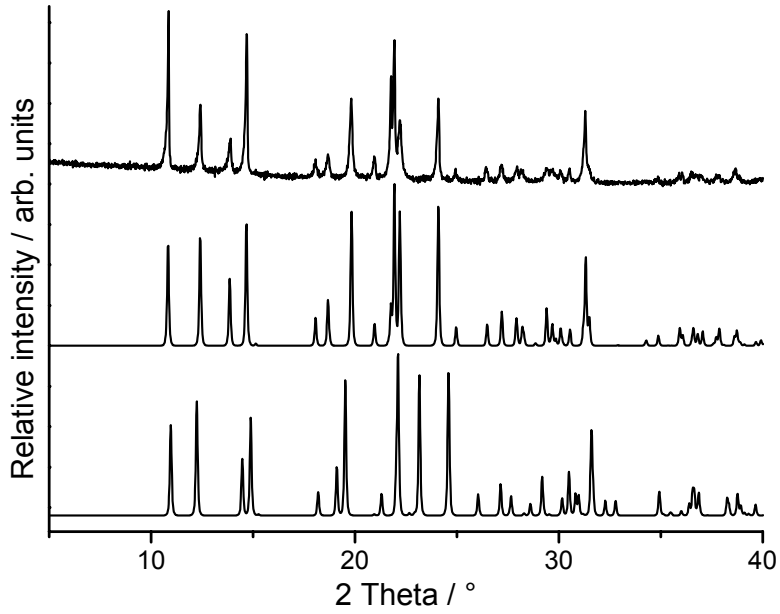

Fig. S7. Experimental XRPD pattern (top) and XRPD pattern calculated at 293 K (middle) and 87 K (bottom) from single crystal data of **1-Mn**.

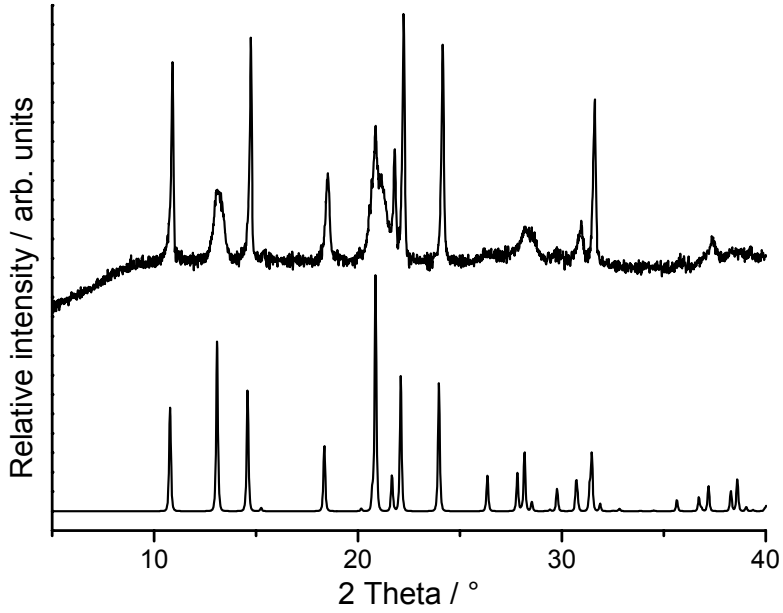

Fig. S8. Experimental XRPD pattern (top) and XRPD pattern calculated from single crystal data (bottom) of **1-Fe**.

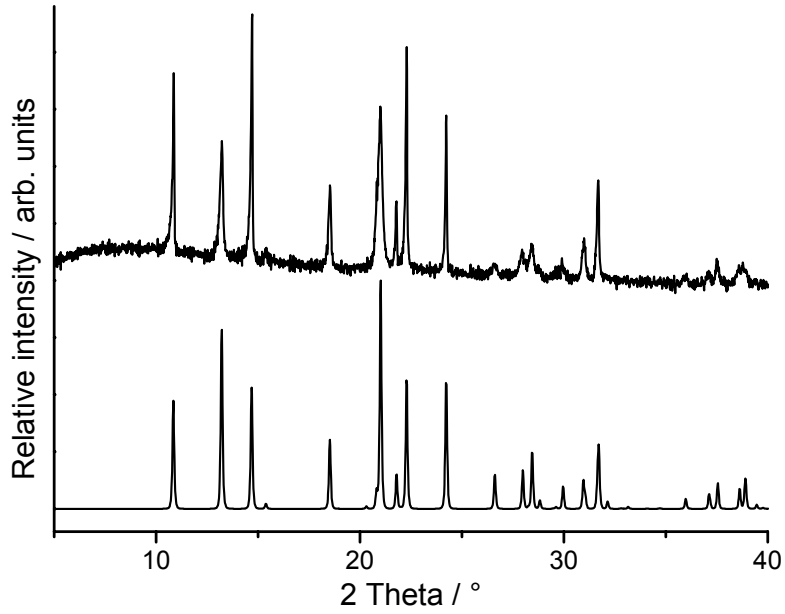

Fig. S9. Experimental XRPD pattern (top) and XRPD pattern calculated from single crystal data (bottom) of **1-Co**.

