Additions and Corrections

Selectively ^{13}C-Enriched DNA: ^{13}C and ^{1}H Assignments of the Lac Operator by Two-Dimensional Relayed HMQC Experiments [*J. Am. Chem. Soc.* **1993**, *115*, 1599–1600]. GÉRARD LANCELOT,* LUC CHANTELOUP, JEAN-MARIE BEAU, AND NGUYEN T. THUONG

Page 1599: The following legends identify Figures 1 and 2.

Figure 1. 500-MHz two-dimensional pure phase absorption ^{13}C-^{1}H HMQC spectrum of the ^{13}C1′-labeled duplex

5′ d-(C G C T C A C A A T T*)
0 1 2 3 4 5 6 7 8 9 10
3′ d-(G*C G A G T G T T A A)

using a 0.6 mM sample, 0.1 M NaCl in D_2O at 17 °C. The spectrum was recorded on a Bruker AM-X500 spectrometer with 1024 complex data points in the t_2 domain. The evolution delay in the t_1 dimension was incremented in 128 equal steps of 248 μs, resulting in a width of 1006 Hz. A GARP broad-band ^{13}C decoupling[19] was applied during the acquisition period. The t_1 dimension was zero-filled to 256 points prior to the Fourier transform. G* and T* are unlabeled residues in the sugar moiety. The delay $1/2J$ was optimized for a coupling constant of 168 Hz.

Figure 2. 500-MHz two-dimensional pure phase absorption ^{13}C1′-^{1}H relayed HMQC-NOESY spectrum of the ^{13}C1′-labeled duplex

5′ d-(C G C T C A C A A T T*)
0 1 2 3 4 5 6 7 8 9 10
3′ d-(G*C G A G T G T T A A)

using a 0.6 mM sample, 0.1 M in D_2O at 17 °C. The spectrum was recorded with 1024 complex data points in the t_2 domain and 128 increments in t_1. A GARP broad-band ^{13}C decoupling was applied during the acquisition period in order to vanish the ^{13}C–^{1}H scalar coupling. The mixing time was 250 ms. ^{13}C1′(i)–^{1}H8(i) or H6(i) and ^{13}C1′(i)–^{1}H8(i+1) or H6(i+1) connectivities for the strand 5′ d-(CGCTCACAAT) [^{13}C1′(i)–H8(i–1) or H6(i–1) connectivities for the strand 3′ d-(GCGAGTGTTAA)] are show. The sequential assignment of the ^{13}C1′ carbons and aromatic protons is show by solid lines. G^*_0 and T^*_{10} were not ^{13}C-labeled and present only the connectivities ^{13}C1′(C_1)–^{1}H8(G^*_0) and ^{13}C1′(T_9)–^{1}H6(T^*_{10}).

Is the Structure of Selenoformamide Similar to Those of Formamide and Thioformamide? [*J. Am. Chem. Soc.* **1992**, *114*, 10089–10091]. JERZY LESZCZYŃSKI,* JOZEF S. KWIATKOWSKI,* AND DANUTA LESZCZYŃSKA

Due to an error which arose during generation of the basis sets the predicted relative energies of selenoformamides contain serious computational errors. The following data should replace reported relative stabilities of selenoformamides (Table I):

	SeF–SeFA
ΔE^{el}	
SCF	61.1
CISD	51.9 (52.5)
MP2	60.3 (60.7)
MP3	52.0 (52.9)
MP4(SDQ)	52.5 (53.2)
MP4(SDTQ)	56.0 (56.6)
ΔZPE	–11.8
$\Delta H(0)$	44.2 (43.8)
$\int_0^T \Delta C_p\,dT$	–0.2
$-T\Delta S$	0.3
$\Delta G(T) - \Delta G(0)$	0.1

Table II (Energies of the Core MOs vs the Number of Frozen MOs) should be disregarded. Selenoformamide follows the relative stability patterns observed and predicted for formamide and thioformamide and our conclusion about the essential role of the core electrons in stabilization of the SeFA tautomer is erroneous. We apologize for any confusion this may have caused.

We would like to acknowledge Professor Gernot Frenking for disclosing his results for selenoformamide prior to publication and for sending us a preprint of his paper [Dapprich, S.; Frenking, G. On the Keto/Enol Tautomerism of Selenoformamide and Telluroformamide. (*Chem. Phys. Lett.* In press)].

Book Reviews

Homogeneous Catalysis: The Applications and Chemistry of Catalysis by Soluble Transition Metal Complexes. By George W. Parshall and Steven D. Ittel (E. I. du Pont de Nemours and Company). Wiley-Interscience: New York. 1992. 315 pp. $49.95. ISBN 0-471-53829-9.

