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Electronic Supplementary Information

Synthesis of New Stable and Metastable Thiocyanato Coordination Polymers by Thermal Decomposition and by Solution Reactions.

Susanne Wöhlert, Jan Boeckmann, Inke Jess and Christian Näther

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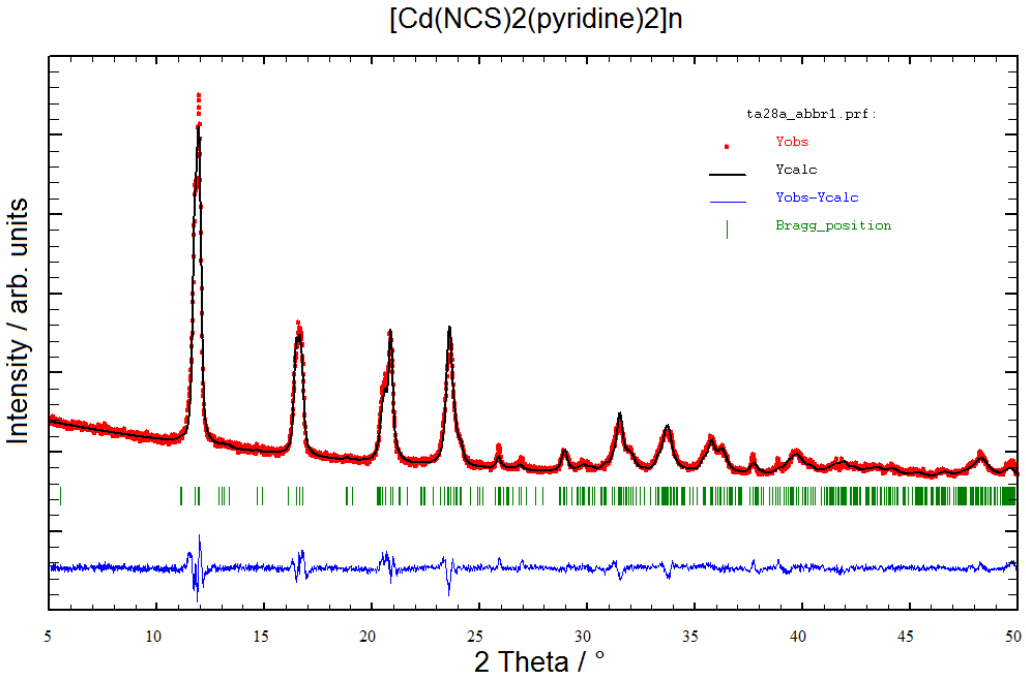

Figure S1. Difference plot of $[Cd(NCS)_2(pyridine)_2]_n$ (**2-Cd/III**).

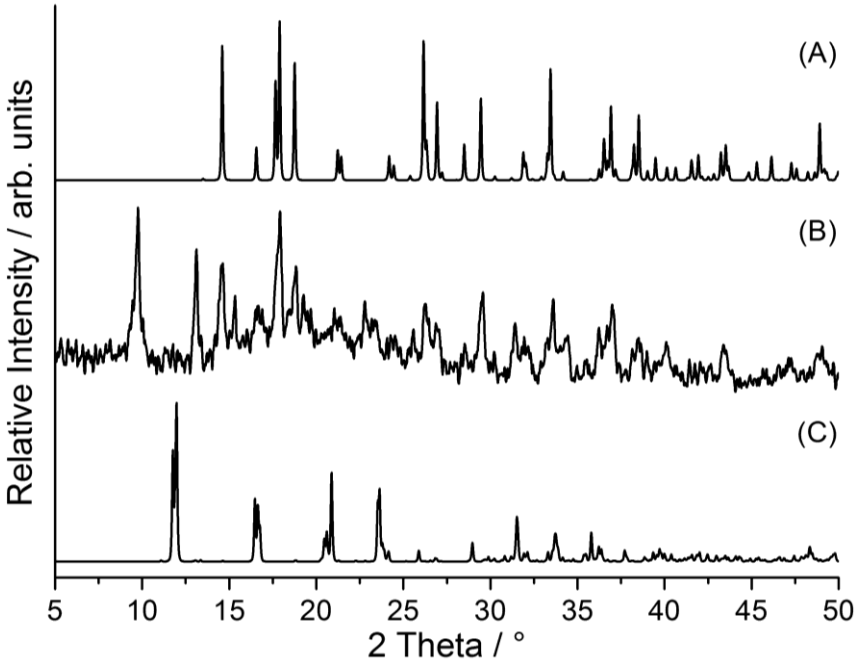

Figure S2. Calculated X-ray powder pattern (XRPD) of $Cd(NCS)_2$ (A) and experimental X-ray powder pattern of the residue formed in the second TG step in the thermal decomposition reaction of **1-Cd** (B) as well as of **2-Cd/III** calculated from Rietveld refinement (C).

