$[Ni(NH_3)_6]SO_4$: Kristallstruktur und Infrarotspektren

$[Ni(NH_3)_6]SO_4$: Crystal Structure and Infrared Spectra

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Hexammine Nickel Sulfate, Ammoniates, Crystal Structure, IR Data, Hydrogen Bonding

The crystal structure of $[Ni(NH_3)_6]SO_4$ has been determined by single-crystal X-ray diffraction ($P2_1/c$; Z = 4; a = 705.0(1), b = 1195.2(2), c = 1180.0(2) pm, β = 96.14(3)°; 2271 reflections; R_1 = 3.94%). In the hitherto unknown structure type, both the $[Ni(NH_3)_6]^{2+}$ and the SO_4^{2-} ions form chains along [100]. The six crystallographically different ammine ligands of the distorted $[Ni(NH_3)_6]^{2+}$ octahedra are involved in hydrogen bonds to six crystallographically equivalent SO_4^{2-} ions (site symmetry C_1). The strength of the hydrogen bonds differs strongly (ν_{OD} of matrix isolated NH_2D molecules: 2378 - 2494 cm^{-1}, N···O distances: 272 - 340 pm). The temperature evolution of the IR bands reveals the decrease of the dynamic orientational disorder of the NH_3 molecules with decreasing temperature.