Ideal-Gas Properties of HCFC's by Quantum Chemical Calculation

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Accurate ideal-gas state functions can be obtained by means of statistical thermodynamics, but the molecular properties are not always available with required accuracy. On the other side, quantum mechanical *ab initio* calculations can be used to obtain molecular properties such as molecular structure, vibrational frequencies, and potential barriers of hindered internal rotation with high accuracy. In this paper we present the geometries and harmonic frequencies of CHF_2-CH_3 (R152a), CF_3-CH_2F (R134a), CF_3-$CHCl_2$ (R123), $CClF_2$-CHClF (R123a), and CF_3-CHClF (R124) as predicted by *ab initio* calculations. We used density functional theory with the B3LYP (Becke three-parameter-Lee-Yang-Parr) method and basis sets of the type cc-pVDZ and cc-pVTZ. The results obtained for the molecules are compared to available experimental molecular data. Comparison of the calculated ideal-gas heat capacities with experimental data show, that an agreement of 1% is achieved, which is the range of agreement of the more recent experimental investigations for R134a.