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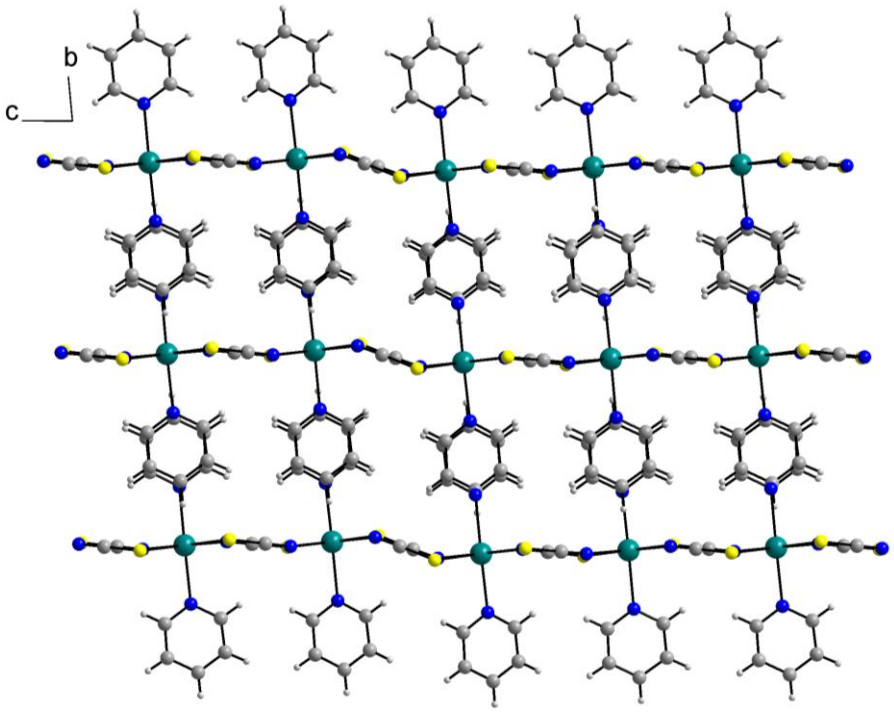

Figure S3. Crystal structure of **2-Cd/II** with view along the crystallographic *a*-axis (green = cadmium, blue = nitrogen, yellow = sulfur, grey = carbon, white = hydrogen).

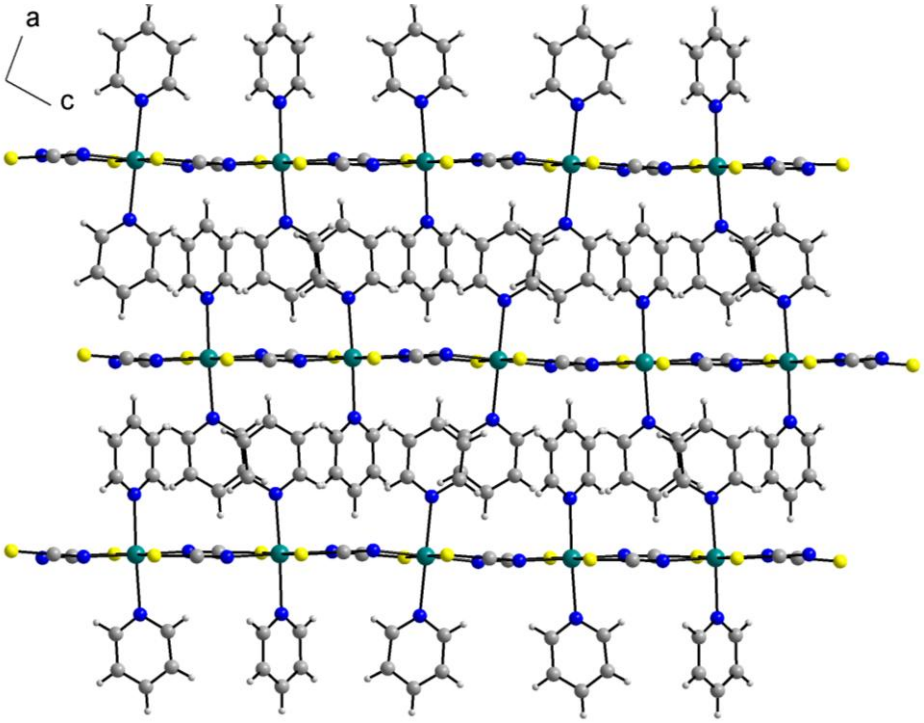

Figure S4. Crystal structure of **2-Cd/III** with view along the crystallographic *b*-axis (green = cadmium, blue = nitrogen, yellow = sulfur, grey = carbon, white = hydrogen).