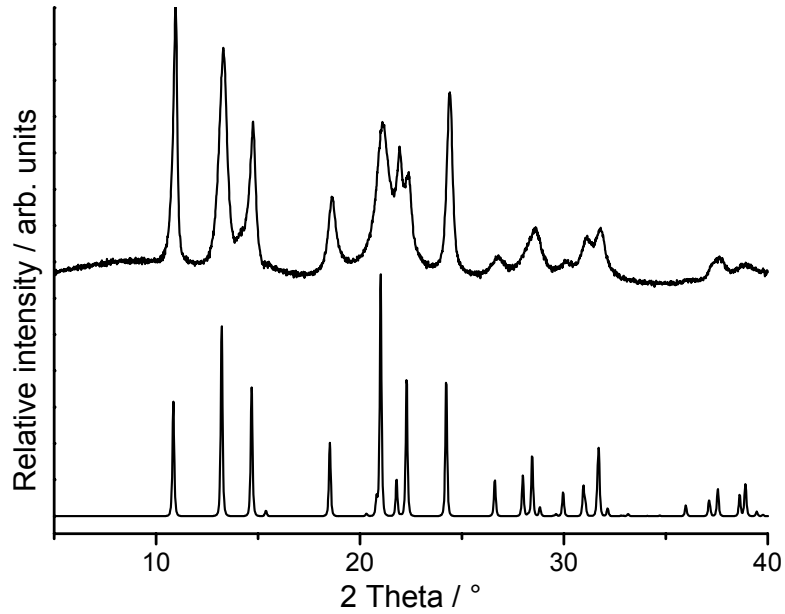

Fig. S10. Experimental XRPD pattern of **1-Ni** (top) and XRPD pattern calculated from single crystal data (bottom) of **1-Fe**.

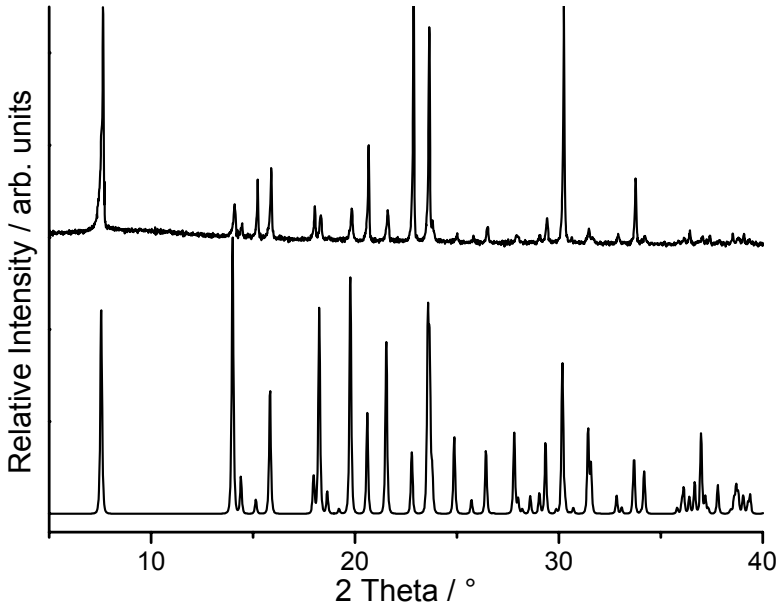

Fig. S11. Experimental XRPD pattern (top) and XRPD pattern calculated from single crystal data (bottom) of **2-Mn**.

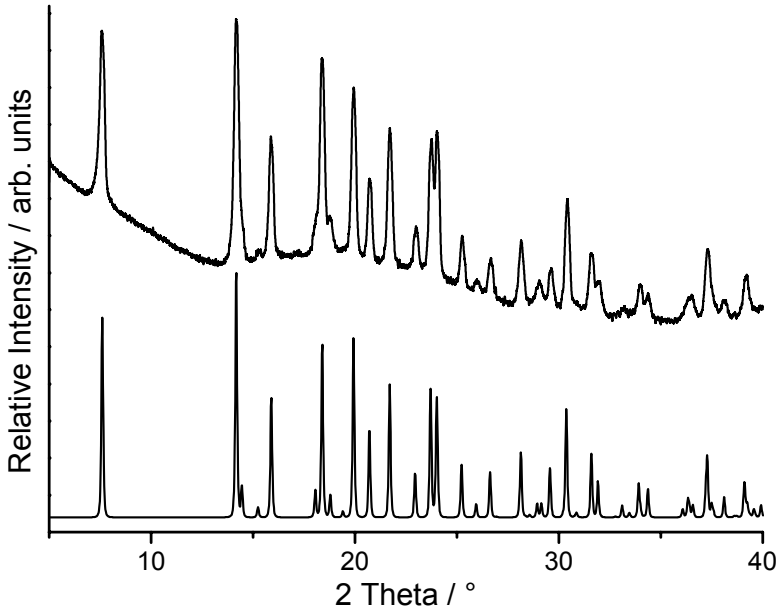

Fig. S12. Experimental XRPD pattern (top) and XRPD pattern calculated from single crystal data (bottom) of **2-Fe**.

