AB INITIO ANHARMONIC FORCE FIELD, SPECTROSCOPIC PARAMETERS, AND EQUILIBRIUM STRUCTURE OF TRIFLUOROSILANE

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All fundamental vibrational states of both $SiHF_3$ and $SiDF_3$ have been measured from microwave up to far-, mid-, and near infrared ranges. This allows us to determine accurately many molecular parameters. In parallel, the force field has been calculated ab initio up to the quartic terms and has been used to calculate the molecular parameters which are found to be in extremely good agreement with the experimental values of the unperturbed states. There are parameters which slightly desagree, but this disagreement is not due to any pitfals of the methods but is a consequence of, at first glance, hidden perturbations that can now be explained. Finally, a new equilibrium structure has been determined.