Charge-Density Analysis of a disordered Aluminium Dihydride BOX Complex

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Today, single crystal X-ray diffraction (SCXRD) experiments are among the most valuable analytical methods for determining the three-dimensional structure of given crystalline substance. Charge-density analyses based on high-resolution datasets are an advanced SCXRD technique significantly more time consuming than the usual standard measurements. However, using the Hansen & Coppens Multipole Model [1], they allow for the modelling of electron density even in interatomic bonding regions. With Bader's Quantum Theory of Atoms in Molecules (QTAIM) [2], various structural properties of interest such as bonding characters and charge distribution can then be determined from a topological analysis of the model [3].

Due to an increased susceptibility to errors in the data, complications such as twinning or disorder are generally considered a dealbreaker in terms of charge-density analysis. Disordered structures come with a wide range of problems for charge-density refinement, first and foremost that many of the structural properties from charge-density analyses can often not be unambiguously determined in disordered parts [4] . In this work, we strive to investigate in how far a successful multipole refinement with subsequent Bader QTAIM analysis of the only slightly disordered compound AlH_2MeBOX [5] (**1**) can be achieved. Bis(benzoxazol-2-yl)methandid (BOX) ligands are a family of readily available ligands with easily customizable steric demand. Therefore, BOX ligands are a promising alternative to the ubiquitous NacNac ligands [6].

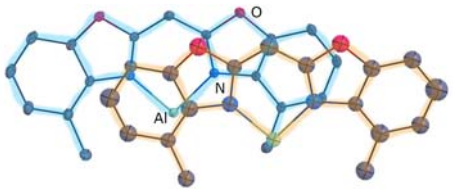

Figure 1: Structure of **1**. Main component highlighted in blue, second component highlighted in orange. Only isotropic displacement parameters were used for the second component Hydrogen atoms omitted for clarity.

Compound **1** is the BOX analogue to an AlH_2-NacNac complex showing catalytic activity, first reported in 2016 [7]. It contains two molecules in the asymmetric unit, both of which show a minor disorder with occupancies around 3% for the second position, respectively.

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