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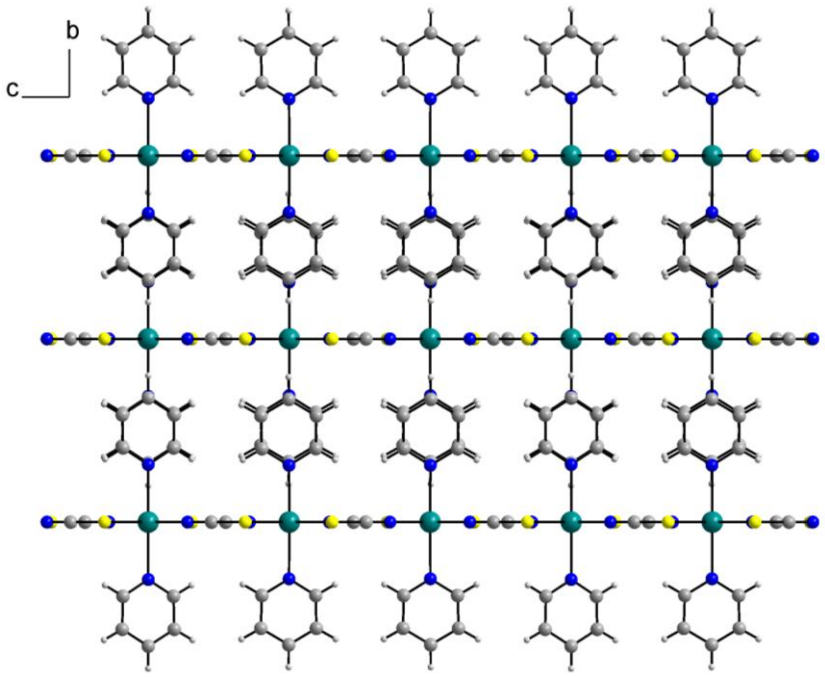

Figure S5. Crystal structure of **2-Cd/IV** with view along the crystallographic *a*-axis (green = cadmium, blue = nitrogen, yellow = sulfur, grey = carbon, white = hydrogen).

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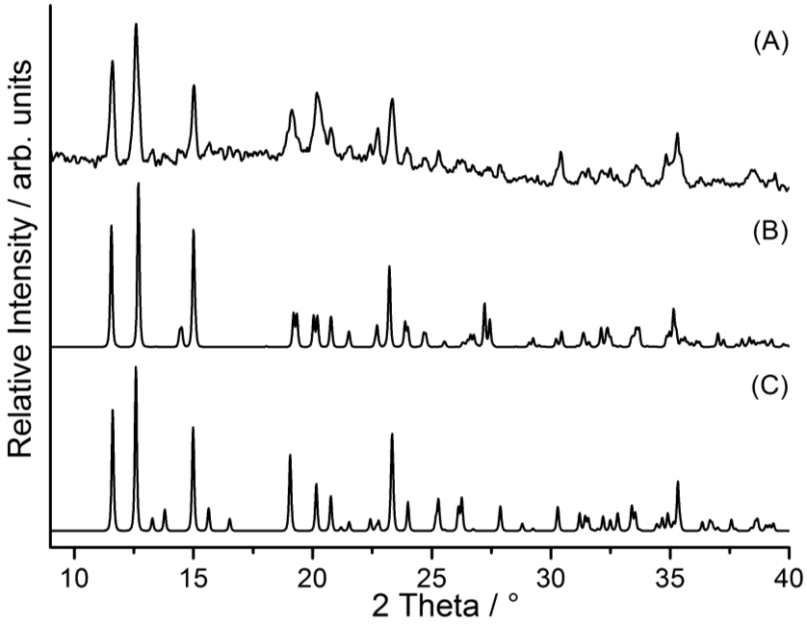

Figure S6. Experimental X-ray powder pattern (XRPD) of a mixture of single crystals of **2-Cd/II** and **2-Cd/IV** (A) and X-ray powder pattern of **2-Cd/II** (B) as well as **2-Cd/IV** (C) calculated from single-crystal data.

