PREDICTION OF FUNDAMENTAL VIBRATIONAL FREQUENCIES AND INFRARED INTENSITIES: A BENCHMARK STUDY

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In this work we investigate the performance of second-order vibrational perturbation theory (VPT2) using force fields computed at the fc-CCSD(T) level in conjunction with different double-, triple-, and quadruple-ζ basis sets[a] for the prediction of fundamental vibrational frequencies and infrared intensities. A benchmark study comprising more than thirty small and medium sized molecules illustrates the accuracy and limitations of the presented scheme.

[a] Atomic natural orbital (ANOY, Y=0,1,2) [J. Almlöf and P. R. Taylor, *J. Chem. Phys.* **86**, 4070 (1987)] and correlation-consistent (cc-pVXZ, X=D,T,Q) [T. H. Dunning, Jr., *J. Chem. Phys.* **90**, 1007 (1989)] basis sets.