VIBRATIONAL SPECTRA AND LATTICE DINAMICS OF THE β-PHASE OF WHITE PHOSPHORUS

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The low-temperature β-form of white phosphorus has been studied by IR and Raman spectroscopy at temperatures of 10 K and above and with a resolution of 0.2 cm^{-1}. For the first time, the structure of splitting of the spectral bands of fundamental vibrations A_1, E and F_2 of the P_4 molecule, caused by the crystal field, is revealed. The band corresponding to the ν_1 (A_1) vibration splits into six components. The bands corresponding to the ν_3 (F_2) and the ν_2 (E) vibrations split into 18 and 12 components, respectively. The half-width (FWHM) of the bands in the infrared spectra range within 0.2–0.3 cm^{-1}, and FWHM for the bands in Raman spectra is about 0.15 cm^{-1}. The nature of the splitting and the number of components correspond to our theoretical calculations. The frequency values of the components of each band predicted by the theoretical calculations are in reasonable agreement with experimental data.

The IR and Raman spectra of the lattice vibrations of the β-phase of white phosphorus are measured for the first time, as well. The number of splitting components of the bands of fundamental vibrations and the vibrational spectra of the crystal lattice correspond completely to the crystalline structure of the β-phase of white phosphorus [1].

Based on *ab initio* calculations, symmetry analysis and our vibrational spectra, conclusions are drawn about the lattice dynamics of the β-phase of white phosphorus.

References

1. A. Simon, H. Borrmann, J. Horakh,. Chem. Ber./Recueil 130 (1997) 1235–1240.