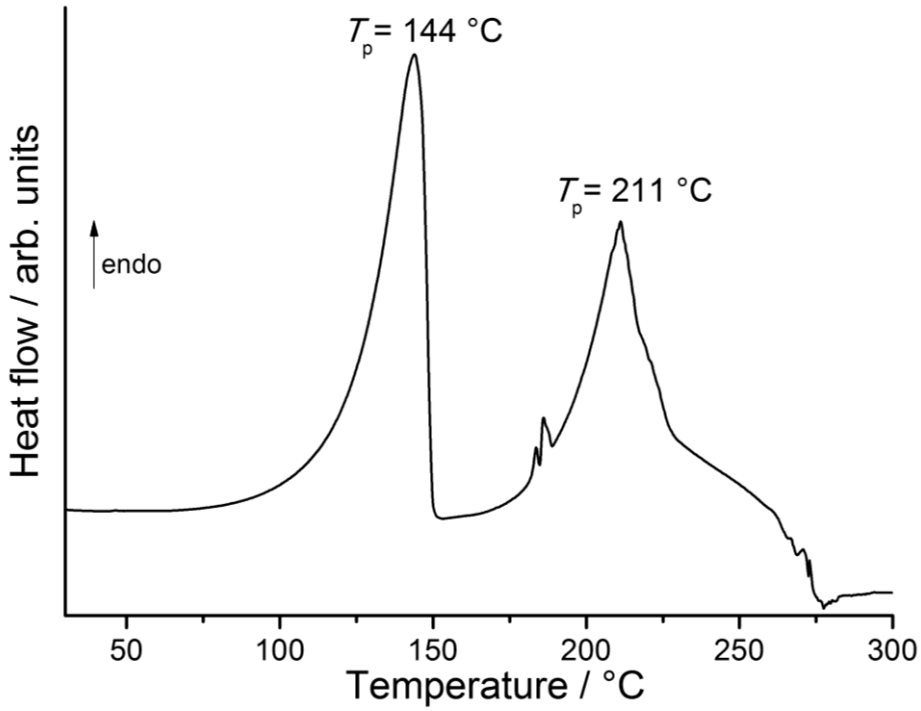

Figure S7. DSC curve for $[Cd(NCS)_2(pyridine)_4]$ (**1-Cd**).

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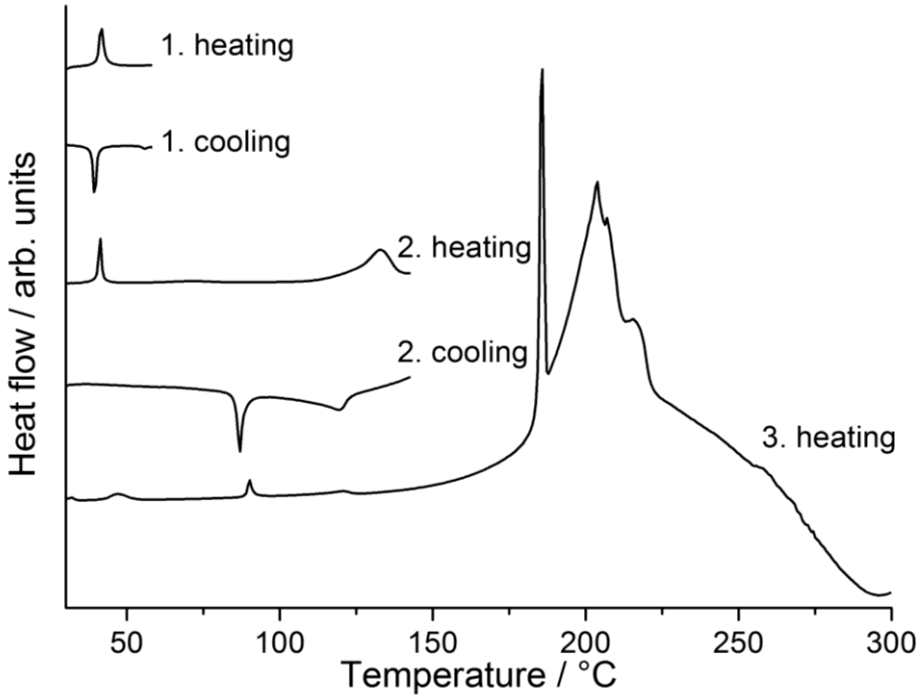

Figure S8. DSC heating and cooling cycles for $[Cd(NCS)_2(pyridine)_2]_n$ (**2-Cd/II**).

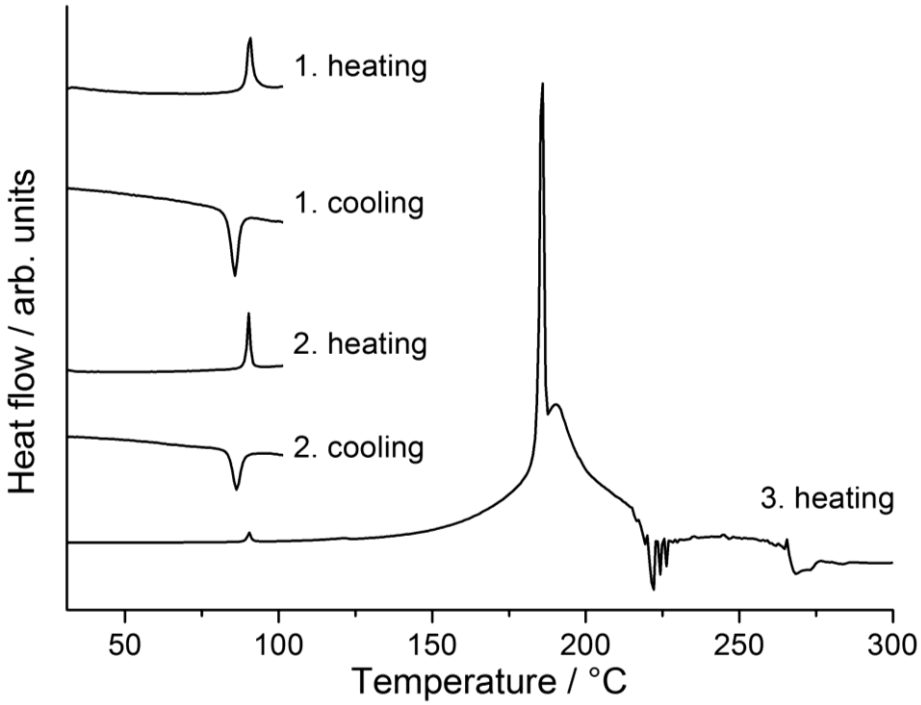

Figure S9. DSC heating and cooling cycles for $[Cd(NCS)_2(pyridine)_2]_n$ (**2-Cd/III**).

