

Thermal Stability, Polymorphism, and Spectroscopic Properties of $[\text{Mn}(\text{DMSO})_6](\text{ReO}_4)_2$

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The structural, thermal, and vibrational properties of hexadimethylsulfoxidemanganese(II) rhenate(VII), $[\text{Mn}(\text{DMSO})_6](\text{ReO}_4)_2$, were investigated using single-crystal X-ray diffraction, thermogravimetric analysis coupled with mass spectrometry (TG-QMS), differential scanning calorimetry (DSC), optical microscopy measurements, infrared (IR), and Raman spectroscopy supported by density functional theory (DFT) calculations. The compound crystallizes at room temperature in the triclinic system (space group) with Mn(II) octahedrally coordinated by six DMSO ligands. DSC revealed two first-order solid-state phase transitions at 338 and 358 K. TG-QMS studies indicate thermal stability up to ~ 405 K, with subsequent stepwise loss of six DMSO molecules upon heating. Detected phase transitions are related to crystal structure changes from triclinic through monoclinic to trigonal symmetry upon heating the sample. A high reorientational disorder is associated with these transformations. The intermediate and high-temperature phases can be classified as a rotationally disordered phases. Optical microscopy measurements confirm that the observed changes are related to evident structural phase transitions in the solid state. Vibrational spectra were assigned based on DFT calculated normal modes for isolated cation and anion models, confirming the compound's molecular structure and purity. FT-IR spectra showed significant changes on heating in the vicinity of phase transitions, proving increasing of the crystal symmetry. These combined results enhance the understanding of the structural dynamics and thermal behavior of this coordination compound.

Słowa kluczowe

Hexadimethylsulfoxidemanganese(II) rhenate (VII), Thermal Analysis, Molecular reorientations, Structural Phase Transitions, Optical microscopy, DFT calculation

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