

Chemistry at Liquid-Liquid Interfaces. Evidence for an S_N1 Reaction Occurring at a Toluene-Water Interface [*J. Am. Chem. Soc.* **1978**, *100*, 7117]. S. L. REGEN* and J. J. BESSE, Department of Chemistry, Marquette University, Milwaukee, Wisconsin 53233

Activation parameters, ΔH^\ddagger , ΔS^\ddagger , and ΔG^\ddagger were computed from observed first-order rate constants and compared with analogous homogeneous reactions. Unfortunately, since hydrocarbon-water liquid-liquid interfaces have not been unequivocally defined (three dimensional vs. two dimensional), absolute values of rate constants and corresponding ΔS^\ddagger and ΔG^\ddagger values cannot be meaningfully compared with those of homogeneous systems.

Deriving Intermolecular Potential Functions for the Water Dimer from Ab Initio Calculations [*J. Am. Chem. Soc.* **1979**, *101*, 2011]. WILLIAM L. JORGENSEN, Department of Chemistry, Purdue University, West Lafayette, Indiana 47907.

The optimized geometries of the cyclic dimers with three point charge models require some correction. In Table I, the cyclic dimer from the CI potential should have 2.78, 52, and 4.62 for $r(\text{OO})$, θ , and $-\Delta E$. The values for the cyclic dimers with the exp and 266 point, 3 point charge potentials in Table III should be 2.73, 49, 3.21 and 2.75, 49, 3.12, respectively. Also, the extraneous cyclic minimum from the CI potential discussed on page 2015 occurs at $r(\text{OO}) = 1.143 \text{ \AA}$, $\theta = -11^\circ$ and with a dimerization energy of -99567 . Finally, the $\sigma_{\text{C-O}}$ in the last column of Table II should be 0.37, not 0.34. The discussions are unaffected.

An Investigation of the Reduction of Arydrazonium Ions by Hydrazines [*J. Am. Chem. Soc.* **1979**, *101*, 4668]. W. T. EVANOCHKO and P. B. SHEVLIN,* Department of Chemistry, Auburn University, Auburn, Alabama 36830

The NMR spectrum reported for 1,4-bis(*p*-nitrophenyl)tetrazine (**10**) has been found to correspond instead to that of its cleavage products *p*-nitrophenyl azide and *p*-nitroaniline. The insolubility of **10** along with its thermal lability has precluded a satisfactory NMR spectrum. The IR band at 2123 cm^{-1} is also due to *p*-nitrophenyl azide. The IR spectrum of **10** in a fluorolube mull shows bands at 3280, 3240, 3090, 3110, and 1502 cm^{-1} . Recrystallization of **10** is accompanied by some cleavage of the tetrazine. We are grateful to D. E. Herbranson of Kansas State University for bringing this matter to our attention.

Asymmetric Addition of Hydrogen Cyanide to Alkenes Catalyzed by a Zerovalent Palladium Compound [*J. Am. Chem. Soc.* **1979**, *101*, 6128]. PATRICIA S. ELMES and ROY JACKSON,* Department of Chemistry, Monash University, Clayton, Victoria, 3168, Australia

A field desorption mass spectrum and new analytical data have now shown that the compound we formulated as $[\text{DIOP}]\text{Pd}$ is in fact $[\text{DIOP}]_2\text{Pd}$. We thank Dr. Penny A. Chaloner and Dr. John Brown, University of Oxford, for informing us of their results which substantiate the $[\text{DIOP}]_2\text{Pd}$ formula.

Organic Electronic Spectral Data. Volume XV [*J. Am. Chem. Soc.* **1980**, *102*, 4284].

The name of one of the editors is incorrect. H. Fever should read H. Feuer.

Monomeric Methyl Metaphosphate: Reactions with Carbonyl Groups [*J. Am. Chem. Soc.* **1980**, *102*, 4464]. ARNOLD C. SATTERTHWAIT and F. H. WESTHEIMER,* James Bryant Conant Laboratory of Chemistry, Harvard University, Cambridge, Massachusetts 02138.

