

Water free neodymium 2,6-naphthalenedicarboxylates coordination complexes and their application as catalysts for isoprene polymerization.

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SUPPLEMENTARY INFORMATION

To be submitted to Inorg. Chem.
Revised version november 22, 2011

Infrared analysis was carried out on a Perkin Elmer Spectrum 2 equipped with a single reflection diamond module (ATR). IR spectrum was recorded in the 400-4000 cm^{-1} range, at 4 cm^{-1} resolution.

Compound 1

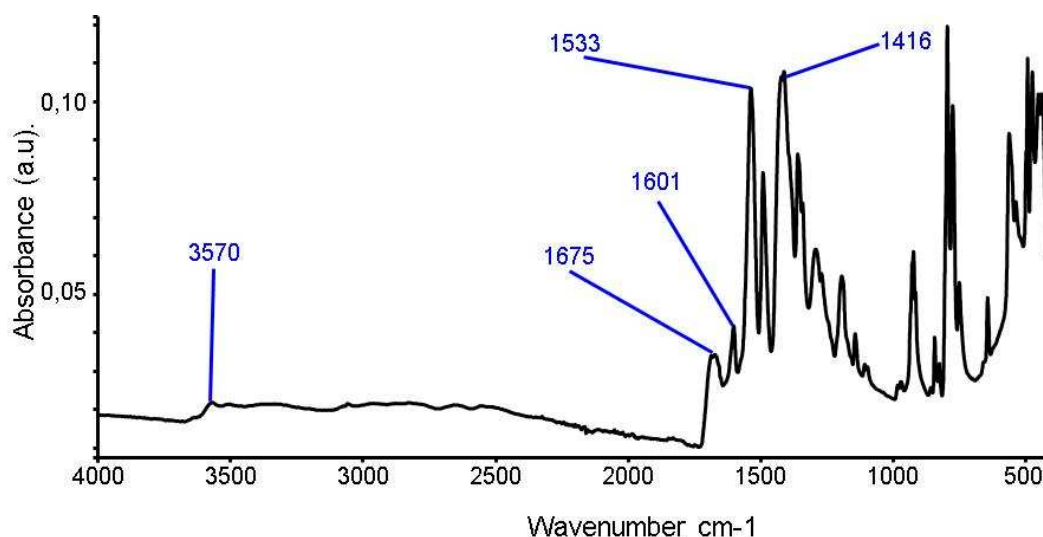


Figure S1a: Infrared spectrum of $\text{Nd}_2(2,6\text{-ndc})_3(\text{H}_2\text{O})_3 \cdot \text{H}_2\text{O}$ (**1**)

Infrared spectrum of $\text{Nd}_2(2,6\text{-ndc})_3(\text{H}_2\text{O})_3$ (**1**) shows a very broad band of absorption in the 3500 – 2500 cm^{-1} range, indicating the presence of hydrogen bonds between the coordinating water and the free water molecules. For the coordinated species, the asymmetric stretching ($\nu_{\text{O-H asym}}$) has been assigned at 3570 cm^{-1} , the $\nu_{\text{O-H sym}}$ occurs in the range of 3500 – 3000 cm^{-1} as a low intensity broad band and the peak at 1601 cm^{-1} has been assigned to the $\delta_{\text{H-O-H}}$ bending. The $\nu_{\text{COO asym}}$ stretching vibrations of carboxylate arms linked to Neodymium were observed at 1533 cm^{-1} . The intense peak appearing at 1416 cm^{-1} has been assigned to the C=C ring vibration of the 2,6-ndc ligand. The peak localized at 1675 cm^{-1} should correspond to DMF ($\nu_{\text{C=O}}$) remaining after the washing procedure.

