

Hydrogen Fluoride: A Tale of Four Fluids

J. Ilja Siepmann^{1, S, C} and Chun-Kai Chang¹

¹*Chemistry, University of Minnesota - Twin Cities, Minneapolis, MN, U.S.A.
siepmann@umn.edu*

Aggregation-volume-bias Monte Carlo simulations in the Gibbs ensemble are carried out to determine the vapor-liquid coexistence curve and the thermophysical properties of the saturated phases for hydrogen fluoride from the critical point to temperatures approaching the triple point. The heat of vaporization and the vapor-phase compressibility factor are found to exhibit a non-monotonic temperature dependence. A detailed analysis of the corresponding structural changes in the liquid and vapor phases is presented.