Ab Initio Theoretical Frequencies and Intensities in the Interpretation of Infrared Spectra [J. Am. Chem. Soc. 1984, 106, 4348]. B. ANDES HESS, JR.,\* L. J. SCHAAD,\* and PRASAD L. POLAVARAPU\*

Page 4351: Figure 5 was accidentally modified in printing. It should appear as follows.



## Book Reviews

**Chemical Thermodynamics.** By Peter A. Rock (University of California, Davis). University Science Books, Mill Valley, CA. 1983. xiii + 548 pp. \$29.00.

This is an introductory textbook, of fourteen chapters and four appendices, written for undergraduates. The first four chapters develop the fundamental concepts of thermodynamics: purpose and scope, temperature, internal energy and the first law, and entropy and the second law. Chapter 5 reviews the partial differential calculus and its applications to thermodynamic state functions. Chapter 6 deals with absolute entropies and the third law. The thermodynamics of chemical reactions (e.g., determinations of  $\Delta H^{\circ}$ ,  $\Delta G^{\circ}$ ,  $\Delta S^{\circ}$ ) is discussed in Chapter 7, while Chapters 8 and 9 deal with chemical potential, phase rule and phase equilibria, and the activity function. Equilibrium constants are discussed in Chapter 10. Chapters 11 and 12 treat activities of solution species and the thermodynamics of ions in solution. Phase equilibria in solutions are handled in Chapter 13, while a cursory examination of statistical thermodynamics is the topic of the final chapter.

In general this is a carefully constructed and well-written text. It is especially good in enunciating the very crucial concepts of work, heat, thermodynamic properties, and the mathematics governing them as they are defined and used in thermodynamic science. Many books are not sufficiently clear on these points. In this reviewer's opinion any physical science undergraduate should be able to comprehend these ideas clearly and completely after reading about them in Rock's book. The author combines a fine writing style with a reasonable economy of words. However, this latter aspect, while generally admirable throughout the text, does on occasion lead to some shallowness in the presentation of certain topics. For example, this reviewer feels that the basic concepts of activities are too superficially covered, and therefore there may be some vagueness and unanswered questions in the mind of an average student. It is unfortunate that the author fails even to mention the "fugacity" of a gas in connection with the ideas of activity, preferring, rather, to develop activity in a more general sense. This is not improper, but this reviewer believes that the student is somewhat short changed in this regard by at least not being made aware of the existence of a thing called "fugacity". It has been with us a long time, and will more than likely continue so.

The only major disappointment for this reviewer is that Rock eschews the contemporary approach to the description of chemical equilibrium in terms of the degree of advancement variable,  $\xi$ , which leads to  $dG/d\xi = \Delta G^\circ + RT \ln Q$  at constant T, P, etc. Rather, the author writes this in the older form,  $\Delta G_{rxn} = \Delta G^\circ_{rxn} + RT \ln Q$  etc., which, unless carefully Design and Reactivity of Topologically Unique, Chiral Phosphonamides. Remarkable Diastereofacial Selectivity in Asymmetric Olefination and Alkylation [J. Am. Chem. Soc., 1984, 106, 5754-5756]. STEPHEN HANESSIAN,\* D. DELORME, S. BEAUDOIN, and Y. LEBLANC

Page 5755, right column, line 5 from bottom: pro-R should be pro-S.

Page 5756, right column, line 4 from top: pro-R should be pro-S.

Page 5756, ref 19, line 5: pro-R should be pro-S.

Mechanisms of Stereochemical Control in Propylene Polymerizations with Soluble Group 4B Metallocene/Methylalumoxane Catalysts [J. Am. Chem. Soc. 1984, 106, 6355-6364]. JOHN A. EWEN

Page 6361, right column, Scheme III, eq 4: The rate constant should be  $k_{2,2}$ .

Page 6363, left column, 37th line: The line should readmethine and methylene groups.

Page 6363, Appendix: The left sides of eq 3 and 4 should be  $M-S\cdots$ . The right side of eq 4 should be  $M-R-S\cdots$ .

and properly interpreted, can be quite misleading and confusing. Because of this the author has missed a golden opportunity to illustrate the manner in which total  $G_{T,P}$  of a system declines with increasing  $\xi$  for a spontaneous reaction until equilibrium is attained for minimum G at  $dG/d\xi = 0$ . Some subtle complications and confusion concerning units also arise from the application of this older approach. For example, in applying the older form of the equation to excercises on pp 307-8, the author obtains answers for  $\Delta G_{rxn}$  and  $\Delta G^{\circ}_{rxn}$  in units of kJ, rather than the proper units of kJ/mol, which automatically result when using the equation in terms of  $dG/d\xi$ ,  $\xi$  having the unit of mol (of *reaction*). In this reviewer's opinion this represents a step backward in the progress of the development of thermodynamic rigor and conceptual understanding.

In spite of these flaws, this reviewer highly recommends the present text for the clientele for whom it is intended. It is well written. There are but very few errors and errata. There are ample, well-selected, and instructive examples and problems. The author obviously knows his subject quite well and puts it across in a better than average manner. The only caveat is that some areas may require greater amplification on the part of an instructor. On a scale of 1 to 10, if 5 is average, then this reviewer would award Peter Rock's book a rating of about 7.5.

James L. Copeland, Kansas State University

**Biological Magnetic Resonance. Volume 5.** Edited by Lawrence J. Berliner (Ohio State University) and Jacques Reuben (Hercules Incorporated). Plenum, New York. 1983. xix + 303 pp. \$45.00.

This volume of the series consists of five chapters. The first chapter by R. L. Baxter, N. E. Mackenzie, A. I. Scott is a concise review of the applications of CMR (<sup>13</sup>C NMR) to study metabolic pathways, in vivo. The power of CMR as a probe in the analysis of metabolic pathways at the level of cells and whole organs by following the fates of <sup>13</sup>C-enriched precursors is well documented. The second chapter is a comprehensive survey of <sup>15</sup>N NMR of molecules of biological interest by F. Blomberg and H. Ruterjans. The authors provided not only extensive tables for the values of chemical shifts and coupling constants of various compounds but also compact sections for the properties of  $^{15}\mathrm{N}$  NMR and experimental considerations to overcome the low sensitivity of the <sup>15</sup>N nucleus. The third chapter, by B. D. Nageswara Rao, describes the application of <sup>31</sup>P NMR to enzyme systems. This chapter starts with the basic considerations pertinent to the problems in <sup>31</sup>P NMR of enzyme systems followed by sections containing examples of several enzyme systems, and of computer simulations of the spectra. M.-D. Tsai and K. Bruzik summarize the use of oxygen isotopes (18O and 17O) in 31P and 17O NMR