

Rb₂P₂S₆ – A New Alkali Thiophosphate: Crystal Structure and Vibrational Spectra of Rubidium Hexathiodiphosphate(V)

Mimoza Gjika, Claus Ehrhardt, and Wolfgang Brockner

Institute of Inorganic and Analytical Chemistry, Clausthal University of Technology,
Paul-Ernst-Straße 4, D-38678 Clausthal-Zellerfeld, Germany

Reprint requests to Dr. M. Gjika. Fax: (+49)5323-722995. E-mail: mimoza.gjika@tu-clausthal.de

Z. Naturforsch. **61b**, 1049 – 1053 (2006); received March 21, 2006

Single crystals of rubidium hexathiodiphosphate(V), Rb₂P₂S₆, have been obtained and investigated by single crystal X-ray diffraction, and IR/FIR and Raman spectroscopy. The title compound crystallizes isotypically to the potassium, caesium and thallium analogues in the orthorhombic space group *Immm* (no. 71) with $a = 8.485(3)$, $b = 6.953(3)$, $c = 9.259(3)$ Å, and $Z = 2$, final $R1 = 0.0579$ and $wR2 = 0.0987$. The crystal structure is characterized by discrete [P₂S₆]²⁻ anions (edge-sharing double-tetrahedra) with D_{2h} symmetry. Rubidium is coordinated by ten sulfur atoms forming a slightly distorted two-capped tetragonal prism with a coordination number CN_{Rb} 10. The FT-Raman and FT-IR/FIR spectra have been recorded and a factor group analysis was carried out.

Key words: Thiophosphate, Rb₂P₂S₆, Crystal Structure, Raman, IR