Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information of the paper:

STEREOREGULAR POLYMYRCENES BY NEODYMIUM-, IRON- and COPPER-BASED CATALYSTS.

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EXPERIMENTAL

X-ray powder diffraction profiles were recorded with Ni filtered Cu Kα radiation by using an Empyrean diffractometer by Malvern Panalytical operating in the reflection geometry with continuous scans of the 2θ angle and scanning rate of 0.02 degree/s.

DSC scans were carried out on a Mettler 822 calorimeter equipped with a liquid nitrogen subambient device. The sample, ca. 4 mg, was placed in a sealed aluminum pan, and the measurements were carried out using heating and cooling rates of 10°C/min.

Compression molded films were prepared by heating the as-polymerized samples at temperatures of 120 °C under a press at low pressure and by slow cooling to room temperature.

The mechanical properties were evaluated performing mechanical tests at room temperature on compression-molded films with a mechanical tester apparatus (Zwicky by Zwick Roell) following the standard test method for tensile properties of thin plastic sheeting ASTM D882-83. Rectangular specimens 3 mm long, 2 mm wide and 0.3 mm thick have been stretched up to the break or up to a given deformation $\varepsilon = [(L_f - L_0)/L_0] \times 100$, where L_0 and L_f are the initial and final lengths of the specimen, respectively. Two benchmarks have been placed on the test specimens and used to measure elongation. In the mechanical tests, the ratio between the drawing rate and the initial length was fixed equal to 0.1 mm/(mm×min) for the measurement of Young's modulus and 10 mm/(mm×min) for the measurement of stress–strain curves and the determination of the other mechanical properties (stress and strain at break and tension set). The reported values of the mechanical parameters are averaged over at least five-eight independent experiments.

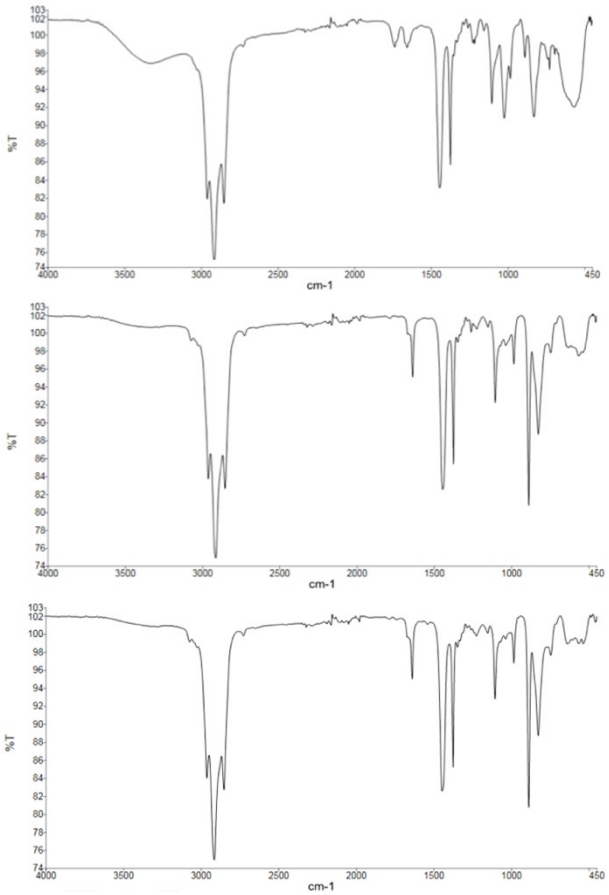

Figure SI_1. FT-IR spectra of poly(myrcene)s (Table 1) obtained with the catalyst systems Nd1/TIBAO(entry 1 of Table 1) (top), Fe1/MAO (entry 2 of Table 2) (middle) and Cu1/MAO (entry 3 of Table 1) (bottom).