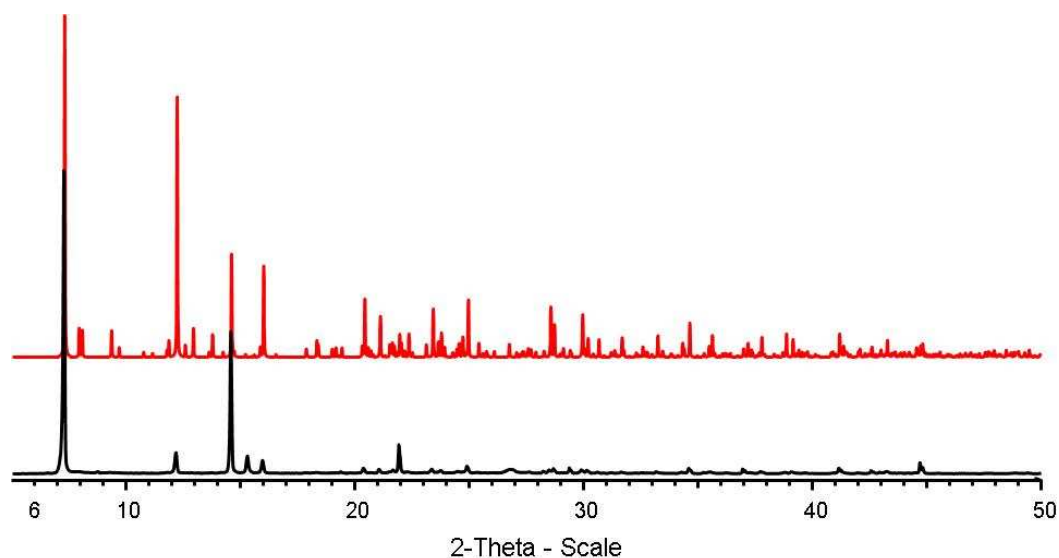


Figure S1b: Calculated (top) and experimental (bottom) X-ray diffraction powder patterns of $\text{Nd}_2(2,6\text{-ndc})_3(\text{H}_2\text{O})_3 \cdot \text{H}_2\text{O}$ (**1**; copper radiation).

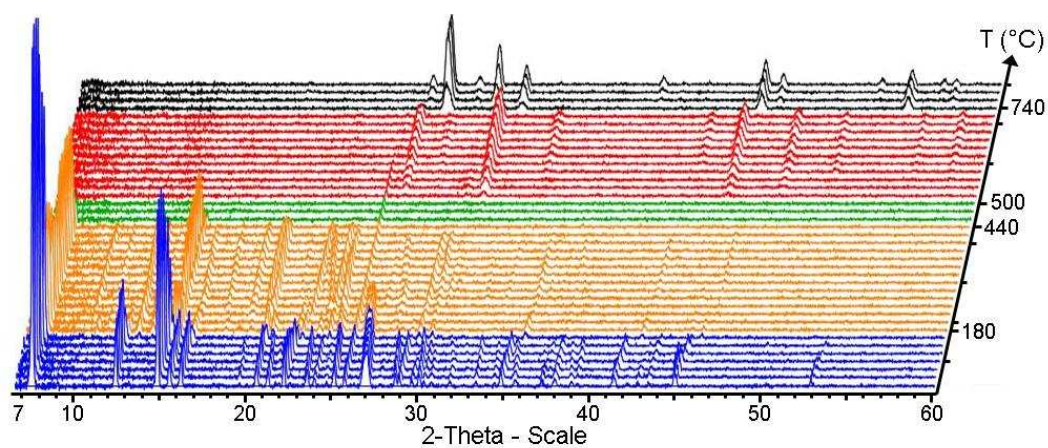


Figure S1c: X-ray thermodiffraction patterns of $\text{Nd}_2(2,6\text{-ndc})_3(\text{H}_2\text{O})_3 \cdot \text{H}_2\text{O}$ (**1**) under air atmosphere (copper radiation).

