

Hexafluoroethane (C₂F₆, R116): Intermolecular Interaction Potential and Thermophysical Properties

L. Zarkova^{C,S}

Institute of Electronics, Sofia, Bulgaria
lzarkova@yahoo.com

U. Hohm and M. Damyanova

Institut für Physikalische und Theoretische Chemie, der TU Braunschweig, Braunschweig, Germany

Recently, the interest in the transport properties of the perfluorocarbons has grown noticeably. The reason for this is not only the wide application of these gases in semiconductor and CVD manufacturing, but also the fact that they are accumulating in the atmosphere. The Global Warming Potential of C₂F₆ is almost as high as that of CO₂, and this is why it has been included in the Kyoto protocol as a greenhouse gas.

Our aim is to determine the potential parameters (PP) of the (n-6) Lennard Jones temperature-dependent potential (LJTDP) for C₂F₆ following our procedure used earlier for a number of different gases, amongst them CF₄ [1] and C_nH_{2n+2}, n < 6 [2]. The PP are obtained by fitting the LJTDP to a set of 70 experimental data points determined in the temperature range between 175 and 1000 K. In particular, there are 40 points for viscosity η [3-6], 19 for the second pVT-virial coefficient B [7,8] and 11 for the second acoustic virial coefficient β [9].

For the PP, our present results are: potential well depth $\varepsilon/k = 438.7(7)\text{K}$, equilibrium distance $r_m = 5.144(7)\text{\AA}$, repulsive parameter $n = 75.0(4)$, and enlargement of the first vibrationally excited level $\delta = 0.023(2)\text{\AA}$. The experimental results are reproduced with a mean deviation of 1.3 from experimental errors. A comparison with the recommended data of NIST demonstrates an acceptable agreement.

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