Homogeneous catalysis has evolved considerably since the appearance of the first edition of this book twelve years ago. The pace of industrial applications, particularly in fine chemicals, has accelerated, and a generation of chemists has been trained in the basic tenets of organometallic chemistry and homogeneous catalysis. As a consequence, the authors have chosen to put less emphasis on the fundamental concepts (e.g. mechanisms are often represented simply in a schematic form) in order to include many examples of actual (or potential) industrial applications. Furthermore, along with the description of the catalyzed synthesis of certain well-known large scale chemical intermediates, there are many (perhaps, less well-known) up-to-date examples of applications in pharmaceuticals, agrochemicals, and fragrances as well as in the production of high performance materials. In particular, the numerous examples given to enantioselective synthesis illustrate the increasingly important role of homogeneous catalysis in this area.

Of the twelve chapters, five are concerned with olefin and diene chemistry. Chapters on isomerization, hydrogenation (and other HX additions), polymerization, oligomerization, and metathesis are illustrated not only with detailed discussions of classical processes such as adiponitrile manufacture (a Du Pont in-house success), the dimerization and polymerization of olefins, or the Shell Higher Olefin Process but also with very topical sections on fine chemical syntheses such as those of *l*-menthol, geraniol, *l*-dopa, and naproxen.

The importance of metal–carbene chemistry in catalytic cyclopropanation and metathesis is illustrated by several examples such as in ROMP polymerization or in the synthesis of imipenem (antibiotic) or permethric acid (insecticide). The chapter on oxidation of olefins shows the gradual shift in interest from Wacker chemistry toward Mo and Ti based processes using hydroperoxides. The enantioselective epoxidation and dihydroxylation of olefins is also seen to be of growing importance.

A major chapter is dedicated to carbon monoxide as a building block. Although a growth chemical in the production of certain large scale intermediates (e.g. oxo alcohols, acetic acid and anhydride), further possible developments are seen in other areas such as adipic acid or isocyanate manufacture. The applications in lower volume products (butanediol, dialkyl oxalates or carbonates) or growing specialty uses (CO/α-olefin copolymers) are also discussed.

Further chapters on arene and acetylene reactions as well as hydrocarbon oxidation are also well treated with examples. The book is completed by two chapters not typically present in such texts—one involving esterification and polycondensation processes (e.g. the synthesis of polyesters and amides, polysiloxanes) and the other on the application of homogeneous catalysis to halocarbon chemistry, a subject which is of immediate general concern.

This is a timely and extremely useful book for those involved in research in catalysis or speciality chemical synthesis. For the organic chemist, it may well serve as a source of ideas for new synthetic routes. For the educator, it can be used for an introductory (if rather substantial) course on homogeneous catalysis—spanning undergraduate/graduate studies but requiring a good base in organometallic chemistry. Overall, the success of this book rests on the authors' ability to span the fundamental/industrial interface. The quality of the presentation and the insights therein are a reflection of the excellence that has characterized research at Central Research at Du Pont in this area during the last thirty years and, in particular, the "old hand" who is the senior author of the text.

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Advances in Electron Transfer Chemistry. A Research Annual. Volume 2. Edited by Patrick S. Mariano (University of Maryland—College Park). JAI Press: Greenwich (Connecticut) and London. 1992. xii + 286 pp. $78.50. ISBN 1-55938-168-X.

Single electron transfer is now appreciated as the central paradigm of a profound number of chemical transformations. The goal of the second volume of this series is to describe current breakthroughs in the rapidly expanding area of electron transfer chemistry and biochemistry.

The broad scope of hole catalysis (HC) in organic synthesis is described in Chapter 1 (by N. L. Bauld), with considerable attention given to the underlying mechanistic theory. Generation of substrate radical cations photochemically and by use of triarylaminium ($Ar_3N^{+\bullet}$) salts is described. For example, whereas the Diels–Alder reaction of electron-rich dienophiles proceeds sluggishly and produces mixtures of isomeric products, such dienophiles readily undergo stereoselective cycloaddition under HC conditions. Sigmatropic, cheleotropic, and electrocyclic reactions are also carefully illustrated with examples.

The extensive field of electron transfer by catalytic redox coenzyme analogues is the subject of Chapter 2 (by S. Fukuzumi). A model compound that serves as an NADH analogue, for example, is 9,10-dihydro-10-methylacridine. Instead of hydride transfer per se, the mechanistic pathway is initial electron transfer from substrate to redox catalyst, followed by proton transfer from catalyst radical cation to substrate radical anion. A second electron transfer then completes the chemical reduction. Competition between proton transfer and other processes leads to an extensive array of mechanistic possibilities. The flavin redox coenzyme analogues are also considered, including enhancement by acids under nonaqueous conditions. Radical chain reactions and photoinduced electron transfer figure prominantly in this thorough chapter.

