Cross Second Virial Coefficients for Mixtures of Hydrogen with Nitrogen, Oxygen, Carbon Dioxide, Methane, Ethane, and Propane from First-principles Calculations

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Hydrogen and its mixtures with many other gases are expected to play a key role in the transition to renewable energy sources, which requires reliable thermophysical property data. In this work, we aim to provide accurate values for the cross second virial coefficients B_{12} of the six binary systems formed by H_2 with the common gases N_2, O_2, CO_2, CH_4, C_2H_6, and C_3H_8 up to very high temperatures of at least 1200 K. This extends our previous work [R. Hellmann, J. Chem. Eng. Data **68**, 2212–2222 (2023)], in which we provided B_{12} values for the mixtures of H_2 with H_2O and H_2S. For all binary mixtures, obtaining B_{12} is essentially a two-step process. In the first step, intermolecular potential energy surfaces for the respective pairs of H_2 with the other molecules are developed on the basis of quantum-chemical *ab initio* calculations using high-level methods such as CCSD(T) and CCSDT(Q). In the second step, B_{12} values are extracted from the potential energy surfaces employing statistical thermodynamics. The results of our calculations will be compared with the available experimental data. In addition, we will present simple but accurate correlations of the calculated B_{12} values for convenience in practical applications.