Poster

Pseudo-centrosymmetry can confuse automatic space group determination

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Enantiopure 1,2-diaminocyclohexane (DACH) and its derivatives are cheap and popular compounds for the chiral resolution in organic synthesis. When they are used as N-coordinating ligands in octahedral metal complexes with the composition $(DACH)_2MX_2$, the X ligands can be arranged in *trans* or *cis* geometry at the metal. In *trans* geometry, pseudo-inversion can be present on the metal positions in the crystal. In *cis* geometry, Λ and Δ enantiomers can be distinguished [1]. Pseudo-inversion centres in the crystal can then be present between the molecules. In all cases, the DACH ligands remain homochiral.

We present the crystal structures of an octahedral DACH complex with a pseudo-inversion centre at the metal (Fig. 1). The ADDSYM algorithm of the PLATON software [2] detects ~85% inversion symmetry for the overall crystal structure [3]. We also show crystal structures where equal amounts of Λ and Δ enantiomers are present in the same crystal (Fig. 2). Here, ADDSYM detects ~89-91% inversion symmetry.

When pseudo-inversion centres are present in the crystal, automatic software tends to propose centrosymmetric space groups. Examples of erroneous publications will be given. In these cases of wrong space group determination, the enantiopurity of the DACH ligands will ultimately cause severe disorder. The error can be avoided by basic chemical knowledge. We will also propose crystallographic tools to confirm the true non-centrosymmetry.

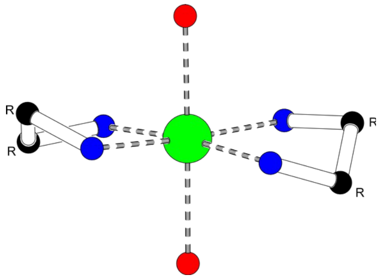

Figure 1. Schematic drawing of the backbone of the *trans*-complex. A pseudo-inversion centre can occur on the site of the metal.

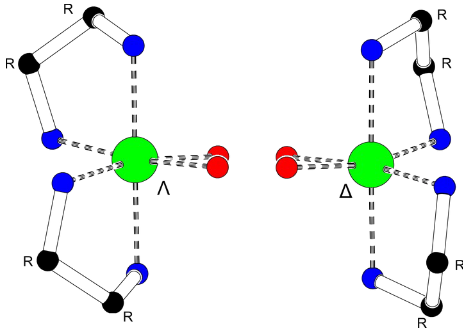

Figure 2. Schematic drawings of the backbones of the *cis*-complex. When Λ and Δ enantiomers are present in equal amounts, pseudo-inversion centres can occur between the molecules.

[1] Ehnbom, A., Ghosh, S. K., Lewis, K. G., Gladysz, J. A. (2016). *Chem. Soc. Rev.* **45**, 6799.

[2] Spek, A. L. (2009). *Acta Cryst.*, D**65**, 148.

[3] Lutz, M. (2023). *J. Mol. Struct.*, **1284**, 135362.