PARTITION SUMS FOR NON-LOCAL THERMODYNAMIC EQUILIBRIUM APPLICATIONS: NLTE-PS

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For high-altitude radiative transfer models, the importance of non-LTE corrections to the vibrational partition sum has been shown to be important with the differences in calculated radiance as large as 30% at 130 km in some cases.[a] In order to apply this correction the rotational and vibrational partition sums must be determined separately. To facilitate this, rotational and vibrational partition sums are calculated in the temperature range 100 - 450K for a number of isotopomers of atmospheric molecules important in NLTE processes: H_2O, CO_2, O_3, N_2O, CO, CH_4, NO, NO_2, and OH. The resulting data are fit to a polynomial expression of the form

$$Q(T) = a_0 + a_1 T + a_2 T^2 + a_3 T^3$$

where the coefficients are determined by a simplex nonlinear minimization routine. The resulting coefficients can then be used in a FORTRAN program for rapid recall of the rotational partition sum. The method of calculation of Q(T) for each isotopomer, convergence of the partition sum in each temperature range, the quality of the fit of the data, and comparisons with other work are discussed. The program NLTE-PS is available from the HITRAN website (http://www.hitran.com/) or from one of the authors (Robert_Gamache@uml.edu).

[a] D. P. Edwards, M. Lópes-Puertas, and R. R. Gamache *J. Quant. Spectrosc. Radiat. Transfer* **59**, 423-436, 1998.