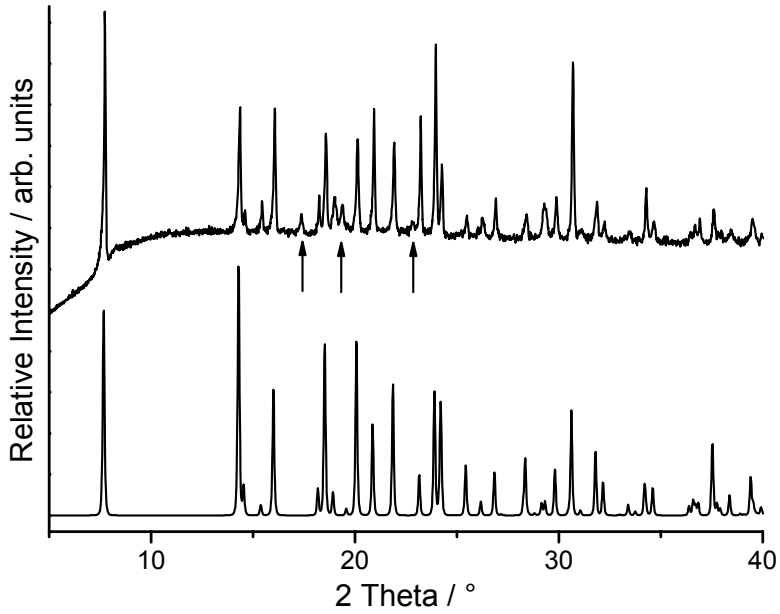

Fig. S13. Experimental XRPD pattern (top) and XRPD pattern calculated from single crystal data (bottom) of **2-Co**. The arrows indicate reflections of $Co(dca)_2$.

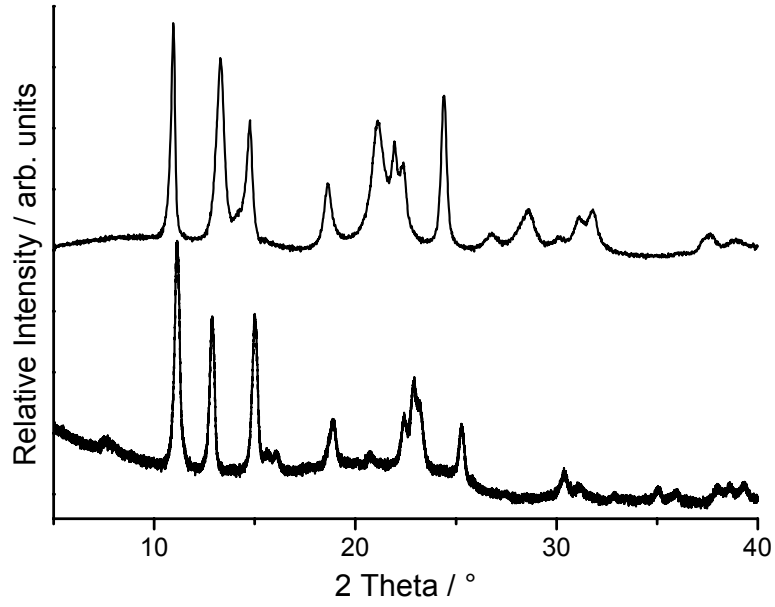

Fig. S14. Experimental XRPD pattern of **1-Ni** (top) and **2-Ni** (bottom).