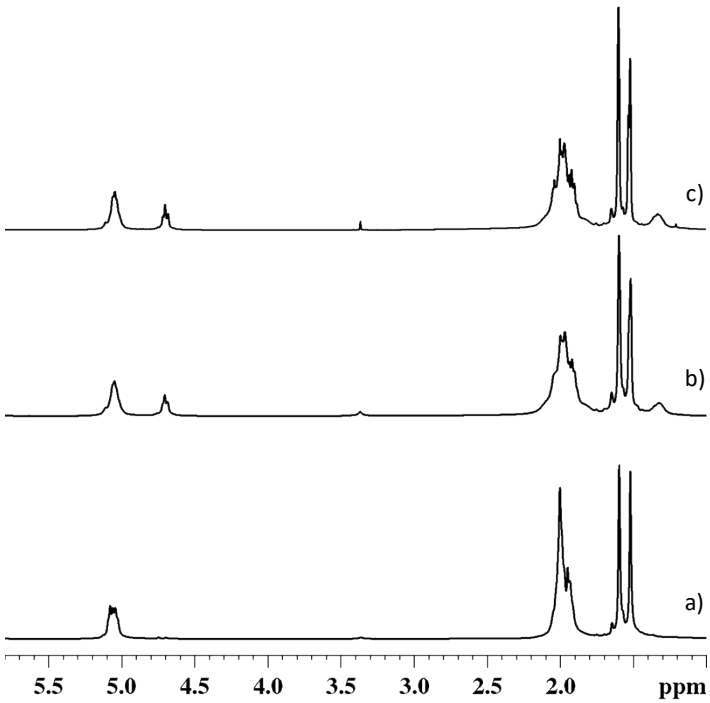

Figure SI_2. ^{1}H NMR spectra of poly(myrcene)s obtained with the catalyst systems Nd1/TIBAO (entry 1 of Table 1) (a), Fe1/MAO (entry 2 of Table 1) (b) and Cu1/MAO (entry 3 of Table 1) (c).

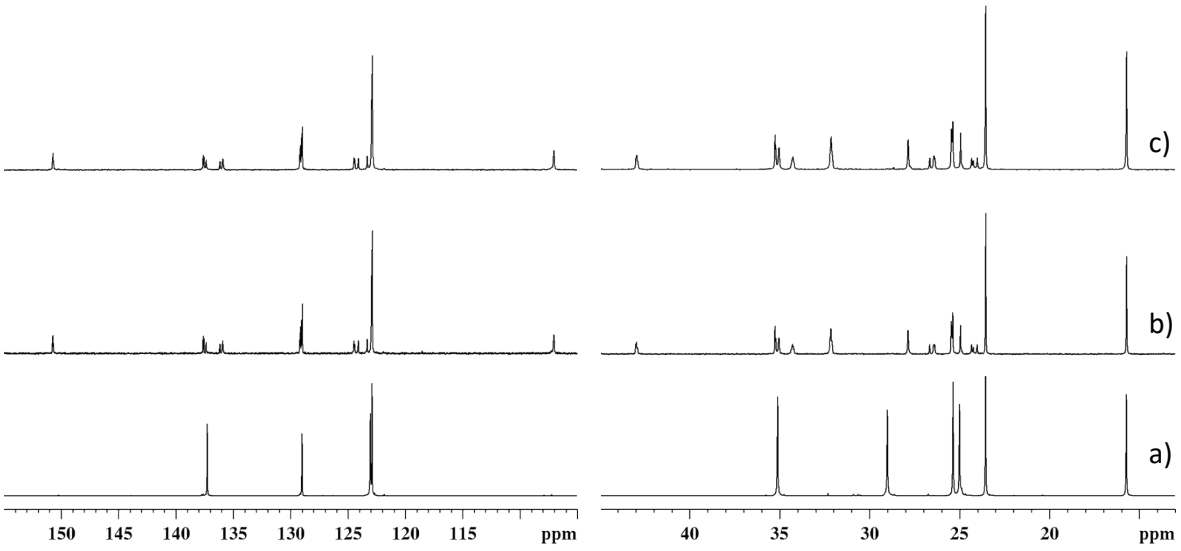

Figure SI_3. ^{13}C NMR spectra of of pol(ymyrcene)s obtained with the catalyst systems Nd1/TIBAO (entry 1 of Table 1 (a), Fe1/MAO (entry 2 of Table 1) (b) and Cu1/MAO (entry 3 of Table 1) (c).

