Poster

Pressure induced phase transition of [Ni(κ^3-Tp*)(acac)(MeCN)]

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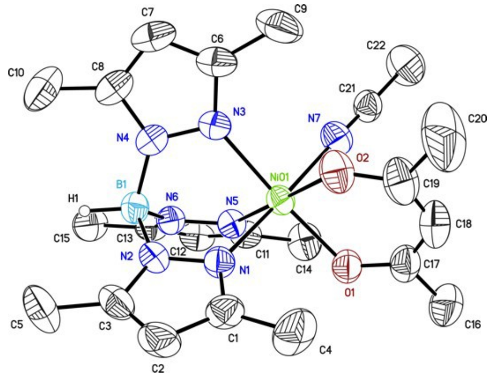
Single crystal X-ray diffraction experiments under ambient as well as high pressure were performed to investigate the solid state structure of [Ni(κ^3-Tp*)(acac)(MeCN)] (Tp* = Tris(3,5-dimethyl)pyrazol-2-ylborate, acac = acetylacetonate, MeCN = acetonitrile). All X-ray diffraction experiments were performed on a unique in-house diffractometer equipped with a Dectris Eiger 2R 1M CdTe detector, 4-circle kappa goniometer and a Metaljet X-ray source utilizing In K_α radiation, which has been shown to be capable of collecting high quality data [1].

Under ambient conditions the compound crystallizes in the monoclinic space group $P2_1/n$ with one molecule in the asymmetric unit as shown in Fig. 1. Between 0.15 GPa to 0.76 GPa a phase transition occurs whereby the symmetry of the structure is reduced to triclinic space group $P\bar{1}$ with two molecules in the asymmetric unit. The structural change is visualised in Fig. 2. A similar pressure induced phase transition for an octahedrally coordinated nickel complex resulting in reduction of symmetry was described by Cameron et al. [2].

To investigate the bonding situation upon phase transition, quantum crystallography tools were used to provide structure-property correlation. The compound exhibits an absorption change upon compression also dependent on the crystal orientation under polarised light.



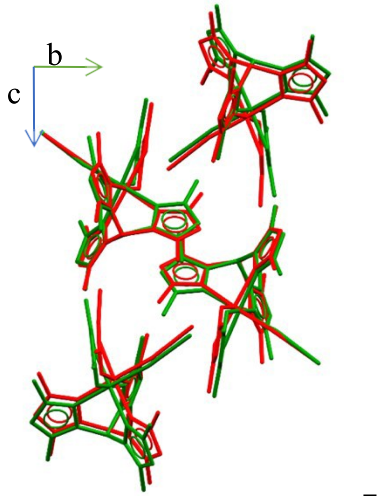


Figure 1. Asymmetric unit of [Ni(κ^3-Tp*)(acac)(MeCN)] at 302 K and ambient pressure. ADPs are depicted at 50% probability level. Hydrogen atoms (except H1) are omitted for clarity.

Figure 2. Overlay of unit cells for the structures determined at ambient pressure in $P2_1/n$ (green) and 0.76 GPa in $P\bar{1}$ (red).

[1] a) N. Graw, P. N. Ruth, T. Ernemann, R. Herbst-Irmer & D. Stalke, *J. Appl. Cryst*. **2023**, *56*, 1315–1321. b) P. N. Ruth, N. Graw, T. Ernemann, R. Herbst-Irmer, & D. Stalke, *J. Appl. Cryst*. **2023**, *56*, 1322–1329.

[2] C. A. Cameron, D. R. Allan, K. V. Kamenev, S. A, Moggach, M. Murrie & S. Parsons, Z. *Kristallogr. – Cryst. Mater.* **2014**, *229*, 200–209.