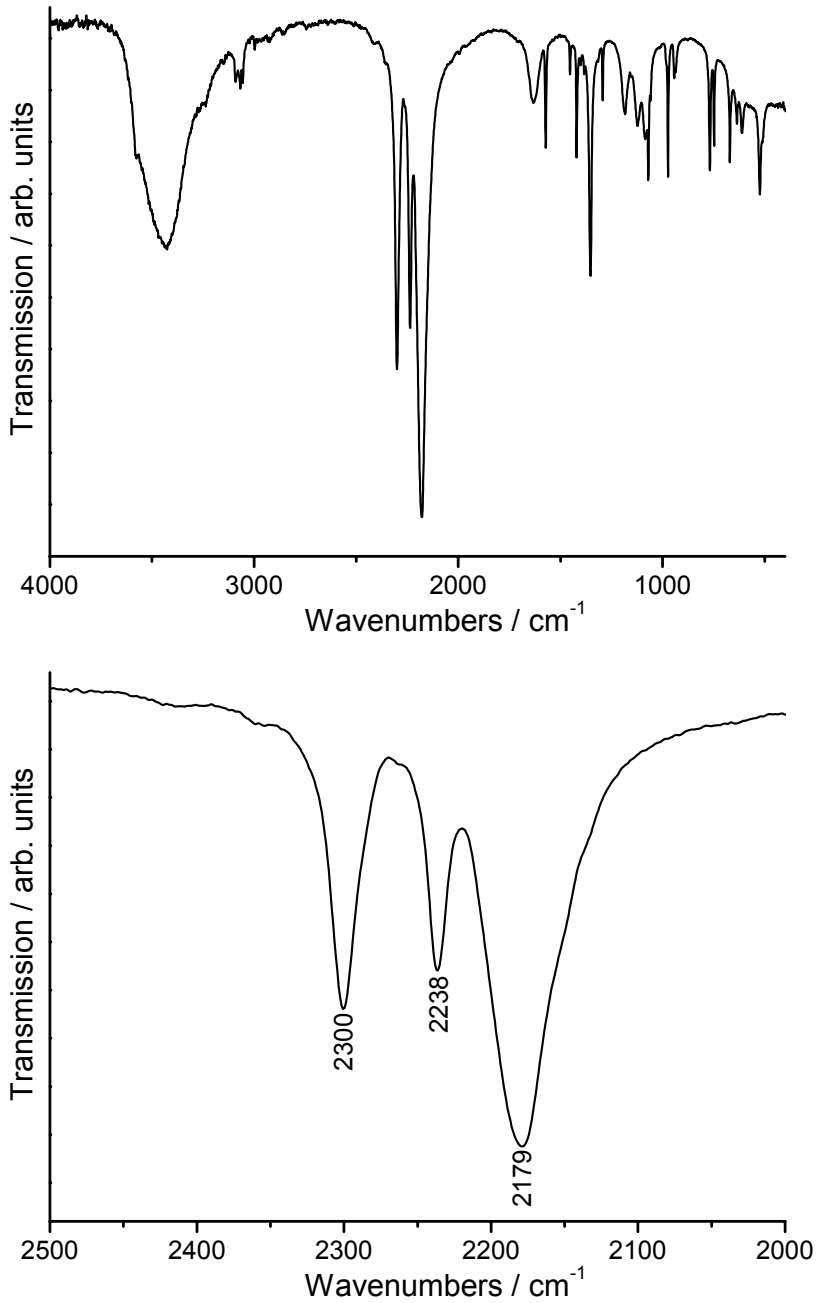

Fig. S15. IR spectroscopic data of **1-Mn** (top) with details of its ν(CN) vibrations bands (bottom).

