

Thermodynamic Properties of Hydrofluorocarbons

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Hydrofluorocarbons (HFCs) are widely used as industrial refrigerants and fire suppressants. Both applications need accurate thermodynamic property information for practical design decisions. Recently, the concerns of climate change initiated the search for new refrigerants with low Global Warming Potential (GWP). Specifically, the use of hydrofluoroolefins (HFOs) is presently considered. HFOs have much lower atmospheric lifetime than the HFC-based refrigerants presently in use. Similar concerns apply to industrial fire suppressants. This work focuses on reevaluation of the existing data and calculation of the ideal-gas thermodynamic properties for HFCs. The available experimental data on the enthalpies of formation for the compounds were compiled and analyzed with the use of composite quantum chemical methods. The developed procedure for evaluation of D_fH for HFCs was used to obtain the enthalpies of formation for promising HFO-based refrigerants unavailable from experiment. The molecular geometries and vibrational spectra for HFCs were calculated by different methods of quantum chemistry. B3LYP and B98 functionals were found to have the best performance for calculation of the considered properties. The equations for scaling of the vibrational frequencies were found using genetic algorithms. The performance of different methods for determination of the parameters of internal rotation in HFC molecules was also considered. Thermodynamic properties for HFO-based refrigerants were calculated over a wide temperature range using the above-mentioned procedures.