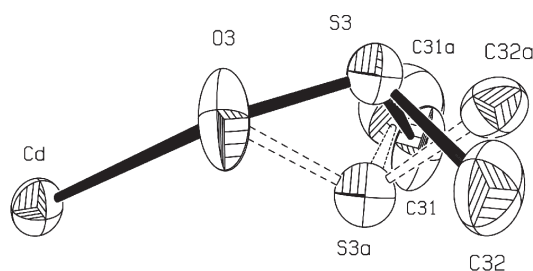


s12.m34.p5 **Influence of Temperature on Disorder of a Coordinated Dimethylsulphoxide Molecule.** Ivan Halasz and Ernest Mestrovic, *Chemistry Department, Faculty of Science, University of Zagreb, Zvonimirova 8, 10002 Zagreb, Croatia.* E-mail: [ihalasz@chem.pmf.hr](mailto:ihalasz@chem.pmf.hr)

**Keywords:** Dimethylsulphoxide; Disorder; Temperature

If some fragment, usually relatively small, of the crystal structure cannot be assigned the same equilibrium position in all unit cells of the crystal or its equilibrium position changes in time, it is said that such fragment is disordered. In the former case disorder is referred to as static whereas in the latter as dynamic. Disordered crystal structures are relatively often encountered, and a dimethylsulphoxide (dms) molecule is particularly often found to be disordered.

In the dimethylsulphoxide adduct of bis(1,3-diphenyl-1,3-propanedion)cadmium(II) complex the two dms molecules are ligated to cadmium(II) ion through oxygen atoms in cis geometry [1]. Electronic density of one of the two dms molecules was modeled assuming positional disorder of that molecule over two positions. In order to gain deeper insight into the nature of the disorder, variable temperature diffraction experiment was performed with one single crystal. The temperature of the sample was in the interval from 100°K to 330°K. It was found that disorder was completely diminished at 100 K and became more expressed as temperature was raised. For this reason disorder was interpreted as dynamic, that is, the results indicate that the position of the dms molecule changes with time. At 300 K refined occupancies of major and minor orientations are 0.82 and 0.18, respectively.



Based on data measured at four temperatures, in the interval from 150 K to 300 K (quality of data collected at 330 K was quite poor), the enthalpy difference [2] of the two orientations was estimated at 4.9 kJ mol<sup>-1</sup>. The disordered dms molecule is situated in a cavity between two phenyl rings which are leaving enough space for the orientation to change without significant energy increase.

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s12.m34.p6  **$\alpha$ -Li<sub>3</sub>InF<sub>6</sub>, a Ternary Fluoride Lithium with a New Structure Type.** M. Hamadene<sup>a</sup>, F. Balegroune<sup>a</sup>, A. Guehria<sup>a</sup>, J. Grannec<sup>b</sup> and J. Ravez<sup>b</sup>, <sup>a</sup>Laboratoire de Cristallographie-Thermodynamique, Faculté de Chimie, USTHB, BP 32, El-Alia, BEZ, Alger, Algérie, <sup>b</sup>Institut de Chimie de la Matière Condensée de Bordeaux, Laboratoire du CNRS, Avenue du Dr. A. Schweiter, Cedex, 33608, Pessac, France. E-mail: [mal\\_hamadene@hotmail.com](mailto:mal_hamadene@hotmail.com)

**Keywords:** New structural type; Disorder

The ternary lithium indium fluoride, Li<sub>3</sub>InF<sub>6</sub>, has been found to undergo three allotropic  $\alpha$ ,  $\beta$ ,  $\gamma$  forms [1]. Evidence of new structural characteristics occurred, due to the larger trivalent cation size, compared with the Li<sub>3</sub>MF<sub>6</sub> (M=Al, V) compounds. The low-temperature  $\alpha$ -Li<sub>3</sub>InF<sub>6</sub> form crystallizes in the monoclinic system with space group P21/m (Z=4) and cell parameters a=4.797(3)Å; b=8.679(1)Å; c=10.366(1)Å and  $\beta$ =90.90(1)°. The structure has been solved from 1381 reflections and refined from least-squares to an R factor of 0.028, using SHELX97 programs [2]. The cell contains two independent In atoms and four Li atoms. The framework is built up from isolated InF<sub>6</sub> octahedra, one-edge sharing LiF<sub>6</sub> octahedra and half-filled [Li<sub>2</sub>F<sub>6</sub>] bitetrahedra. The one-edge shared LiF<sub>6</sub> octahedra form infinite zigzag chains of the formula (LiF<sub>4</sub>)<sub>n</sub><sup>3n-</sup>, running along b-axis and connected together via common vertices. Single InF<sub>6</sub> octahedra share common corners with surrounded half-filled [Li<sub>2</sub>F<sub>6</sub>] entities to form double files along b-axis. As a consequence, alternating LiF<sub>6</sub> chains and double files occur along [100] and [001] directions. A comparison with other two known  $\alpha$ -Li<sub>3</sub>AlF<sub>6</sub> [3] and  $\beta$ -Li<sub>3</sub>VF<sub>6</sub> [4] compounds reveals one common feature which is the isolated MF<sub>6</sub> octahedra, but shows different polyhedra networks. Moreover, this structure is noteworthy for the thermal motions of octahedrally linked Li atoms, implying a statistical distribution between two positions. Partial occupation of tetrahedral sites leads to another disorder. The observed antiparallel displacements of atoms from the octahedron centers, are consistent with an antiferroelectric behaviour studied elsewhere [1]. Further researches are in progress about the electrical properties of the ternary indium fluoride (conductivity) in order to establish the relationship between the mobility of Li<sup>+</sup> cations and structural characteristics.

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