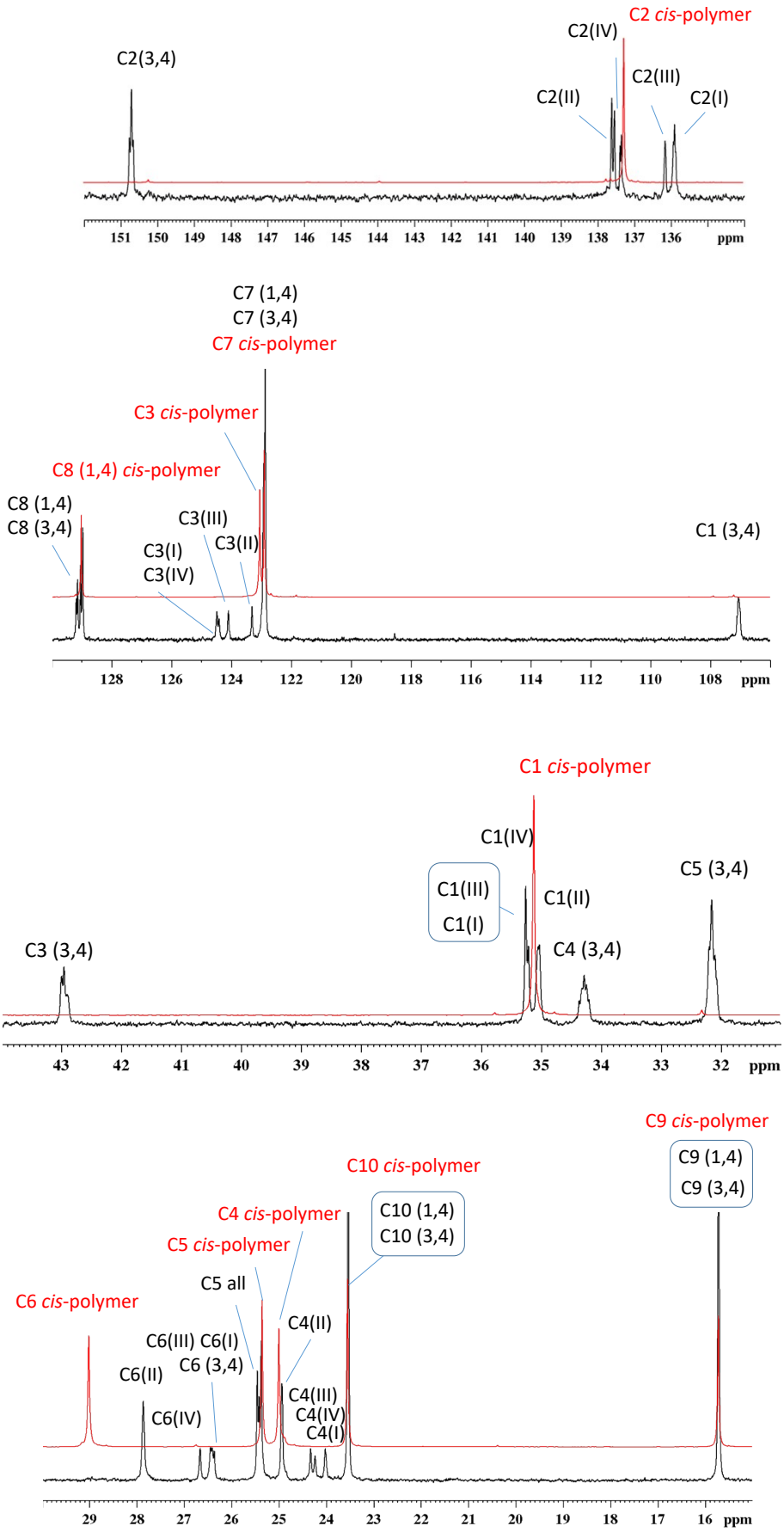

Figure SI-4. Peaks attribution in the ^{13}C NMR spectra of Nd-polymyrcenes (in red) and Fe-polymyrcenes (in black).