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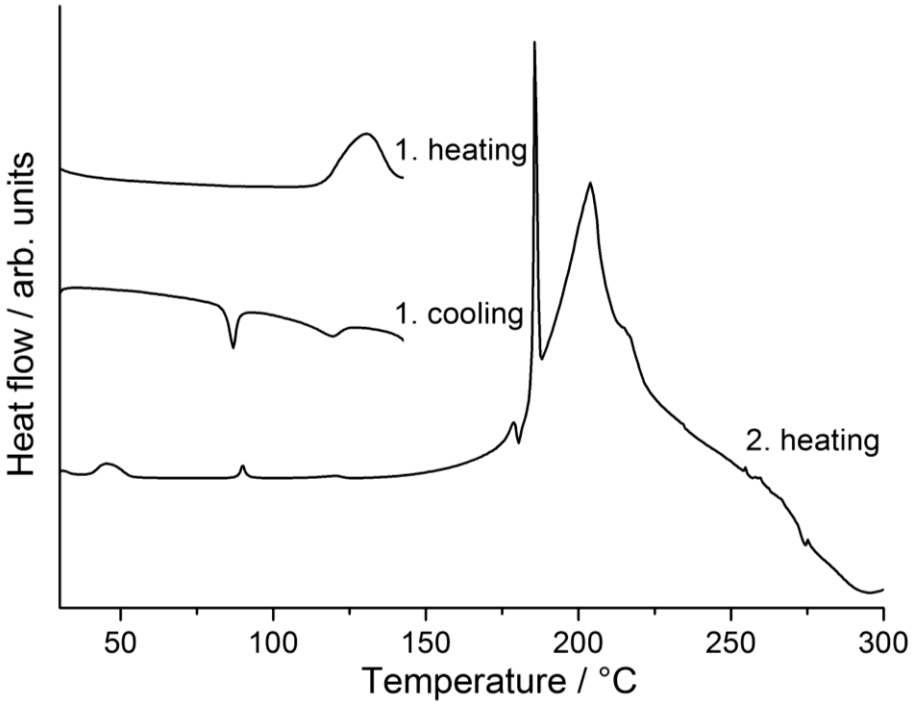

Figure S10. DSC heating and cooling cycles for $[Cd(NCS)_2(pyridine)_2]_n$ (**2-Cd/IV**).

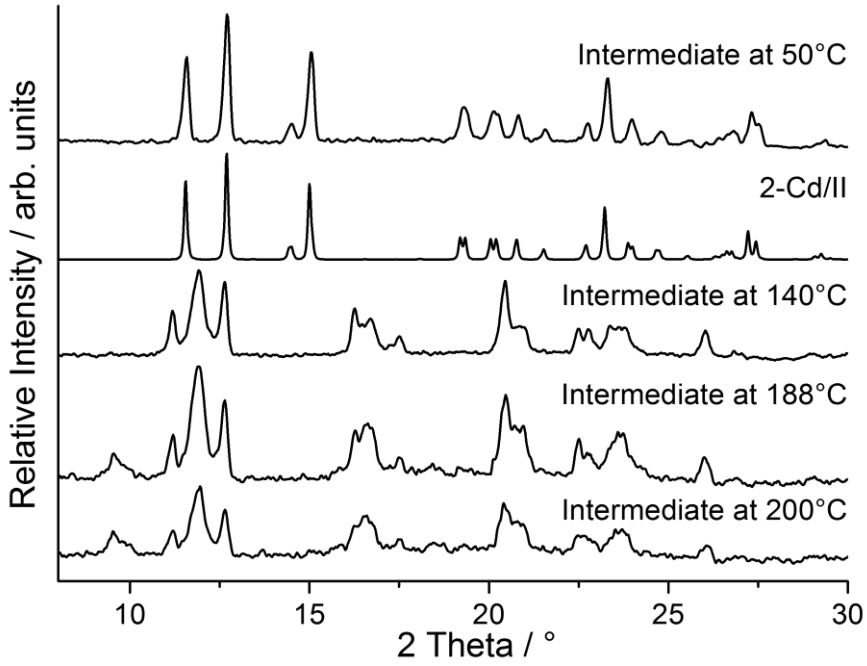

Figure S11. X-ray powder pattern of the intermediates obtained at different temperatures in the DSC measurement of compound **2-Cd/II** and X-ray powder pattern of $[Cd(NCS)_2(pyridine)_2]_n$ (**2-Cd/II**) calculated from single-crystal data.

