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NASA TECH BRIEF

Computer Program for Calculation of Ideal Gas Thermodynamic Data

The problem:

To calculate ideal gas thermodynamic properties for any species for which molecular constant data are available.

The solution:

A computer program which calculates the required partition functions and derivatives from formulas based on statistical mechanics.

How it's done:

The program can perform any combination of the following: calculate thermodynamic functions (heat capacity, enthalpy, entropy, and free energy) for any set of 1 to 200 temperatures; fit the functions to empirical equations; and calculate, as a function of temperature, heats of formation and equilibrium constants from assigned reference elements and/or from these elements in their atomic gaseous state.

The thermodynamic functions for ideal gases may be calculated from molecular constant data using any one of several partition function variations provided by the program. For monatomic gases, any one of three partition function cutoff techniques may be selected and electronic energy levels which are unobserved but predicted may be included by the program. For diatomic and polyatomic gases, it is possible to select any one of five partition functions which differ in the correction factors for nonrigid rotation, anharmonicity, and vibration-rotation interactions. Excited electronic states may also be included.

For the purpose of additional processing, known thermodynamic functions for solids, liquids, or gases may be calculated from heat capacity equations or read from IBM cards.

Notes:

1. This program is written in Fortran IV and MAP for use on the IBM 7094 computer. The equations, the program, and some examples of input and output are given in NASA Technical Note D-4097, *Fortran IV Program for Calculation of Thermodynamic Data,* by Bonnie J. McBride and Sanford Gordon.
2. An option is provided to punch cards containing least squares coefficients in the form required by the program described in NASA Technical Note D-1454, *A General IBM 704 or 7090 Computer Program for Computation of Chemical Equilibrium Compositions, Rocket Performance, and Chapman-Jouguet Detonations,* by Frank J. Zeleznik and Sanford Gordon.
3. Copies of the NASA Technical Notes are available from the Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia 22151; price: $3.00 each; microfiche $0.65 each.
4. Thermodynamic data resulting from the program have applications in such fields as thermodynamics, kinetics, and fluid dynamics. The data may be used, for example, in calculating combustion compositions, transport properties, propellant performance, detonation parameters, or shock tube parameters.
5. Inquiries concerning this program may be directed to:

   COSMIC
   Computer Center
   University of Georgia
   Athens, Georgia 30601
   Reference: B68-10025

(continued overleaf)

Patent status:

No patent action is contemplated by NASA.

Source: Bonnie J. McBride and Sanford Gordon
Lewis Research Center
(LEW-10254)