$RbAsF_6$, $CsAsF_6$ und $RbSbF_6$: Kristallstrukturen, Thermische Phasenumwandlungen und Schwingungsspektren

$RbAsF_6$, $CsAsF_6$ and $RbSbF_6$: Crystal Structures, Thermal Phase Transitions, and Vibrational Spectra

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Alkaline Hexafluoropnictates, Crystal Structure, Thermal Phase Transitions, Vibrational Spectra

The title compounds are isostructural to $CsSbF_6$ and crystallize with the $KOsF_6$ structure type (space group R3, Z = 3) with the lattice constants a = 749.7(1) pm, c = 758.9(1) pm ($RbAsF_6$), a = 772.3(1) pm, c = 805.0(1) pm ($CsAsF_6$) and a = 767.0(1) pm, c = 786.1(2) pm ($RbSbF_6$). The structures exibit nearly ideal $[MF_6]^-$ octahedra, the alkaline cations are coordinated by 12 fluorine ions in a distorted cuboctahedral geometry. Cations and complex anions form a slightly distorted CsCl arrangement. On heating, the arsenates transform to a NaCl arrangement with disordered $[AsF_6]$ ions, whereas the antimonates of Rb and Cs form the corresponding disordered CsCl type at higher temperatures. The phase transitions and the i. r. and Raman spectra as well as the structural relations to the remaining hexafluoropnictates $A^I[M^VF_6]$ are discussed.

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