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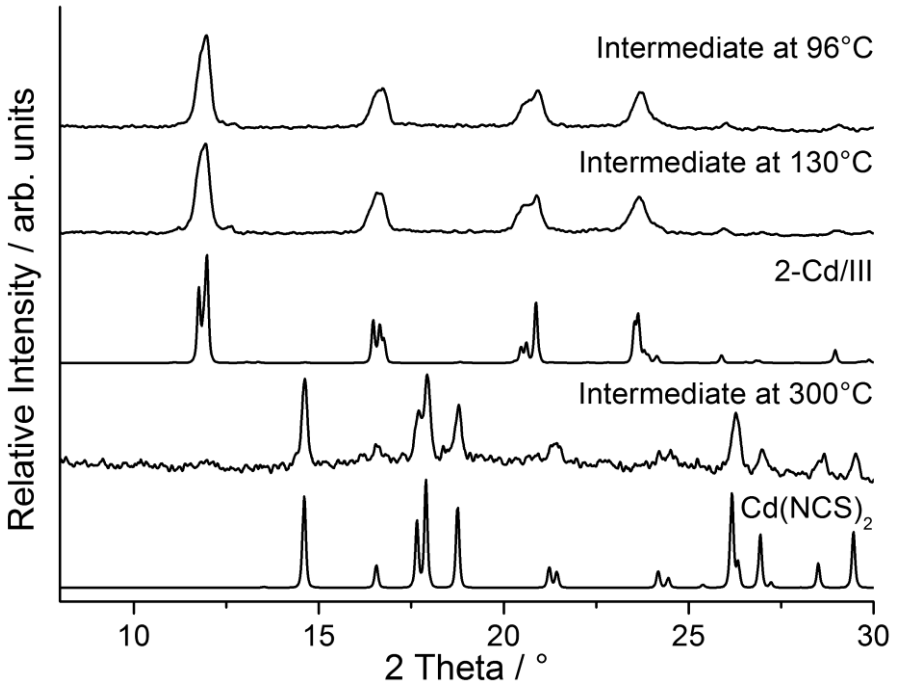

Figure S12. X-ray powder pattern of the intermediates obtained at different temperatures in the DSC measurements of compound **2-Cd/III** and X-ray powder pattern of $[Cd(NCS)_2(pyridine)_2]_n$ (**2-Cd/III**) calculated from Rietveld refinement and of $Cd(NCS)_2$ calculated from single-crystal data.

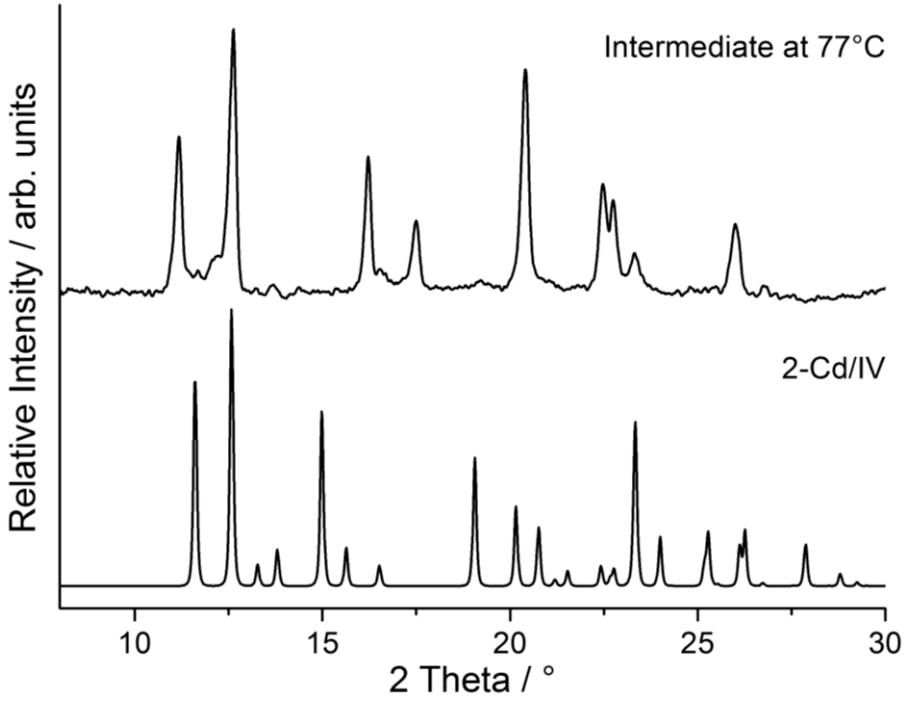

Figure S13. X-ray powder pattern of the intermediate obtained at 77°C from the DSC measurement of compound **2-Cd/IV** (top) as well as the X-ray powder pattern calculated for $[Cd(NCS)_2(pyridine)_2]_n$ (**2-Cd/IV**) from single-crystal data.