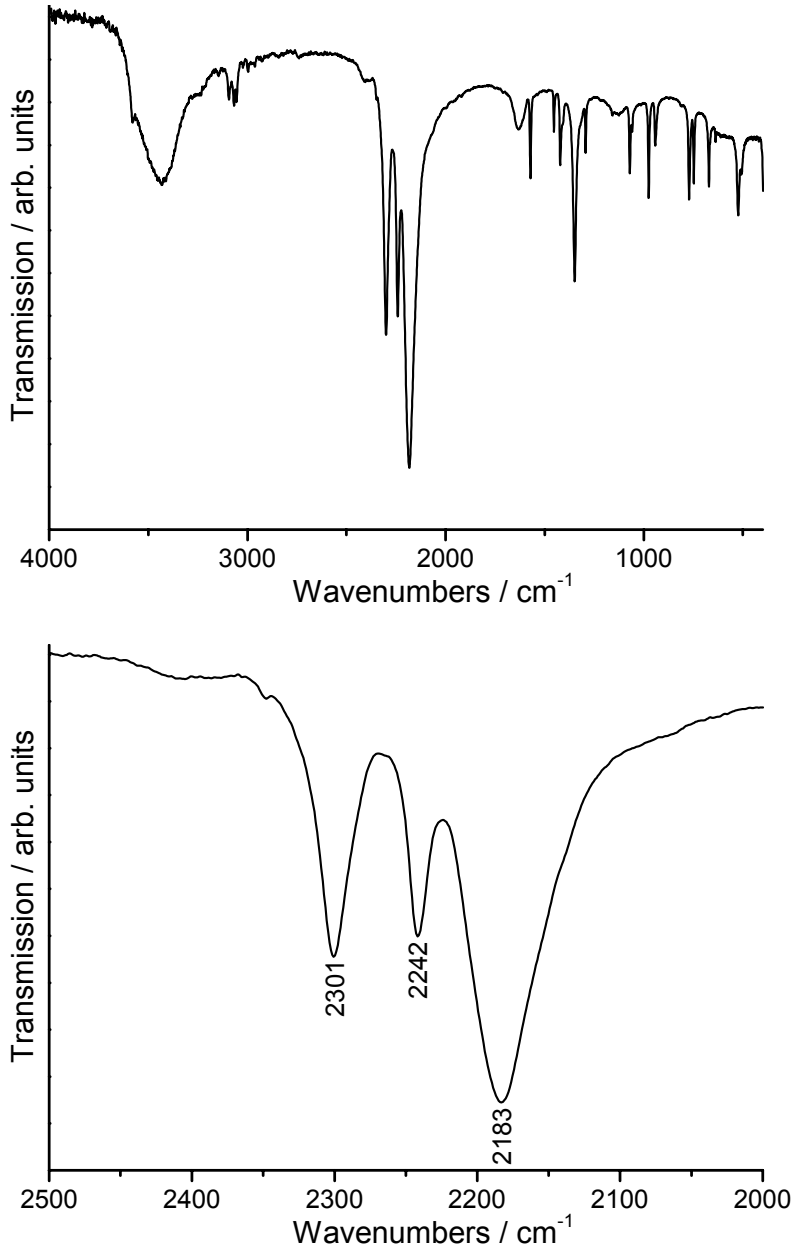

Fig. S16. IR spectroscopic data of **1-Fe** (top) with details of its ν(CN) vibrations bands (bottom).

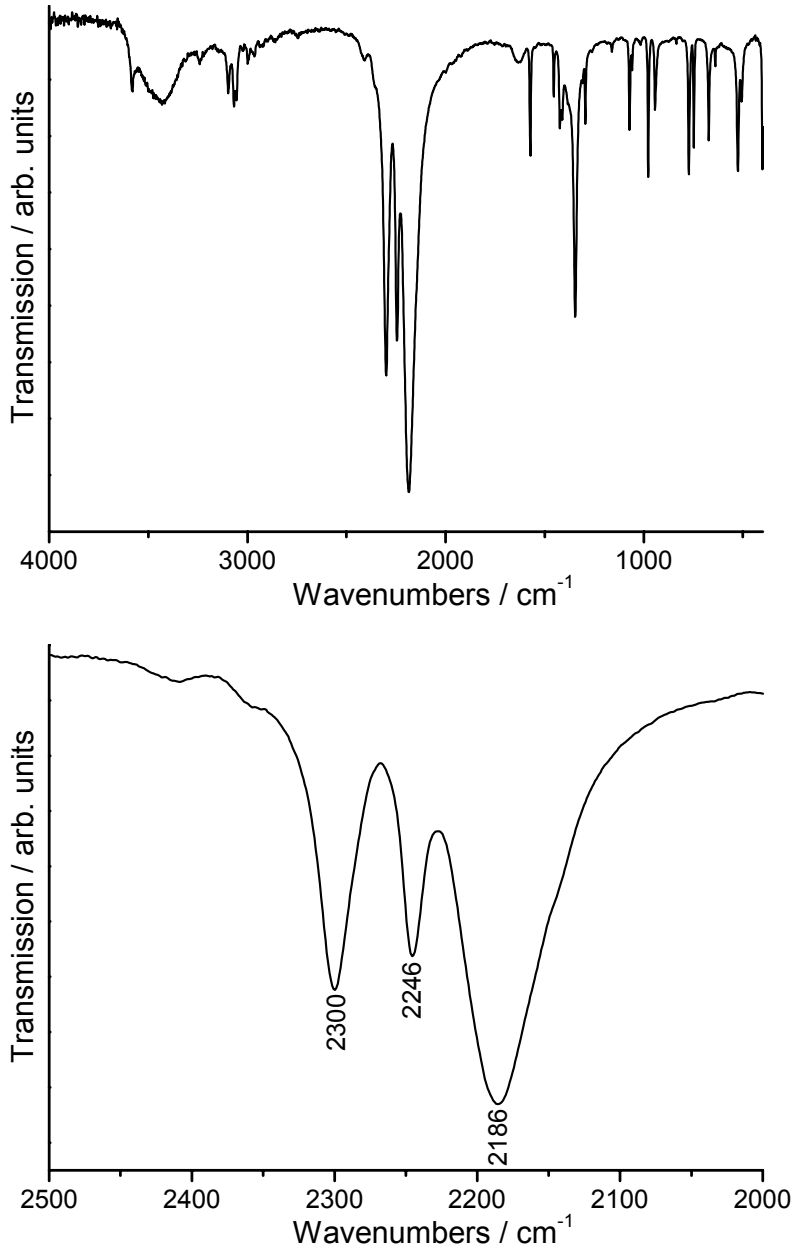

Fig. S17. IR spectroscopic data of **1-Co** (top) with details of its ν(CN) vibrations bands (bottom).

