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Symmetry Influence on the Rotation of Molecules in Crystals

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Abstract

© 2017 American Chemical Society. It was shown that rotational mobility of molecules in crystals is affected by the symmetry of their surroundings. A hypothesis was proposed for the discovered correlation. Three cases are possible for the location of the molecules with respect to the crystallographic symmetry elements: I - the location in a general position; II - the location in special positions without symmetry disordering; III - the location in special positions with symmetry disordering. According to the experimental data, the rotation barrier heights at the location of the molecules in cases I and III are lower than in case II. This fact is explained by the amplitude and p hase shifts of the rotational energy profiles of two parts of the molecule in case I and by increasing the number of minima on the rotation barrier profile at disordering the molecules by symmetry in case III. The way is proposed for lowering the rotational barrier of molecules in crystals.

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