

## Search for molecular crystals with NLO properties: 5-sulfosalicylic acid with nicotinamide and isonicotinamide.

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### Streszczenie

Two proton transfer hydrogen-bonded complexes of 5-sulfosalicylic acid (3-carboxy-4-hydroxybenzenesulfonic acid, 5-SSA) with the aromatic amides: nicotinamide (NA) and isonicotinamide (INA), are characterized by X-ray diffraction and spectroscopic studies. In the crystal structures of nicotinamidium 3-carboxy-4-hydroxybenzenesulfonate, **1**, and isonicotinamidium 3-carboxy-4-hydroxybenzenesulfonate monohydrate, **2**, the ions are linked into three dimensional frameworks by a combination of O–H···O, N–H···O and C–H···O hydrogen bonds and cation–anion  $\pi$ – $\pi$  stacking interactions. The hydrogen-bonding behavior of the pyridine N atom is different in the two crystals, bonding to a sulfonate O atom of anion in **2** but to a carbonyl O atom of cation in **1**. The complex **1** shows relatively efficient second harmonic frequency generation.

### Słowa kluczowe

Nicotinamide, Isonicotinamide, 5-Sulfosalicylic acid, Hydrogen bonds, Crystal structure, SGH

### Adres publiczny

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