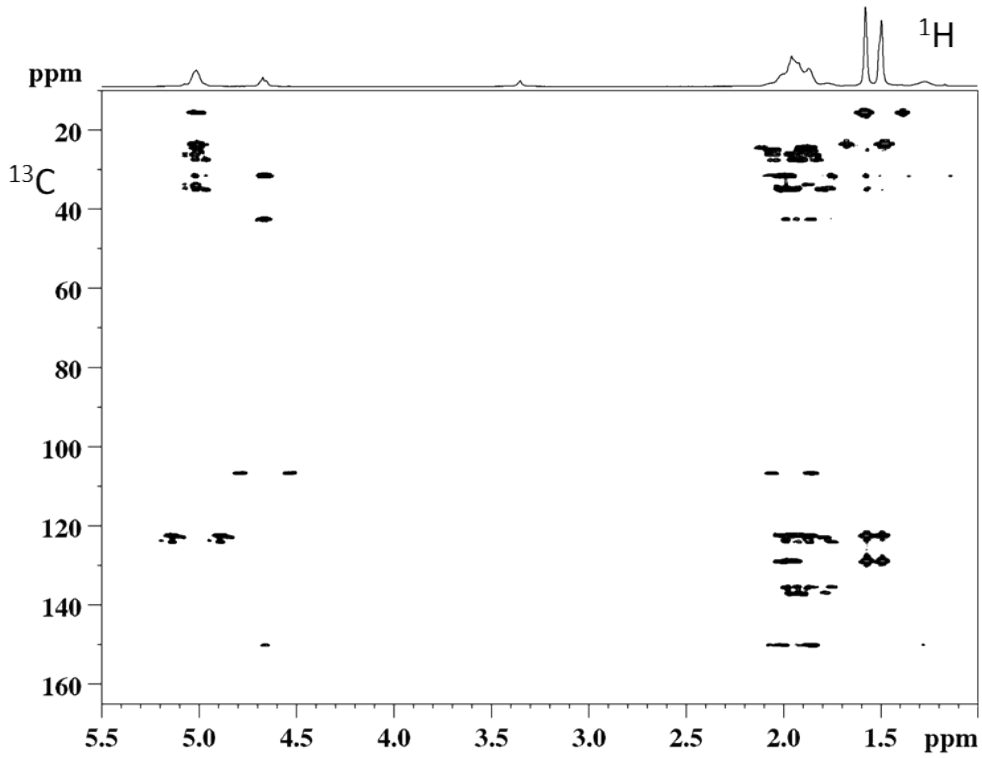

Figure SI-5. ^{1}H-^{13}C HMBC (full spectrum) of sample entry 2 in table 1, @600 MHz and 330 K.

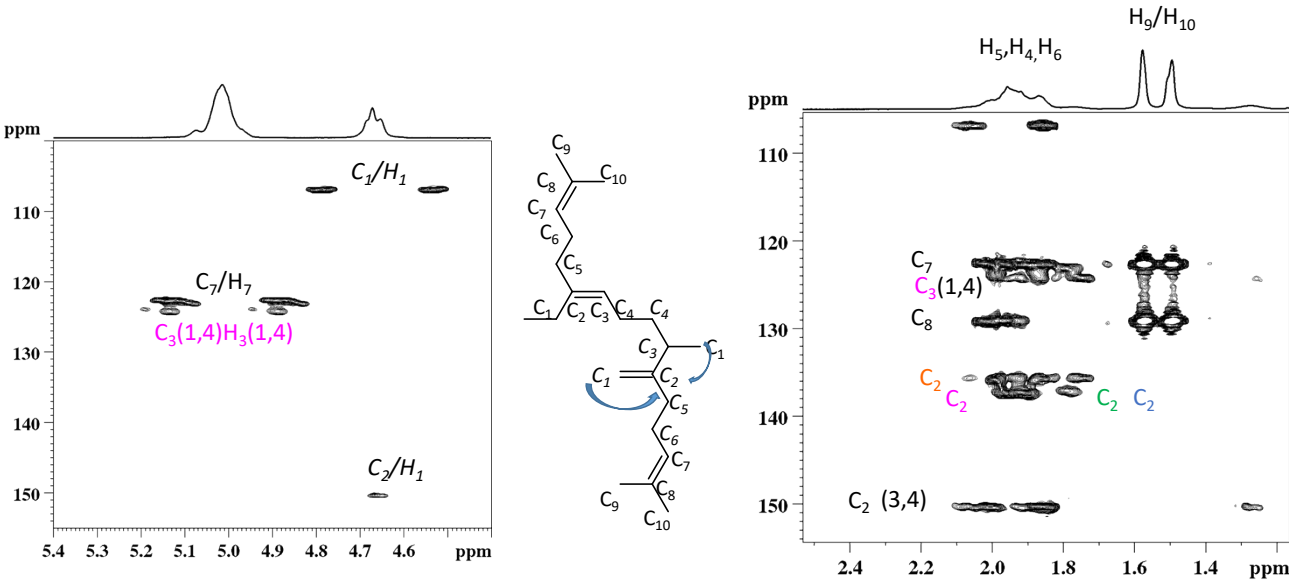

Figure SI-6. ^{1}H-^{13}C HMBC (expanded olefinic on the left, and aliphatic region, on the right) of sample entry 2 in table 1, @600 MHz and 330 K