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AB INITIO CALCULATION OF ENERGY LEVELS AND RO-VIBRATIONAL SPECTRA FOR SiH₄ MOLECULE

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New potential energy surface (PES) and dipole moment surfaces (DMS) of molecule SiH₄ are constructed using extended ab initio CCSD(T) calculations at 19882 nuclear configurations. The PES ¹ and DMS ² analytical representation are determined through an expansion in symmetry adapted products of internal nonlinear coordinates involving 282 and 692 parameters up to the 8th order and 6th order. Lower vibrational and rovibrational levels are calculated ³. Good agreement of calculated fundamentals with observed values was found. The integrated intensities of lower polyads was calculated .

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¹[doi:10.1016/j.cplett.2010.11.008](https://doi.org/10.1016/j.cplett.2010.11.008), A.V. Nikitin, M. Rey, VI.G. Tyuterev, *Chem. Phys. Lett.*, **501**, 179–186 (2011).

²[doi:10.1016/j.cplett.2013.02.022](https://doi.org/10.1016/j.cplett.2013.02.022), A.V. Nikitin, M. Rey, VI.G. Tyuterev, *Chem. Phys. Lett.*, **565**, 5–11 (2013).

³[doi:10.1039/c3cp50275a](https://doi.org/10.1039/c3cp50275a), M. Rey, A.V. Nikitin, VI.G. Tyuterev, *Phys. Chem. Chem. Phys.*, **15**, 10049–10061 (2013).