

Struktura a nieelastyczne rozpraszanie neutronów przez kryształy molekularne z wiązaniami wodorowymi = Structure and inelastic neutron scattering by the molecular crystals with the hydrogen bonds.

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The molecular crystals, which are built of organic or organic-inorganic molecules, are characterized by the weak intermolecular interactions. From the viewpoint of the potential applications in electronics or optoelectronics the electric properties of the crystals are essential. In turn these properties are related to their crystal structure as well as the dynamics of the molecules in the solid state. The existence of the hydrogen bonds in the crystal structures, conventional and unconventional, is crucial from the viewpoint of the electric properties of the crystals. The dynamics of methyl groups present in the structure can be a measure of the molecular interactions in the crystals. In this work the dynamical properties, first of all taking into account the research results concerning the neutron scattering, will be discussed. The neutron technique is very effective as regards the methyl group dynamics investigations. The relationship between a formation of the conventional and unconventional hydrogen bonds and a tunneling of the methyl groups at low temperature will be discussed. The method of the interpretation of the INS spectra will be described taking into account the theoretical model, the parameters of which are fitted to the experimental data. The examples will regard the following molecular crystals: p-N,N'-1,10-tetraacetyldiaminodurene (TADD) (Figs. 2 and 4), 2,3,5,6-tetramethylpyrazine with chloranilic acid (TMP·CLA) (Figs. 5, 6 and 7), 2,3,5,6-tetramethylpyrazine with bromanilic acid (TMP·BRA) (Figs. 5 and 6) and the crystal of 3,4,7,8-tetramethyl-phenantroline (Me4phen) and its complex with picric acid (Me4phen·PIC) (Figs. 8 and 9). In this paper we have shown that the surrounding of the methyl group and its interactions with the adjacent molecules has a stronger effect than the changes in the electronic charge density in the molecule.

Słowa kluczowe

molecular complexes, hydrogen bonds, crystal structure,
neutron scattering, molecular dynamics in the solid state

kompleksy molekularne, wiązanie wodorowe, struktura
krystaliczna, rozpraszanie neutronów, dynamika cząsteczek w
fazie stałej

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