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标题: Crystal structures and physical properties of 5-sulfosalicylate and violurate metal-organic crystals - experimental versus theoretical study

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摘要: Crystal structures, theoretical, and experimental physical properties of six coordination compounds of violuric and 5-sulfosalicylic acid (5SSA) with silver and potassium ions (1-6) are reported. The correlation between crystallographic data of the potassium violurate methanol solvate (2), potassium 5-sulfosalicylic acid salts (3 and 4), the redetermined structure for the potassium violurate dihydrate (1), and the already reported complexes of silver(I) with 5SSA (5 and 6) as well as the optical properties in the condensed phase was performed using the electronic-absorption, diffuse reflectance and fluorescence spectroscopies. The vibration characteristics of the crystals were studied by solid-state Raman spectroscopy. Special attention is focused on elucidation of the specific excitation phenomena within the THz-region, allowing unambiguously defining of the metal-organic polymorphs. The physical behavior and related processes under soft electrospray ionization (ESI) and matrix-assisted laser desorption/ionization (MALDI) mass spectrometric conditions are elucidated by corresponding methods, including imaging mass spectrometry (MS). A discussion on the stabilization of complex species and adducts in the gas phase depending on the type of metal ion was performed, with a view to their further application as matrices in the MALDI-Orbitrap MS method. The thermal properties were elucidated using the thermogravimetric and differential scanning calorimetric methods. Quantum chemical DFT calculations of the optical properties and selected thermodynamic quantities in solid-state were performed, supporting and elucidating some of the observed phenomena.

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