POTENTIAL PARAMETERS OF PH_3 OBTAINED BY SIMULTANEOUS FITTING OF *AB INITIO* POTENTIAL POINTS AND EXPERIMENTAL VIBRATIONAL BAND ORIGINS

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Experimental information about rotation-vibration energies plays a very important role in the analysis of molecular potential energy surfaces (PES). The parameters of an analytical representation of the PES are normally obtained from a nonlinear least squares method. However, it is usual for polyatomic molecules to have few observed data and very many potential parameters. This makes it necessary to constrain some of the parameters to zero or to their *ab initio* values. As a result the optimized potential surface becomes a rather effective one, and it could be different from the real PES or even unrealistic.

We present here a simultaneous fitting of potential parameters to experimental band origins and to *ab initio* energies for the PH_3 molecule. The vibrational energies have been calculated using the following basis set: a) Morse oscillator functions for the stretching modes; b) harmonic oscillator functions for the nonsymmetrical bending modes, and c) symmetrical bending functions, obtained by the Numerov-Cooley approach. Different weights have been applied in the fitting procedure to describe appropriately the importance of the large *ab initio* set and the small experimental data set. Preliminary fittings to PH_3 data have been carried out; the resulting PES predicts well the known band origins for PD_3.