Compound **3**

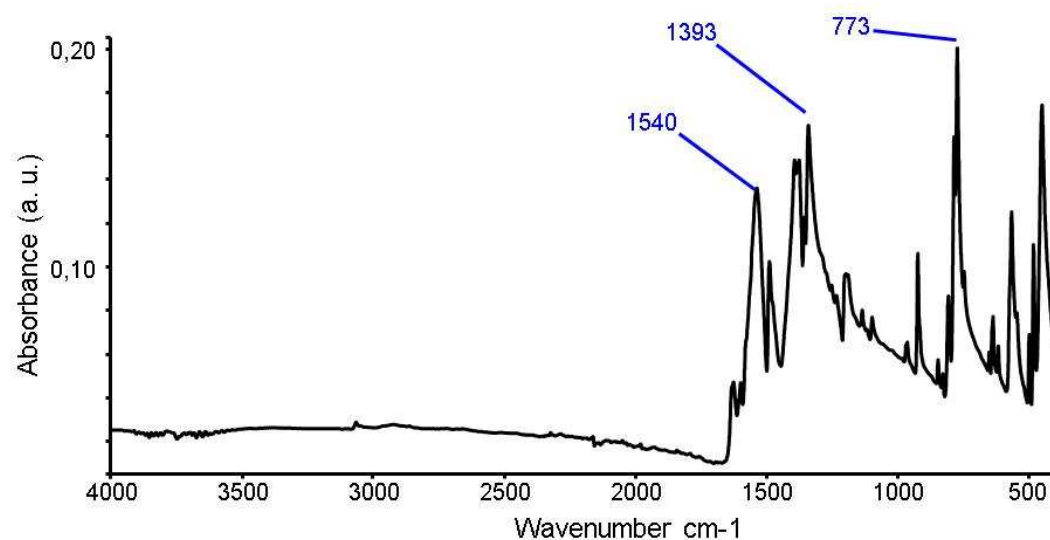


Figure S2a: Infrared spectrum of Nd(2,6-ndc)(form) (**3**)

Infrared spectrum of Nd(2,6-ndc)(form) (**3**) confirm the presence of coordinating carboxylate functions ($\nu_{\text{COO asym}}$ at 1540 cm^{-1}). The Nd-O related vibrations give absorbance in the domain $800\text{--}400\text{ cm}^{-1}$. In our case only the peak appearing at 773 cm^{-1} can be assigned to Nd-O asymmetric stretching vibration ($\nu_{\text{Nd-O asym}}$). The intense peak at 1393 cm^{-1} can be attributed to the C=C ring vibration.

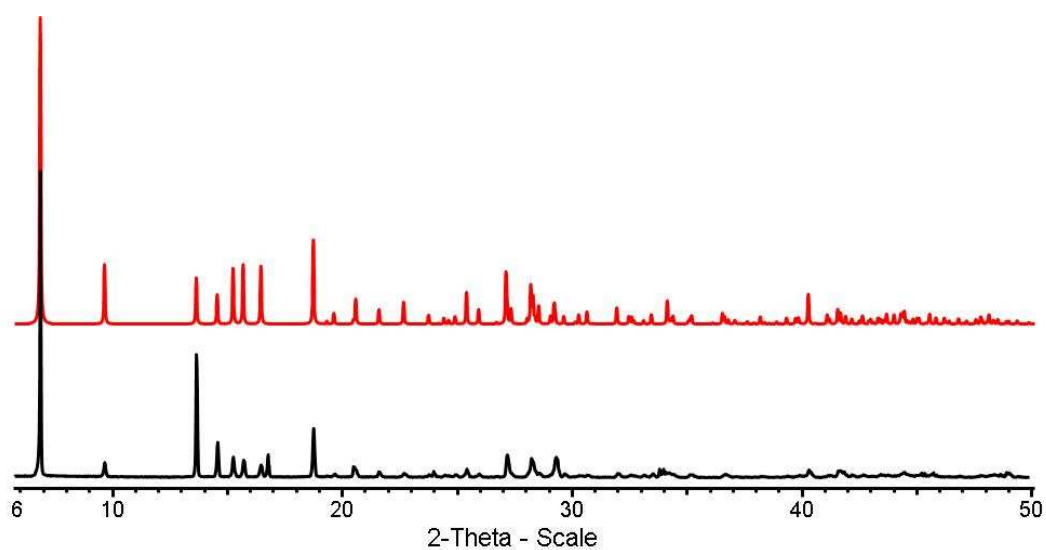


Figure S2b: Calculated (top) and experimental (bottom) X-ray diffraction powder patterns of Nd(2,6-ndc)(form) (**3**; copper radiation).

