Second Pressure and Acoustic Virial Coefficients and Transport Properties for Ethylene Oxide Gas from an Ab Initio Pair Potential

Johann-Philipp Crusius C.5 and Tatiana Vasiltsova
University of Rostock, Department of Technical Thermodynamics, Rostock, Germany
johann-philipp.crusius@uni-rostock.de

Robert Hellmann
University of Rostock, Institute of Chemistry, Rostock, Germany

Egon Hassel
University of Rostock, Department of Technical Thermodynamics, Rostock, Germany

Eckard Bich
University of Rostock, Institute of Chemistry, Rostock, Germany

Ethylene oxide is a key substance in industrial processes. As the starting material for the production of ethylene glycol and PET it is indispensable. Due to its risk of explosion and toxicity obtaining experimental thermophysical data for ethylene oxide is fraught with difficulties. A solution to this is offered by theoretical methods. In combination with todays advances in computer technology it is possible to calculate thermophysical properties entirely from theory. Based upon quantum-chemical ab initio calculations a new pair potential function for ethylene oxide has been developed. Using statistical mechanics we have calculated the second pressure and acoustic virial coefficients including corrections for quantum effects and compare them to experimental data. Eventually we want to develop an ab initio three-body potential to be able to accurately determine higher virial coefficients. Furthermore we have applied kinetic theory to calculate transport properties in the zero-density limit. Here the available experimental data are scarce and we hope to improve this situation with our results.