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Infrared Lattice Vibration Spectra of Monoclinic ZnP₂

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The lattice vibrational properties of ZnP_2 which is known to crystallize in a monoclinic and tetragonal modification with space groups P $2_1/c$ and one of the enantiomorphs P $4_1^2 1^2$ or P $4_3^2 1^2$, respectively /1/, have been studied in detail only in tetragonal ZnP_2 mainly by Raman scattering measurements /2 to 4/ but also by infrared reflectivity and absorption measurements /5, 6/. In the case of monoclinic ZnP_2 the only experimental data available at present is from unpolarized infrared transmission measurements on very thin samples with thicknesses in the range of about 3 μ m from which approximate values for several transverse optical mode frequencies in the wave-number range $\bar{\nu}=200$ to 500 cm⁻¹ have been derived /6/. In the present communication we report the results of polarization-dependent infrared reflectivity measurements on sufficiently large vapour-grown monoclinic ZnP_2 single crystals with their twofold symmetry axis (b-axis) oriented parallel to the large surface plane of the samples. All measurements are made at room temperature in the wave-number range $\bar{\nu}=50$ to 4000 cm⁻¹.

Monoclinic ZnP_2 contains eight molecules per unit cell which means that we have 72 phonon branches. According to group theory /7/ the irreducible representation of the phonon normal modes at the point Γ of the Brillouin zone is given by

$$\Gamma = 18 \text{ A}_g \oplus 18 \text{ B}_g \oplus 18 \text{ A}_u \oplus 18 \text{ B}_u$$

The even parity 18 A_g and 18 B_g modes are Raman active. Of the A_u and B_u modes one A_u and two B_u are acoustic modes whilst the remaining 17 A_u and 16 B_u modes are infrared active for the polarization directions $\vec{E} + \vec{b}$ and $\vec{E} + \vec{b}$, respectively.

The experimental reflectivity spectra observed in the wave-number range $\bar{v} = 50$ to 500 cm^{-1} are shown in Fig. 1. At $\bar{v} > 500 \text{ cm}^{-1}$ no additional

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