

## Poster Presentation

CC.P06

*When crystallography can use help from tin-119 Mössbauer spectroscopy*

G. Denes<sup>1</sup>, M. Madamba<sup>1</sup>, H. Merazig<sup>2</sup>, A. Muntasar<sup>1</sup>

<sup>1</sup>Concordia University, Department of Chemistry and Biochemistry, Montreal, QC, Canada, <sup>2</sup>Universite de Constantine 1, Departement de Chimie, Constantine, Algeria

Crystallography, the most powerful method for obtaining structural data, can benefit from help from other techniques. In this work, <sup>119</sup>Sn Mössbauer spectroscopy was used to assist crystallography, for finding the tin(II) positions in the unit-cell and determine a tin(II) coordination in agreement with both the diffraction data and the tin electronic structure. Even high quality single crystal data do not guarantee that the right solution will be obtained. A first attempt at the structure of  $\alpha$ -SnF<sub>2</sub> yielded the tin positions with very reasonable R and R<sub>w</sub> residuals, 0.23-0.25. However, the fluorine positions could not be found (Bergerhoff, 1962). After many other attempts, the full crystal structure was finally solved 14 years later (R.C. McDonald et al. 1976). The difference in the tin position with the initial solution (1962) was that, in the latter, half of the tin atoms were on special sites, however, the tin sublattice was identical. Because the tin sites in the initial solution gave very reasonable residuals, 14 years of hopeless efforts were wasted. The presentation will show that this could have been avoided using <sup>119</sup>Sn Mössbauer spectroscopy. This was possible since the spectrum had already been recorded (A.J.F. Boyle et al., 1962). Mössbauer spectroscopy can also help determine the tin coordination, when combined with powder diffraction data, in case of disordered structures. The presence of tin(II), disordered with a metal ion in cubic coordination, when diffraction shows there is no lattice distortion and no superstructure, suggests that tin has also a cubic coordination. This would require the tin lone pair to be non-stereoactive; however Mössbauer spectroscopy shows it is stereoactive.

[1] G. Bergerhoff, *Acta Cryst.* 1962, 15, 509., [2] R.C. McDonald, H. Ho-Kuen Hau and K. Eriks, *Inorg. Chem.* 1976, 15, 762-765., [3] A.J.F. Boyle, D.St.P. Bunbury and C. Edwards, *Proc. Phys. Soc.* 1962, 79, 416-424.

**Keywords:** Site symmetry, Lone pair stereoactivity, Mossbauer spectroscopy