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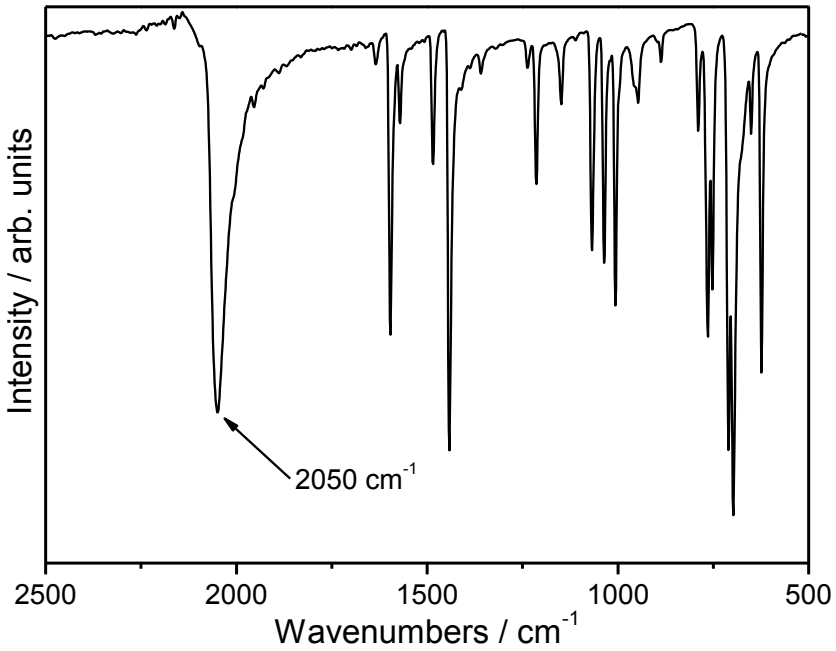

Figure S14. IR spectrum of [Cd(NCS)$_2$(pyridine)$_4$] (**1-Cd**).

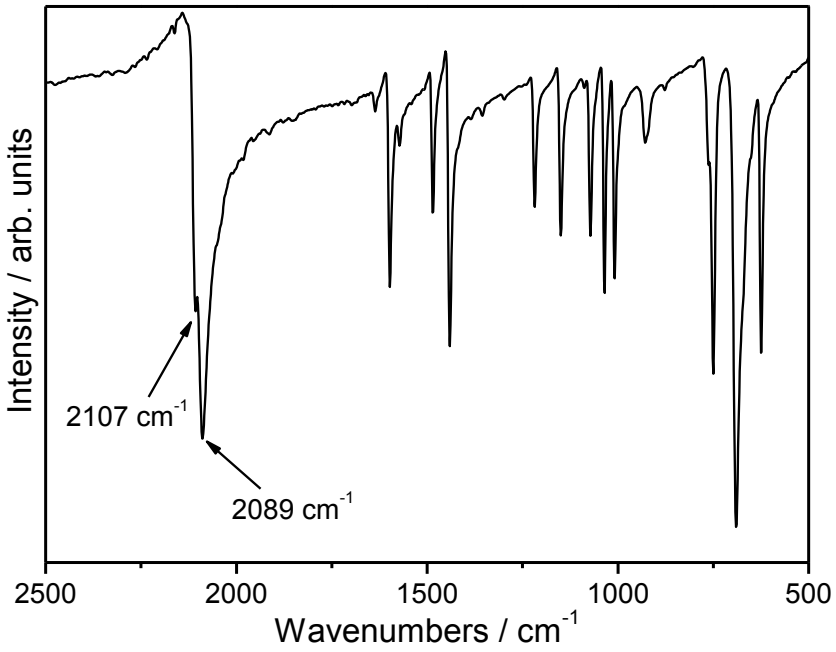

Figure S15. IR spectrum of the ligand-deficient 1:2 compound [Cd(NCS)$_2$(pyridine)$_2$]$_n$ (**2-Cd/II**).

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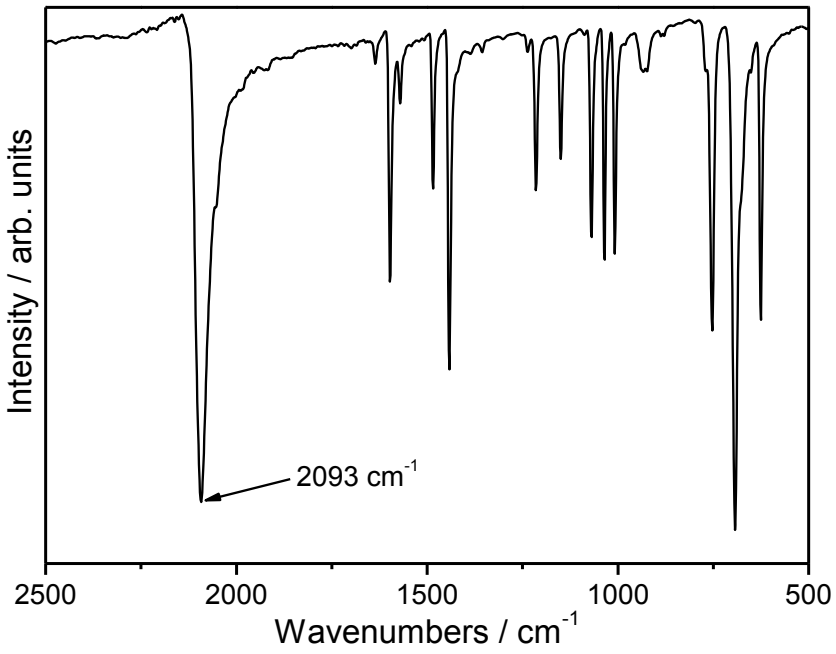

