

## On 2:1 melamine—squaric acid dihydrate complex : the structure and vibrational spectra.

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In the present paper we would like to describe the structural and dynamical properties of crystalline dihydrated complex of melamine (2,4,6-triamino-1,3,5-triazin-1-ium) with squaric acid (3,4-dihydroxycyclobut-3-ene-1,2-dione) abbreviated as MH·SQ. The X-ray diffraction studies show the presence of deprotonated units (C<sub>4</sub>O<sub>4</sub>)<sup>2-</sup> and single protonated melamine cations surrounded by tetrameric water assemblies (H<sub>2</sub>O)<sub>4</sub>. The formation of the water tetramers deserves a special attention. IR absorption and Raman spectra reflect a richness of structural units and numerous hydrogen bonds. The presence of the continua in the IR spectra, with a characteristic presence of the Hadži's trio enriched by a numerous submaxima, may be ascribed to the structural units and to the various types of hydrogen bonds. The density functional theory calculation with the periodic boundary conditions was use to precise analysis of experimental data.

### Słowa kluczowe

Melamine - squaric acid dihydrate, X-ray structures, FT-IR spectroscopy, Raman spectroscopy, density functional calculations

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