

Optically Active Amines. XVIII. Spectral Observations on Optically Active N-Substituted Pyrroles [*J. Am. Chem. Soc.*, **97**, 3126 (1975)]. By HOWARD E. SMITH,* RICHARD K. ORR, and FU-MING CHEN, Departments of Chemistry, Vanderbilt University, Nashville, Tennessee 37235, and Tennessee State University, Nashville, Tennessee 37203.

On page 3129, right column, line 22 of the Experimental Section should read: “(**R**)-1-(1,2,2-Trimethylpropyl)pyrrole [(**R**)-**1**] was prepared in 57% yield from (*R*)-2,2-dimethyl-3-aminobutane, $[\alpha]^{24D} -5.6^\circ$ (neat) [lit.¹⁰ $[\alpha]^{24D} -5.6^\circ$ (neat)]”.

Conformational Studies on Peptides. X-Ray Structure Determinations of Six N-Methylated Cyclic Dipeptides Derived from Alanine, Valine, and Phenylalanine [*J. Am. Chem. Soc.*, **98**, 6676 (1976)]. By ETTORE BENEDETTI, RICHARD E. MARSH, and MURRAY GOODMAN,* Department of Chemistry, University of California, San Diego, La Jolla, California 92039, and the A. A. Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California 91125.

In Figure 3, center, the left-hand drawing represents cyclo(L-Val-L-Val) rather than cyclo(L-Val-D-Val). To obtain the correct structure for cyclo(L-Val-D-Val), one isopropyl group and the hydrogen on the same α carbon should be interchanged. Torsion angles in the right-hand drawing refer, as indicated, to cyclo(L-Val-D-Val), whose crystal structure has been worked out.³⁸

Hydration of NH_4F [*J. Am. Chem. Soc.*, **98**, 6820 (1976)]. By P. A. KOLLMAN* and I. D. KUNTZ, Department of Pharmaceutical Chemistry, School of Pharmacy, University of California, San Francisco, California 94143.

We have noticed an error in eq 2; it should read [D. L. Beveridge and G. W. Schnuelle, *J. Phys. Chem.*, **79**, 2562 (1975)]:

$$-\Delta E = \frac{\epsilon - 1}{2\epsilon} \frac{q^2}{a} \quad (2)$$

Also, our choice of 2.6 Å as the radius of the cavity around solvated NH_4^+ and solvated F^- is probably too small. Choosing a distance from the NH_4^+ or F^- to the external hydrogen in the first shell water leads to cavity radii of 3.35 Å around NH_4^+ and 3.19 Å around F^- . Using these radii in the corrected equation (2) leads to a reaction field stabilization of 100.3 kcal/mol for infinitely separated NH_4^+ and F^- in H_2O ($\epsilon = 80$), instead of the 24.6 incorrectly entered as the last entry of column 5 of Table VIII. This leads to a net relative energy of this structure of -21.5 kcal/mol (last entry of column 6 in Table VIII). This relative stability is sensitive to the choice of the cavity radius; if one chooses the edge of the cavity at one-half the distance between the first and second shell waters, the reaction field stabilization is 90.8 and the net relative energy -12.0. However, the main point is that all the ionic NH_4^+ F^- structures are of comparable stability in aqueous solution and more stable than neutral $\text{NH}_3 \cdots \text{HF}$ (Table VIII), in marked contrast to the relative stabilities in the gas phase (first row of Table VII).

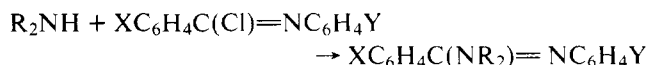
Proton Magnetic Resonance Studies of sym-Oxepin Oxide [*J. Am. Chem. Soc.*, **98**, 6353 (1976)]. By DANIEL D. HAAS and WILLIAM H. RASTETTER,* Departments of Chemistry, Harvard University, Cambridge, Massachusetts 02138, and Massachusetts Institute of Technology, Cambridge, Massachusetts 02139.

J. P. Snyder and D. N. Harpp [*J. Am. Chem. Soc.*, **98**, 7821 (1976)] have published recently a careful reexamination of the nitrogen extrusion behavior of azo compound **11** and have found $E_a = 24.1 \pm 0.3$ kcal/mol and $\Delta S^\ddagger = 6.3 \pm 0.9$ eu (CHCl_3) for the extrusion process. These authors suggested experimental factors possibly responsible for the very great differences between their activation parameters and those originally found by E. L. Allred and J. C. Hinshaw [*Chem. Commun.*, 1021 (1969)], $E_a = 14.9 \pm 1.5$ kcal/mol and $\Delta S^\ddagger = -21$ eu. The method we employed for the kinetic analysis of azo diepoxide **8** (pulse Fourier transform NMR and metal-free reaction mixtures) most closely resembles the method of Snyder and Harpp. Further, these authors provide error limits for their value of ΔS^\ddagger ; Allred and Hinshaw do not.

A comparison of Snyder and Harpp's data for **11** with that found for azo diepoxide **8** ($E_a = 26.5 \pm 0.4$ kcal/mol and $\Delta S^\ddagger = 13.2 \pm 1.5$ eu) suggests that the nitrogen extrusion processes for **8** and **11** are similar in character; i.e., both sets of data are in good accord with a concerted extrusion of N_2 . The new data for **11** strongly suggest that a similar degree of small ring strain is released from **8** and from **11** in going to the respective transition states for nitrogen extrusion.

Nucleophilic Attacks on Carbon-Nitrogen Double Bonds. 3. Diversity of Mechanisms for the Substitution of Diarylimidoyl Chlorides by Amines in Acetonitrile [*J. Am. Chem. Soc.*, **98**, 8460 (1976)]. By RACHEL TA-SHMA and ZVI RAPPOPORT,* Department of Chemistry, The Hebrew University, Jerusalem, Israel.

Equation 1 on p 8461 should be:



On page 8465, second column, line 11 from bottom, the concentrations should be 0.0007-0.005 M.

Structure and Absolute Configuration of Strictamine and Strictalamine from *Rhazya stricta*. Stereochemistry of the *Picalima* Alkaloids [*J. Am. Chem. Soc.*, **99**, 1943 (1977)]. By YUSUF AHMAD,* KANIZ FATIMA, ATTA-UR-RAHMAN, JOHN L. OCCOLOWITZ, BARBARA A. SOLHEIM, JON CLARDY,* ROBERT L. GARNICK, and PHILIP W. LE QUESNE*, P.C.S.I.R. Laboratories, Lahore-16, Pakistan, H.E.J. Postgraduate Institute of Chemistry, University of Karachi, Karachi-32, Pakistan, Lilly Research Laboratories, Indianapolis, Indiana 46206, Ames Laboratory and the Department of Chemistry, Iowa State University, Ames, Iowa 50011, and the Department of Chemistry, Northeastern University, Boston, Massachusetts 02115.

The configurations of the ethylidene groups in compounds **6** and **7** are the same as in compound **4**.