Figure S16. IR spectrum of $[Cd(NCS)_2(pyridine)_2]_n$ (**2-Cd/III**).

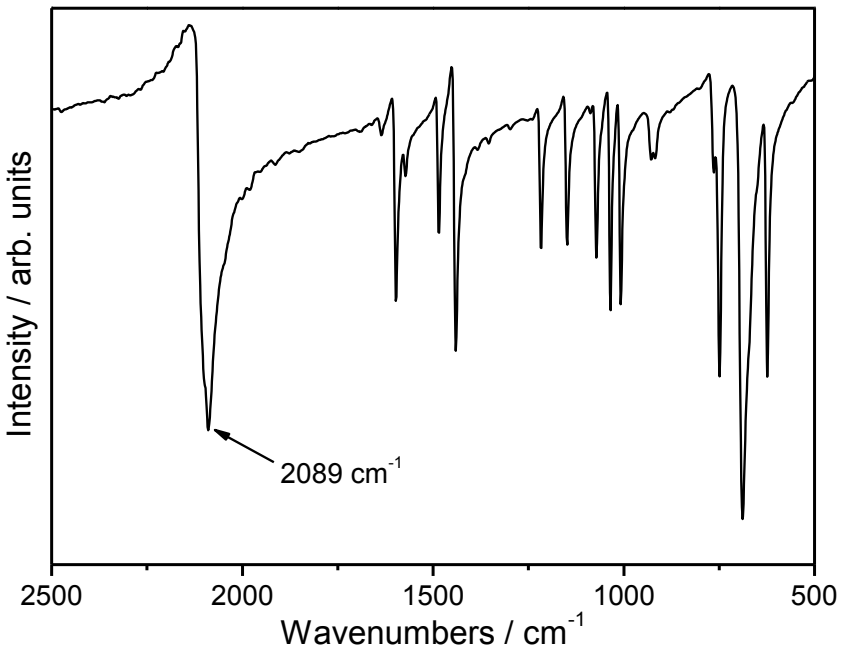

Figure S17. IR spectrum of $[Cd(NCS)_2(pyridine)_2]_n$ (**2-Cd/IV**).

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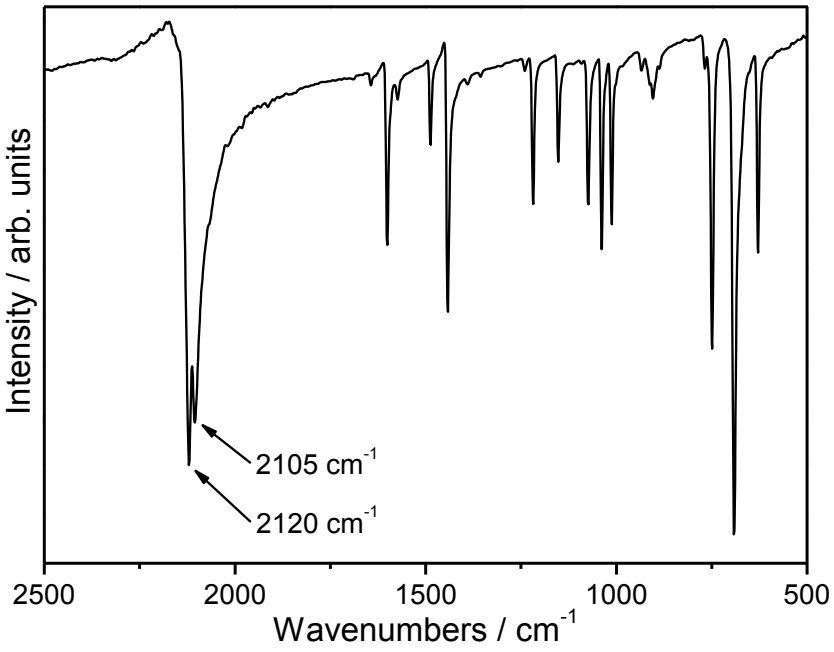

Figure S18. IR spectrum of $[Cd(NCS)_2(pyridine)]_n$ (**3-Cd**).