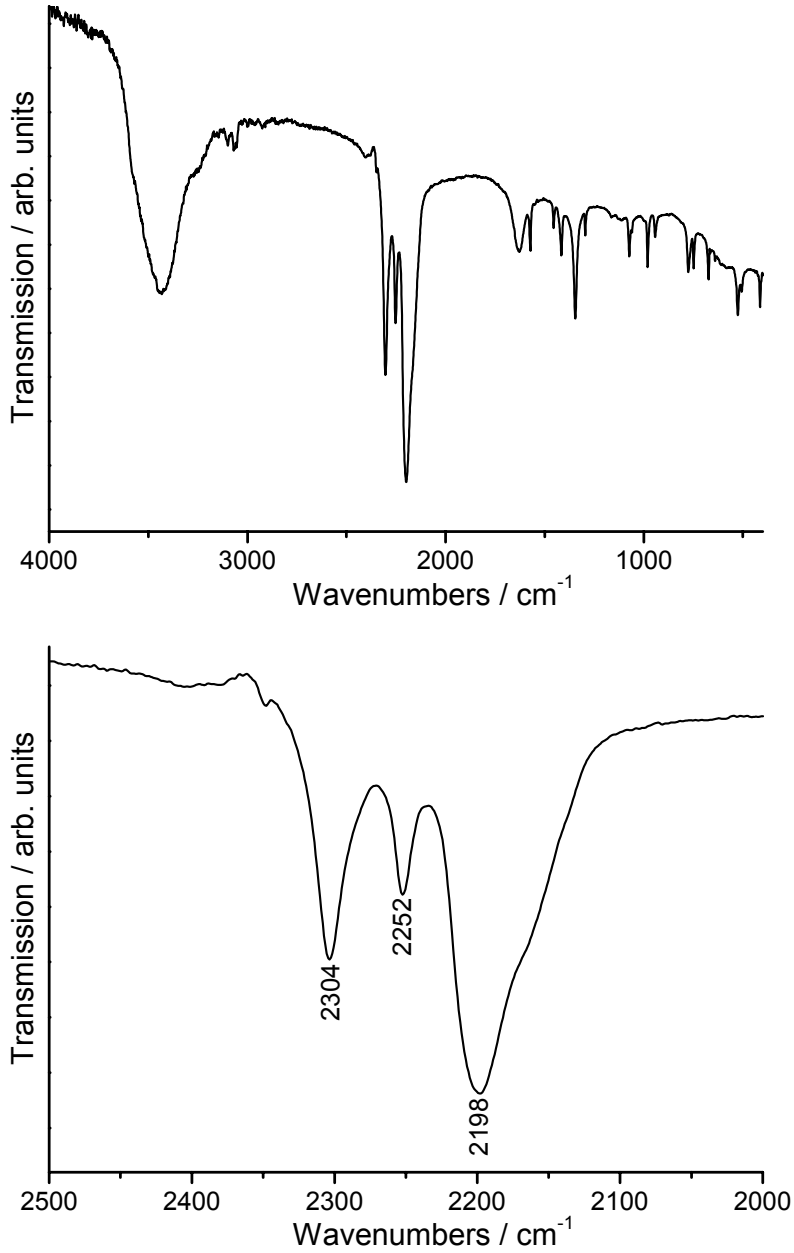

Fig. S18. IR spectroscopic data of **1-Ni** (top) with details of its ν(CN) vibrations bands (bottom).

