Vibrational and scaled quantum chemical study of O,O-dimethyl S-methylcarbamoylmethyl phosphorodithioate, dimethoate

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Infrared and Raman spectra of O,O-dimethyl S- methylcarbamoylmethylphosphorodithioate, dimethoate, have been recorded. Density functional theory, DFT, with the B3LYP functional was used for the optimization of the ground state geometry and simulation of the infrared and Raman spectra of this molecule. Calculated geometrical parameters fit very well with the experimental ones. Based on the recorded data, the DFT results and a normal coordinate analysis based on a scaled quantum mechanical (SQM) force field approach, a complete vibrational assignment was made for the first time.