Calculation of Thermophysical Properties of Hydrogen Sulfide in the Gas Phase Based on an Ab Initio Intermolecular Potential Energy Surface

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Advances in computer technology make it possible to determine the thermophysical properties of dilute gases with high accuracy entirely from theory. For very low and very high temperatures, and also for highly corrosive or toxic substances, ab initio computations represent a reasonable way to obtain accurate values for thermophysical properties. The kinetic theory of gases is a very powerful tool to predict the transport and relaxation properties of a gas directly from its intermolecular potential energy surface. Based on a classical mechanical description of the intermolecular collision process, transport and relaxation properties of important gases such as carbon dioxide, methane, and water vapor have been computed. The deviations from the best experimental data were generally smaller than ±1 % for viscosity and thermal conductivity, except for the thermal conductivity of water vapor. Hydrogen sulfide is a gas for which experimental data are practically non-existent due to its extremely corrosive and toxic nature. Hence we have started calculations on its intermolecular potential energy surface based on high level coupled-cluster ab initio methods. Based on a preliminary potential surface, results for viscosity and thermal conductivity, as well as for the second pressure virial coefficient, will be presented. The uncertainties of the calculated values of the transport properties are estimated to be less than ±2 %. The ultimate goal is to decrease these uncertainties below ±1 %.