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Georges Denes

Concordia University, Canada

When crystallography alone fails, it can use help from tin-119 Mossbauer spectroscopy

Crystallography is unquestionably the most powerful method for obtaining structural data about crystalline solids. However, there are some cases where even the most powerful method can benefit from help from techniques that are not used for structural determination. In the current work, 119Sn Mossbauer 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. The first case will show that even high-quality single crystal data do not always guarantee that the right solution will be obtained. A first attempt at the structure of α–SnF_2 yielded the tin positions with very reasonable R and Rw residuals, 0.23-0.25. However, the fluorine positions could not be found. After many other attempts, the full crystal structure was finally solved 14 years later. The difference in the tin position between the two solutions 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 efforts were wasted. The presentation will show that this could have been avoided using 119Sn Mossbauer spectroscopy. This was possible since the spectrum had already been recorded. It will also be shown how Mossbauer spectroscopy can help determine the tin coordination, when combined with powder diffraction data, in the 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-stereo active; however, Mossbauer spectroscopy shows it is stereo active. The same technique helps to suggest an alternate disordered structure in agreement with the X-ray powder diffraction data. Furthermore, 119Sn Mossbauer spectroscopy was also used to assist diffraction for solving the crystal structure of a compound suffering from an extreme case of preferred orientation. The presentation will show the hurdles faced by diffraction methods alone and how we designed the use of Mossbauer spectroscopy in order to rescue crystallography.

Biography

Georges Dénès is a Professor in Department of Chemistry & Biochemistry at Concordia University, Canada. He has completed his PhD at Universite de Rennes 1. His research interests are solid state inorganic chemistry. He has been teaching general chemistry, inorganic (main group) chemistry and he has published articles in various journals.

gdenes@algol.concordia.ca

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