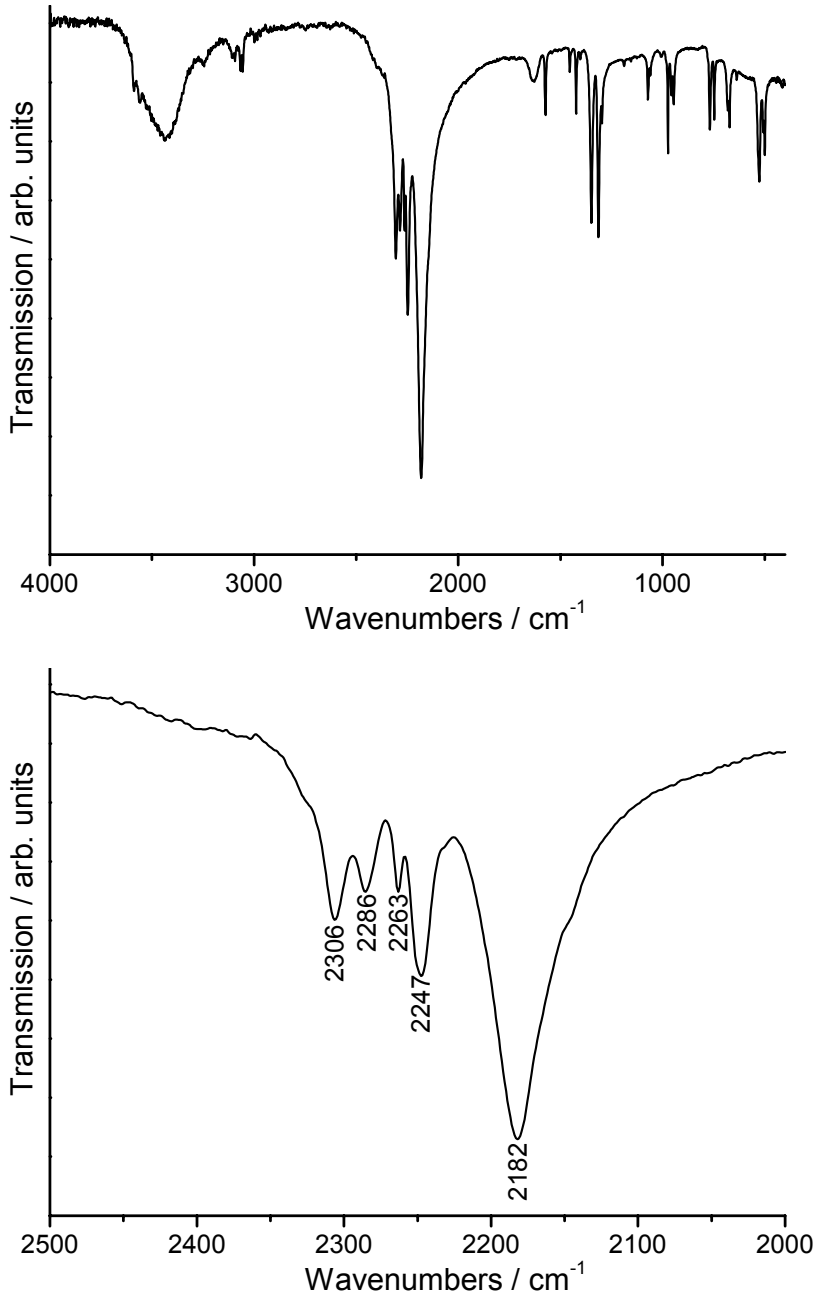

Fig. S19. IR spectroscopic data of **2-Mn** (top) with details of its ν(CN) vibrations bands (bottom).

