Ab Initio Virial Equation of State for Carbon Dioxide

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Advances in computer technology make it possible to determine thermophysical properties of simple molecular fluids with high accuracy entirely from theory. For very low and very high temperatures and also for highly corrosive or toxic substances, *ab initio* approaches represent a reasonable way to obtain accurate values for thermophysical properties. Virial coefficients of gaseous and supercritical fluids up to high order can be calculated using the Mayer-sampling Monte Carlo procedure of Singh and Kofke [1]. For carbon dioxide, a virial equation of state up to eighth order will be presented. A highly accurate *ab initio* two-body potential [2] and a new *ab initio* nonadditive three-body potential were used for the Mayer-sampling computations. Both the two-body and the nonadditive three-body potential are based on counterpoise-corrected supermolecular calculations at the CCSD(T) level of theory. The quadratic Feynman-Hibbs modification to the pair potential [3] was used to account for quantum effects. The resulting virial equation of state will be compared with the best experimental $p\rho T$ data for gaseous and supercritical carbon dioxide.

References

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[2] R. Hellmann, Chem. Phys. Lett. 613, 133 (2014).
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