MICROWAVE SPECTRUM AND CONFORMATIONAL COMPOSITION OF ALLENYLPHOSPHINE, $H_2C{=}C{=}CHPH_2$

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The microwave spectrum allenylphosphine has been investigated in the 8-62 GHz spectral region. Two conformers exist for this compound. The lone electron pair is *syn-periplanar* with the C=C-P link of atoms in one conformer, and *anti-clinal* in the other form. A full assignment of the microwave spectrum of the more stable *syn-periplanar* rotamer has now been achieved. Its dipole moment has been measured. The high-K_{-1} transitions of the *a*-type *R*-branch lines of the less stable *anti-clinal* conformer has also been assigned. The MW work has been augmented by high-level quantum chemical calculations to determine the energies of the two conformers at the G3 level of theory. They were also useful for a first prediction of the rotational constants and the dipole moment components. Finally, the structure of both conformers has been determined.