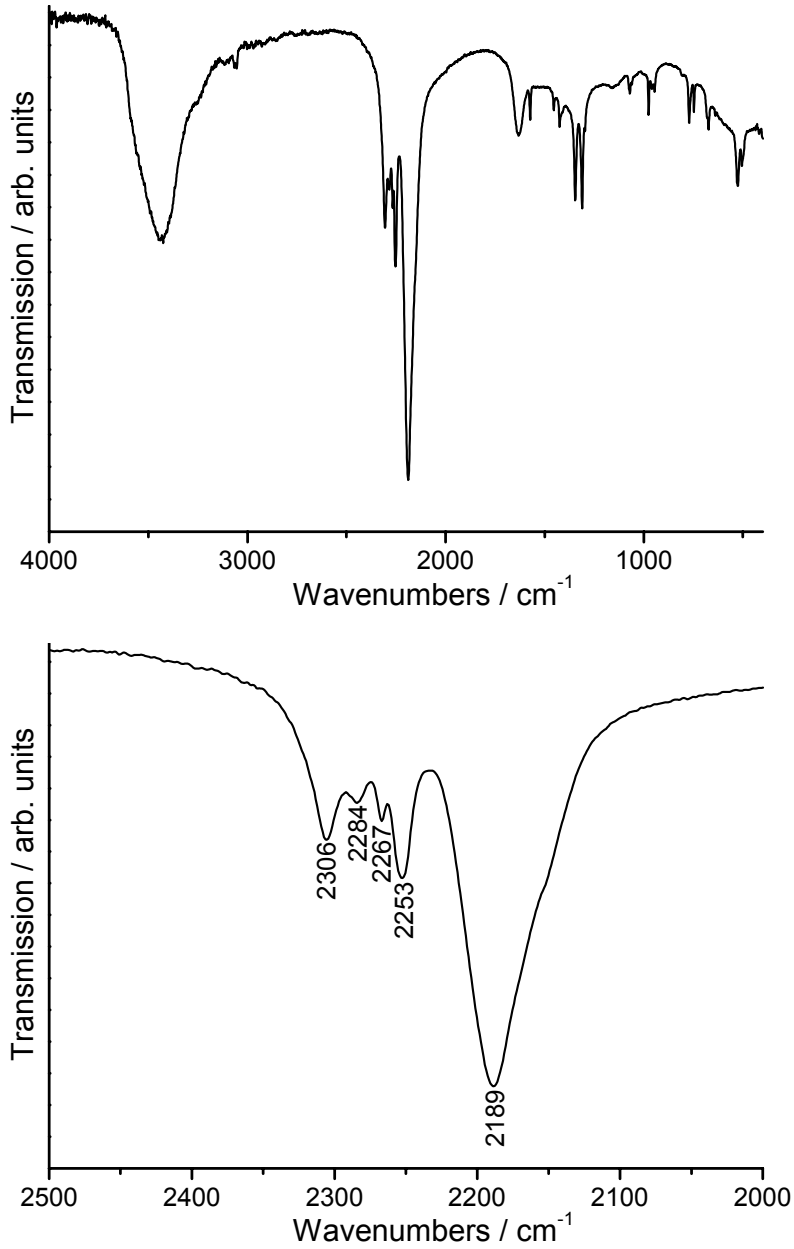

Fig. S20. IR spectroscopic data of **2-Fe** (top) with details of its ν(CN) vibrations bands (bottom).

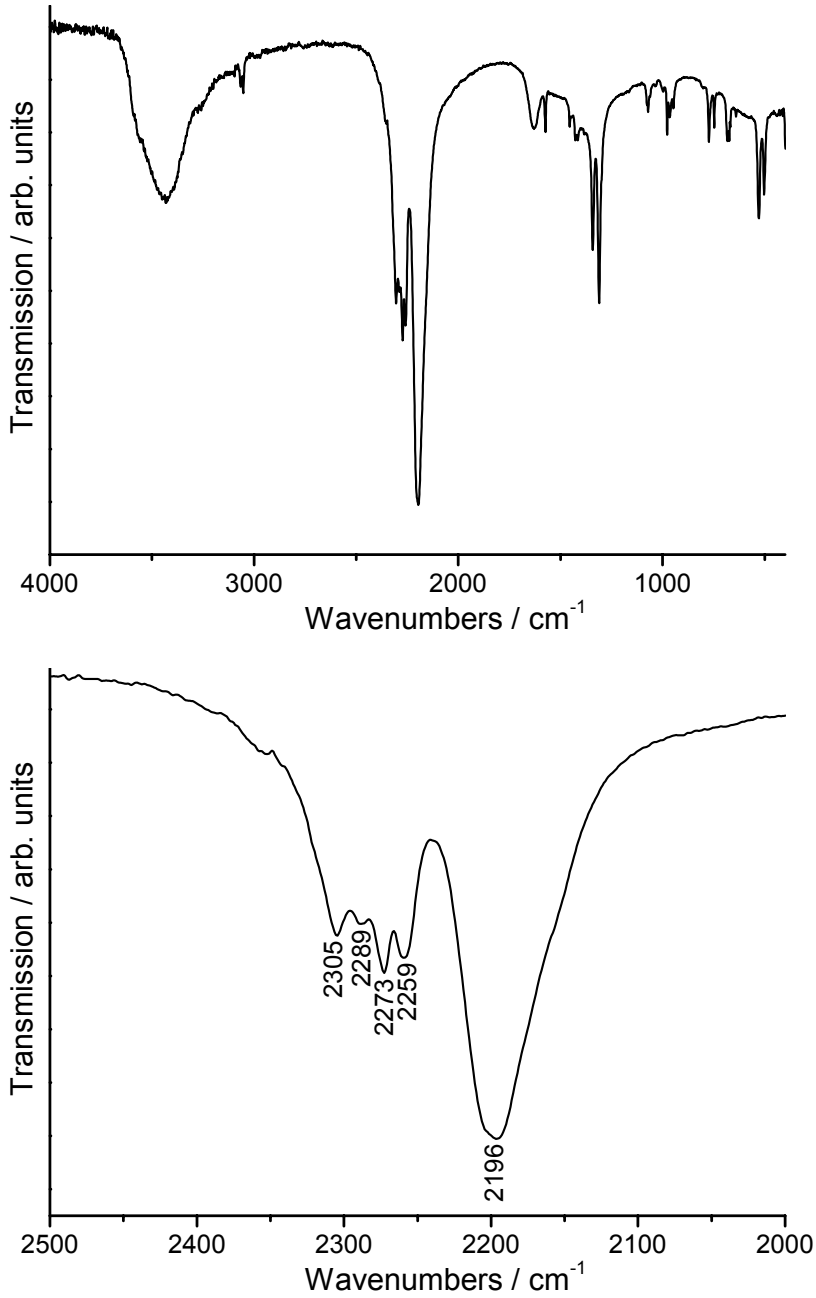

Fig. S21. IR spectroscopic data of **2-Co** (top) with details of its ν(CN) vibrations bands (bottom).