METHOD AND RESULTS OF DETERMINATION IN ANALYTICAL FORM THE PARAMETERS OF TETRAHEDRAL SPLITTINGS AND BAND CENTERS IN THE XY_4 SPHERICAL TOP MOLECULES: $^M GeH_4$ AS AN APPLICATION

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The mathematical basis is discusses the for solving an important and up to the recent time unsolved problem of analytical describing a complicated tetrahedral structure of the spectra of spherical top molecules. The main difficulty of the problem until recently was the impossibility of an analytical presentation of the quantum–mechanical wave functions of such type molecules. Using the theory of irreducible tensor sets, we solved this problem and obtain the necessary results in the most general form for the vibrational problem (possible vibrational resonance interactions are also taken into account). Results are obtained for states of arbitrary symmetry which are united in polyads with a polyad quantum number $P \leq 8$. As an illustration, band center values are predicted for all bands of the five isotopologues of $^M GeH_4$ ($M = 70, 72, 73, 74, 76$) up to 10000 cm^{-1}.

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