New Data Compilations

NBS Tech. Note 438, Compendium of *ab initio* Calculations of Molecular Energies and Properties. MORRIS KRAUSS. Superintendent of Documents, U. S. Government Printing Office, Washington, D. C., 20402–Price 70 cents.

The number of *ab initio* molecular electronic calculations has increased markedly in the last few years. This compendium references the work from 1960 to the present and abstracts from the mass of data the best values for several observable properties including the total energy, dissociation energy, electron affinity, spectroscopic constants, electric moments, field gradients, polarizabilities, and magnetic constants. In order to provide an insight into molecular electronic structure, tables of orbital energies are also included.

This document has been reviewed by Professor C. J. Pings.

NBS Tech. Note 270–3, Selected Values of Chemical Thermodynamic Properties. DONALD W. WAGMAN, WILLIAM H. EVANS, VIVIAN B. PARKER, IVA HALOW, SYLVIA M. BAILEY, AND RICHARD H. SCHUMM. Superintendent of Documents, U. S. Government Printing Office, Washington, D. C., 20402–Price $1.25.

The tables contain values, where known, of the enthalpy and Gibbs energy of formation, enthalpy, entropy and heat capacity at 298.15° K. (25° C.), and the enthalpy of formation at 0° K., for all inorganic substances and organic molecules containing not more than two carbon atoms. In some instances such as metal-organic compounds, data are given for substances in which each organic radical contains one or two carbon atoms.

No values are given in these tables for metal alloys or other solid solutions, fused salts, or for substances of undefined chemical composition.

This document has been reviewed by Professor B. H. Sage.

NSRDS-NBS-10, Selected Values of Electric Dipole Moments for Molecules in the Gas Phase. RALPH D. NELSON, JR., DAVID R. LIDE, JR., AND ARTHUR A. MARYOTT. Superintendent of Documents, U. S. Government Printing Office, Washington, D. C., 20402–Price 40 cents.

This table revises, brings up to date, and extends the coverage on numerical values for dipole moments which was included in NBS Circular 537, Tables of Dielectric Constants and Electric Dipole Moments of Substances in the Gaseous State, prepared by Maryott and Buckley in 1953. A recommended value with an estimate of accuracy is presented for more than five hundred organic and inorganic compounds. Extensive comments are given on the definition of dipole moment and principal methods of dipole moment measurement, as well as an exposition of the criteria employed in selecting the tabulated data.

NSRDS-NBS-9, Tables of Bimolecular Gas Reactions. A. F. TROTMAN-DICKENSON AND G. S. MILNE. Superintendent of Documents, U. S. Government Printing Office, Washington, D. C., 20402–Price $2.00.

This survey covers the kinetics of bimolecular and termolecular gas reactions that do not involve atoms or molecules in electronically excited states. Bimolecular reactions are here defined as reactions in which two molecules are involved as reactants, that yield two or more molecules as products. Those reactions in which two molecules combine to form one molecule are most usefully considered as the reverse of unimolecular reactions which will be dealt with in another survey. Reactions of oxygen and nitrogen atoms have been omitted as they will also form the subject of another survey.

The literature from 1954 to December 31, 1965 has been exhaustively searched and it is hoped that for this period nothing has been omitted that should have been included.

The survey of earlier work has been based on one of the writers' books on "Gas Kinetics" which covered the literature to 1954. Use of the book for over ten years has revealed few omissions and these have been included in these tables. Data for the period January to August 1966 has been included where possible.

These documents have been reviewed by the Editorial Board of the National Bureau of Standards.