

Charge density analysis of two proton transfer complexes : understanding hydrogen bonding and determination of in-crystal dipole moments.

Autorzy

R. Thomas

S. Pal

A. Datta

Mariusz K. Marchewka

Henryk Ratajczak

S. K. Pati

G. U. Kulkarni

Rok wydania

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Streszczenie

An experimental charge density study has been carried out on proton-transfer complexes exhibiting nonlinear optical (NLO) properties-melaminium tartrate monohydrate and l-asparaginium picrate employing high-resolution X-ray diffraction at 100 K. Both the complexes crystallize in non-centric space group P21 and the structures exhibit interesting patterns of N-H...O and O-H...O hydrogen bonding. Experimental determination of the dipole moment (μ) for the asymmetric unit reveals that for both the crystals, there is a large cooperative enhancement in the crystalline μ arising essentially due to hydrogen bond mediated charge transfer between the melaminium ion and the l-tartrate in one case, between the l-asparaginium ion and the picrate in the other complex. We have additionally performed theoretical calculations at the density functional theory (DFT) level to understand the origin of enhancement of the dipole moments in the two systems.

Słowa kluczowe

x-ray diffraction, experimental charge density, hydrogen bonding, dipole moment

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