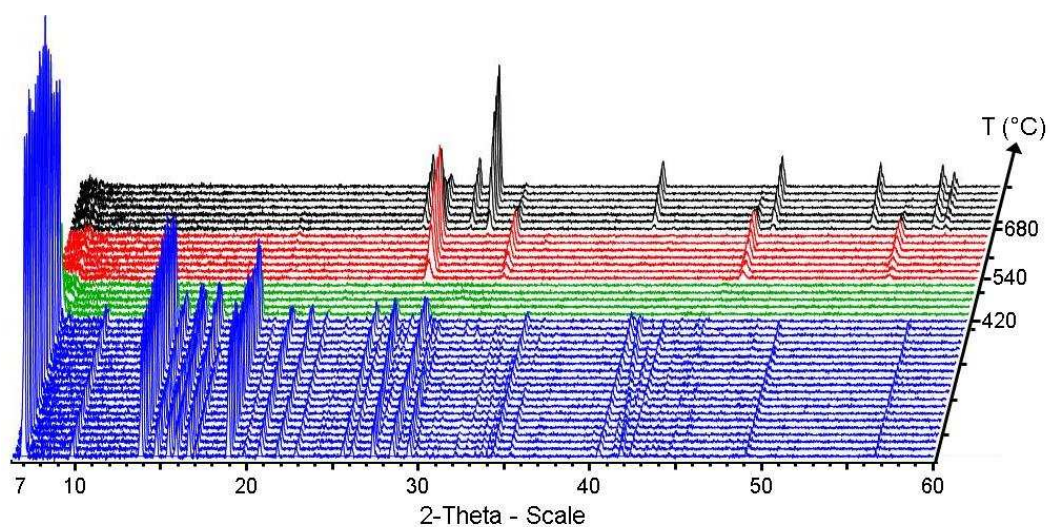


Figure S2c: X-ray thermodiffraction patterns of Nd(2,6-ndc)(form) (**3**) under air atmosphere (copper radiation).

Compound 4

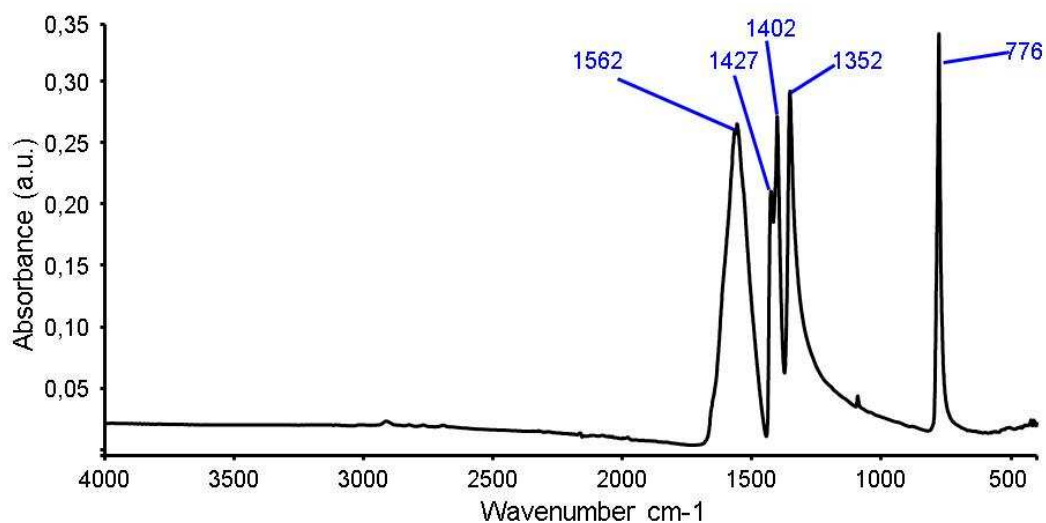


Figure S3a: Infrared spectrum of Nd(form)₃ (**4**)

Infrared spectrum of Nd(form)₃ (**4**) shows a broad band centered at 1562 cm⁻¹ and a sharper one at 1427 assigned respectively to the asymmetric ($\nu_{\text{COO as}}$) and symmetric ($\nu_{\text{COO sy}}$) stretching of the carboxylate function linked to Nd³⁺. The vibrational modes of C-H are localized at 1402 and 1352 cm⁻¹. The intense peak observed at 776 cm⁻¹ corresponds to Nd-O asymmetric stretching vibration ($\nu_{\text{Nd-O asym}}$).