Several lines were omitted in the printing of this article. The last paragraph of p 4468 (continued on p 4469) should read as follows:

Previous observations might be reconsidered in the light of the nonselectivity of monomeric methyl metaphosphate. Monomeric

alkyl metaphosphates have been proposed as active phosphorylating agents in chemical oligonucleotide synthesis.¹⁸ Knorre et al.¹⁹ reported a ^{31}P NMR signal for an active phosphorylating agent formed in pyridine from a nucleoside-5'-phosphate and a condensing agent, triisopropylbenzenesulfonyl chloride...

Photocalorimetric Studies of Singlet Oxygen Reactions [*J. Am. Chem. Soc.* **1980**, *102*, 66]. JOHN OLMSTED, III, Chemistry Department, California State University, Fullerton, Fullerton, California 92634.

Owing to use of an incorrect conversion factor, the reaction enthalpies listed in Column 4 of Table II of this paper are uniformly incorrect. Actual reaction enthalpies can be obtained from the tabulated values by multiplying by 0.47, giving the following corrected table:

Table II. Calorimetric Results for Tetraphenylporphine-Sensitized Photooxygenations^a

| substrate | solvent | Φ_{reaction}^b (± 0.03) | $\Delta H_{\text{reaction}}$, kJ/ mol (± 20 kJ) |
|-------------------|------------------------|--|--|
| DMF ^c | CCl_4 | 0.90 | -45 |
| DPBF ^d | CCl_4 | 0.88 | -95 |
| TME ^e | CCl_4 | 0.87 | -85 |
| CHD ^f | CCl_4 | <i>h</i> | -80 |
| DPA ^g | CCl_4 | <i>h</i> | -25 |
| DPBF | toluene | 0.88 | -85 |
| TME | toluene | <i>h</i> | -75 |
| DPBF | Freon 113 ⁱ | 1.00 | -90 |
| TME | Freon 113 ⁱ | 0.98 | -80 |

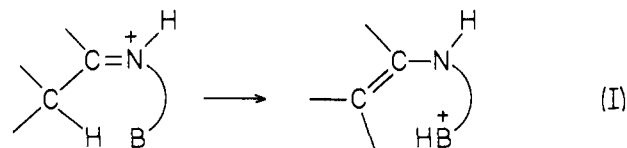
^a 546-nm excitation except where noted. ^b Lower limit of sensitizer triplet yield. ^c 2,5-Dimethylfuran. ^d 1,3-Diphenylisobenzofuran. ^e 2,3-Dimethyl-2-butene (tetramethylethylene). ^f 1,3-Cyclohexadiene. ^g 9,10-Diphenylanthracene. ^h Concentration dependent; see Figure 3. ⁱ 404-nm excitation.

Competitive Oxidation Processes in the Reaction between (Dicyclopentadienyl)zirconium Bis(phosphine) Complexes and Alkyl Halides [*J. Am. Chem. Soc.* **1980**, *102*, 3660-3662]. G. M. WILLIAMS, K. I. GELL, and J. SCHWARTZ,* Department of Chemistry, Princeton University, Princeton, New Jersey 08544

- (1) Paragraph 1, line 16: The compound should be Cp_2ZrL_2 .
- (2) Paragraph 5, line 5: The compound should be *n*-bromobutane rather than "in bromobutane."
- (3) Paragraph 5, line 7: The rate constant is $5.4 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$.

Stereoselective Bifunctional Catalysis of Dedeuteration of Cyclopentanone-2,2,5,5-*d*₄ by (1R,2S,3R,4R)-3-Dimethylamino-methyl-1,7,7-trimethyl-2-norbornanamine [*J. Am. Chem. Soc.* **1980**, *102*, 4403-9]. JACK HINE,* WU-SHYONG LI, and JAMES P. ZEIGLER, Department of Chemistry, The Ohio State University, Columbus, Ohio 43210.

Equation I should be as follows:



In the fifth line of ref 21, " f_i " should be " f_i ".

Disproportionation among Aryloxyphosphoranes [*J. Am. Chem. Soc.* **1979**, *101*, 5329]. IRVING S. SIGAL and F. H. WESTHEIMER,* James Bryant Conant Laboratory of Chemistry, Harvard University, Cambridge, Massachusetts 02138.

In eq 8, p 5330, the summation in the denominator should extend from $i = 0$ to $i = 4$ (rather than from $i = 1$ to $i = 4$).