Monoamine oxidase is the subject of Chapter 3 (by R. B. Silverman). Early in the chapter it is shown that electron transfer mechanisms are more plausible than hydride transfer, carbanionic, or addition–elimination mechanisms. Key to the understanding of results is the mechanism in which single electron transfer from amine nitrogen lone pair to enzyme-bound flavin produces an aminium ion that is subsequently deprotonated at the α-carbon atom to produce an aminyl radical. The fate of this radical (e.g., electron loss or coupling to other radicals followed by β-elimination) is dependent on its oxidation potential. Strained-ring opening of cyclopropylamine substrates points to radical intermediates. The mechanistic implications of kinetic isotope effects, isotopic labeling studies, and enzyme inactivation are clearly and concisely discussed.

Chapter 4 (by A. Sancar) describes DNA repair by photolyases, light-utilizing enzymes that split pyrimidine dimers. The understanding of this photobiochemical reaction has advanced tremendously since the enzymes have become available in relatively large amounts through cloning. The roles of the chromophores and the characteristics of substrate recognition are also described. The probable mode of action is enzyme-mediated electron transfer from the photoexcited reduced flavin to the pyrimidine dimer, followed by cycloreversion of the resulting dimer radical anion. Attention is given to the results of enzymological, model, and in vivo studies. Additionally, some discussion of the current understanding of phenomena that were quite puzzling when first discovered makes this a clarifying, up-to-date review.

Each chapter has nearly 100 references or more (many in 1991), and there is a good subject index. The book is a valuable work describing the role of electron transfer in a wide variety of interesting biochemical and organic chemical processes.

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Diffusion in Zeolites and Other Microporous Solids. By Jörg Kärger (University of Leipzig, Germany) and Douglas M. Ruthven (University of New Brunswick, Fredericton, NB, Canada). John Wiley & Sons: New York. 1992. xxix + 605. $150.00. ISBN 0-471-50907-8.

This book is a welcome addition to the literature on porous crystals and carbon molecular sieves. As the title suggests, zeolites provide the main subject matter. Both the authors have made diffusion in such crystals a major part of their research programs, and their significant contributions over many years have tended to be complementary. Thus Jörg Kärger has, inter alia, been a pioneer and major contributor in self-diffusion measurements; and Douglas Rutheven has contributed in important ways to measurements of diffusivities by mass transport. Their collaboration in writing this book has resulted in an excellent survey of the subject as it has developed to date. After an introductory section on diffusion (pp 1–20) the contents are presented in three parts. Part I is devoted to the theory of diffusion (pp 23–122); Part II covers, with illustrative material, theory and limitations of methods for the measurement of self and mass transport diffusivities (pp 125–337); and Part III, entitled Diffusion in Selected Systems (pp 341–585), presents and discusses, mostly critically and sometimes more speculatively, a large amount of the published literature material. This was a difficult task well done, because of differences among the results obtained from different laboratories even on a single system and because, particularly in interpreting mass transport kinetics, a variety of complicating factors may have been present. There are occasional printer's errors in the text, but these are not such as to obscure meanings. *Diffusion in Zeolites* is a scholarly book which should become a standard reference work for years to come.

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Studies in Physical and Theoretical Chemistry. Volume 80. Theoretical Treatment of Liquids and Liquid Mixtures. By C. Hoheisel (Ruhr-University Bochum). Elsevier: Amsterdam and New York. 1993. xvii + 347 pp. $200.00. ISBN 0-444-89835-2.

This very useful monograph concerns mostly the statistical mechanics of Lennard-Jones liquids and their mixtures. The work is divided into two parts: A [Time independent phenomena = (Introduction; The Monte-Carlo method; The molecular dynamics methods; Performing of computer calculations; Structure and thermodynamics of liquids and dense fluids and Lennard-Jones type systems)] and B [Time dependent phenomena = (Continuum, distribution functions, kinetic theory; Time correlation Functions (TCF's); Single particle dynamics; Collective space and time correlation functions; Transport coefficients; Nonequilibrium methods)]. The focus of the monograph derives largely from the author's own extensive research on Lennard-Jones systems. Overall, the work is tersely, but logically, constructed with emphasis on theory rather than experiment. A good subject index is included with references that are, for the most part, up to date as of 1992. The references in a number of places could have been more specific, so the reader may have to do some work to find supplementary discussions. A general reader, however, who has an interest in the statistical mechanics of Lennard-Jones liquids, and especially in their mixtures, will find this book of immense value.

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