

ANALYSIS OF EXPERIMENTAL SPECTRA OF PHOSPHINE IN THE TETRADECAD NEAR 2.2 μM USING *AB INITIO* CALCULATIONS

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In support of planetary atmosphere remote sensing and exobiology, we studied spectroscopy of phosphine (PH_3) in the full TetradeCAD range, involving 26 rotationally resolved bands, for the first time. For this, we analyzed high-resolution FT-IR spectra in the 3769 - 4763 cm^{-1} region recorded at temperatures 200 K and 296 K. Overall 3242 line positions were assigned and modeled by using a combined theoretical model based on *ab initio* calculations. The total nuclear motion Hamiltonian, including *ab initio* Potential Energy Surface (PES), was reduced to an effective Hamiltonian using the high-order contact transformation method adapted to vibrational polyads of the AB_3 symmetric top molecules, followed by empirical optimization of the parameters. At this step, the measured line positions could be reproduced with a standard deviation of 0.0026 cm^{-1} , providing unambiguous identification for the observed features. We also obtained the effective dipole transition moments of the bands by fitting to the intensities from variational calculations using the *ab initio* Dipole Moment Surface (DMS). The assigned lines were used to additionally determine 1609 vibration-rotational levels up to $J_{\text{max}} = 18$ with their energy in the range of 3896-6037 cm^{-1} . Transitions for all 26 sublevels of the TetradeCAD were identified but with noticeably a fewer number of transitions for fourfold excited bands due to their weaker intensity. We present the latest results and comparison with existing experimental spectra in the discussion of their validation and applications toward planetary atmosphere characterization.