The Transport Properties of Sodium Atoms and the Heat Capacity of Sodium Dimers at High Temperatures

Louis Biolsi [C, S]
Chemistry Department, University of Missouri-Rolla, Rolla, MO, U.S.A.

Paul Holland
Thorleaf Research, Inc., Santa Barbara, CA, U.S.A.

Including the contribution of excited state atoms can improve calculations of dilute gaseous transport properties at high temperatures. For sodium, experimental and/or theoretical information is available about the potential energy curves associated with each of eight low-lying states of the sodium dimer. These include the $X^1\Sigma_g^+$ and $^3\Sigma_u^+$ states, that dissociate to two ground state (^{2}S) Na atoms, and the $^3\Sigma_g^+$, $^1\Sigma_u^+$, $^1\Pi_g$, $^1\Pi_u$, $^3\Pi_g$, and $^3\Pi_u$ states, that dissociate to a ground state ^{2}S atom and an excited state ^{2}P atom. Seven of these are bound states and have been fitted with either the Hulburt-Hirschfelder potential, perhaps the best general purpose atom-atom potential, or with the Morse potential. The $^3\Pi_g$ state is not bound and has been fitted with the exponential repulsive potential. We have used these potentials to calculate transport collision integrals as a function of temperature, and employed degeneracy weighted averaging to determine the viscosity and translational contribution to the thermal conductivity of Na atoms. We have also used these same interaction potentials to calculate the heat capacity, C_p, of Na_2 using an approach that depends on the second virial coefficient and its first two temperature derivatives. Again, the inclusion of molecular states that dissociate to an excited state atom allows C_p to be determined with improved accuracy at higher temperatures. This has allowed us to extend thermophysical property calculations for sodium to 15,000 K. These results are compared with previous results, including heat capacities given in the NIST Thermochemical Tables.