Ab Initio Predictions of Thermophysical Properties of Refrigerant Mixtures.

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We present the results of a completely *ab initio* study of fluid mixtures of CO_2 and fluorinated methane derivatives. Intermolecular pair and three-body interaction potentials are obtained from a combination of molecular orbital theory and perturbation theory. The resulting pair potentials are used in Gibbs ensemble simulations of the liquid/gas equilibrium, at a range of temperatures below the critical temperature. Three-body interaction potentials are included in the simulations by several different techniques, including thermodynamic perturbation theory and the construction of density-dependent effective interaction potentials. The results show impressive agreement with experimental data, when proper account is taken of the one-particle basis set and the electron correlation in the *ab initio* calculations, the anisotropy of atoms within the interacting molecules, and the effects of non-pair-additivity in the intermolecular potential.