

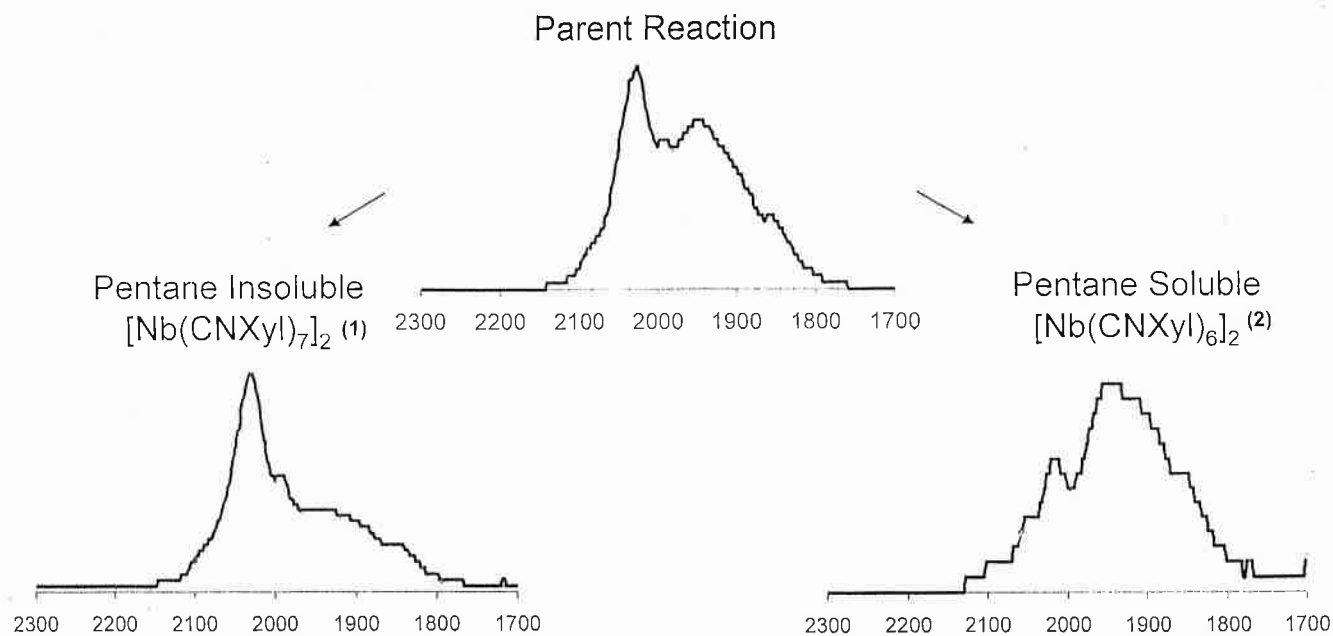


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Supporting information for article:

Niobium isocyanide complexes, Nb(CNAr)₆, with Ar = 2,6-dimethylphenyl (Xyl), a diamagnetic dimer containing four reductively coupled isocyanides, and Ar = 2,6-diisopropylphenyl (Dipp), a paramagnetic monomer analogous to the highly unstable hexacarbonylniobium(0)

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Compound	ν_{CN} in cm^{-1} (solvent)
Parent Reaction	2024, 1990, 1946, 1857 (THF)
$[\text{Nb}(\text{CNXyl})_6]_2$ (2)	2015, 1943, 1857 (THF)
$[\text{Nb}(\text{CNXyl})_7]_2$ (1)	2029, 1992, 1943*, 1855* (THF)

* minor peaks due to (2)

Scheme 1. Infrared spectral data for the reaction of bis(mesitylene)niobium(0) with 6-7 equivalents of CNXyl in tetrahydrofuran at 293K, where the spectrum at the top is that of the initial reaction mixture ("parent reaction"). IR spectra in tetrahydrofuran of the pentane insoluble product, mainly (1), and the pentane soluble component, mainly (2), are shown at the lower left and right, respectively. Major peak values are shown in the table for these spectra.