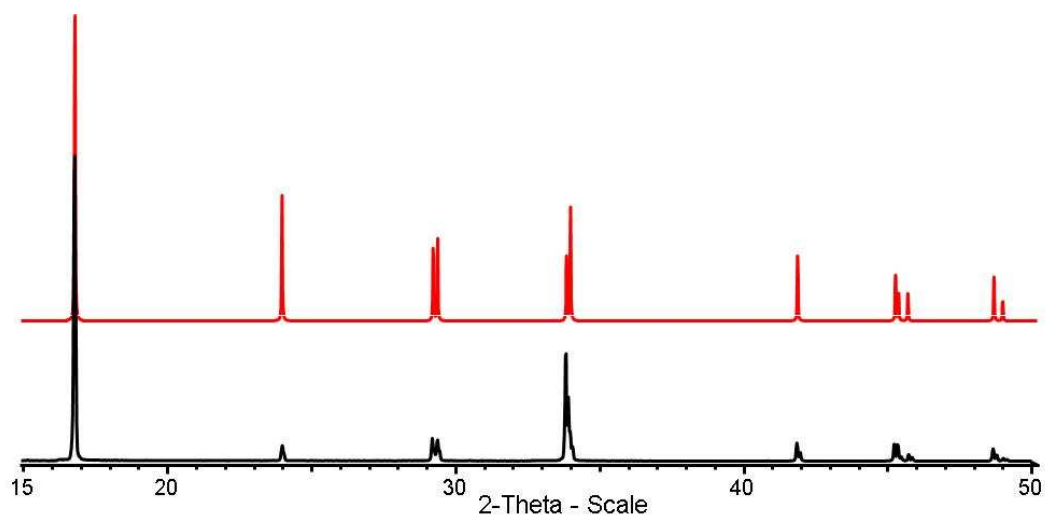


Figure S3b: Calculated (top) and experimental (bottom) X-ray diffraction powder patterns of $\text{Nd}(\text{form})_3$ (**4**; copper radiation).

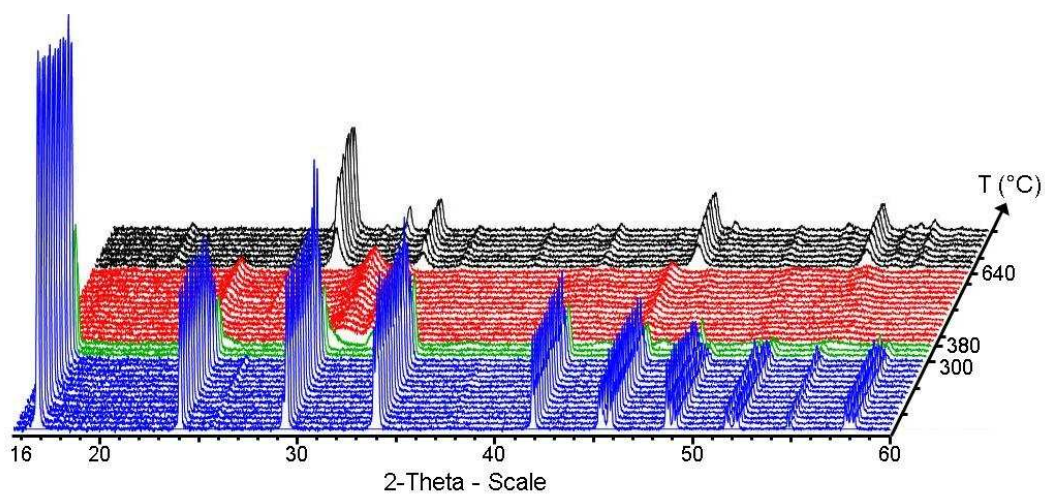


Figure S3c: X-ray thermodiffraction patterns of $\text{Nd}(\text{form})_3$ (**4**) under air atmosphere (copper radiation).