

# Additions and Corrections

Vol. 36, 1971

**Howard E. Smith\* and Ann A. Hicks:** Optically Active Amines. XII. Synthesis and Spectral Properties of Some Optically Active  $\alpha$ -Oximino Ketones and  $\alpha$ -Amino Ketone Hydrochlorides. Dimerization of  $\alpha$ -Amino Ketones.

Page 3665. Column 2, line 47. Change Cyclopentanone to Cyclopentylamine.

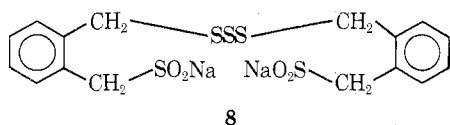
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**R. O. Hutchins,\* M. G. Hutchins, and C. A. Milewski:** Selective Dehydration of Secondary Alcohols with Methyltriphenoxyphosphonium Iodide in Hexamethylphosphoramide.

Page 4192. Figure 2 caption, lines 4 and 5. ● and ○ should be reversed.

**Pramod K. Srivastava and Lamar Field\*:** Organic Disulfides and Related Substances. 36. Some Oxodisulfide Cleavage Reactions to Form Disulfides and Trisulfides.

Page 4197. Column 1, eq 6. The compound shown as 8 should be



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**G. A. Olah\* and Y. K. Mo:** Stable Carbocations. CXXXIV. Protonation of Mono- and Dihydroxybenzenes and Their Methyl Ethers in Superacids.

Page 362. In our paper, the site of protonation in ion 24 was incorrectly assigned. It should be at the 6 position (not the 5).

**William E. Parham,\* David C. Egberg, and W. Charles Montgomery:** 1,3-Bridged Aromatic Systems. VIII. Rearrangements of Strained Systems.

Page 1209. The proton decoupled cmr spectrum of 3b should read "ten aromatic peaks at  $\delta_c$  139.7, 139.0, 133.6, 133.2, 131.9, 128.1, 126.8, 126.1, 124.2, 123.9 and six aliphatic peaks at 32.3, 32.0, 30.8, 29.4, 28.0, and 24.6 ppm downfield from tetramethylsilane.

<sup>13</sup>C enriched 3b had an enhanced resonance at  $\delta_c$  133.6."

The proton decoupled cmr spectrum of 6b should read "ten aromatic peaks at  $\delta_c$  142.0, 137.6, 133.9, 130.5, 130.4, 128.1, 127.0, 126.8, 126.3, and 124.4 and six aliphatic peaks at 34.4, 33.7, 29.6, 29.1, 26.9, and 26.3.

<sup>13</sup>C enriched 6b had an enhanced resonance at  $\delta_c$  137.6."

The proton decoupled cmr spectrum of 11 should read "four aromatic peaks at  $\delta_c$  140.8, 133.3, 127.4 (wt 2), and 125.4 (wt 1) and three aliphatic peaks at 33.5, 32.7, and 26.4. Selective off-resonance decoupling gave singlets at  $\delta_c$  140.8 and 133.3 indicating quaternary carbons and doublets at 127.4 [ $J_r(\text{CH}) = 46$  Hz] and 125.4 [ $J_r(\text{CH}) = 50$  Hz] indicating methine carbons; these results show the integral validity.

<sup>13</sup>C enriched 11 exhibited an enhanced resonance at  $\delta_c$  140.8.

**B. A. M. Oude-Alink, A. W. K. Chan, and C. D. Gutsche\*:** Photolysis of 2-Keto-2,3-dihydrobenzofurans, *O*-Hydroxy-styrenes, and 1-(*O*-Hydroxyphenyl)-1,5-hexadienes.

Page 1993. The phrase "2-methyl-3-acetoxy-5-nitro (and 7-nitro)-2,3-dihydrobenzofuran [M. P. Mertes, L. J. Powers, and E. Shefter, *J. Org. Chem.*, **36**, 1805 (1971)]" should be deleted from footnote 14.

**V. M. Csizmadia, S. A. Houlden, G. J. Kaves, J. M. Boggs, and I. G. Csizmadia\*:** The Stereochemistry and Ultraviolet Spectra of Simple Nitrate Esters.

(The following comments of M. F. Fox are published in this space with the assent of I. G. Csizmadia: Ed.)  
Page 2281.

## The Need for Caution in Absorption Profile Resolution by Computer

The use of computers to "fit" several synthetic Gaussian (normal) curves to an electronic absorption profile can be a powerful

method of band resolution if used cautiously. A frequent result obtained consists of a set of closely overlapped individual absorption bands, e.g., as reported recently by Csizmadia, *et al.*<sup>1,2</sup> However, the use of symmetric Gaussian functions for fitting to the electronic absorption spectra of large organic molecules must be carefully examined. The resolved spectra presented in the references cited, and of many others increasingly presented in the literature, often show two asymmetric bands to be so closely overlapped that replacement by one asymmetric band would appear to be not only reasonable but probably indistinguishable.

In contrast, it has been demonstrated that the log-normal function is a better representation of component band shapes for the absorption profiles of large organic molecules.<sup>3</sup> The log-normal curve has the appearance of an asymmetric Gaussian with two different half widths, ratio  $\rho$ . For the spectra of organic molecules the best-fitted log-normal curves have  $\rho$  values lying between 1.3 and 1.5. For the charge-transfer-to-solvent spectrum of iodide in water  $\rho$  is  $\leq 1.04$ , i.e., very close to that for a Gaussian (normal) curve.

I would urge the need for caution in fitting series of symmetric functions to electronic absorption bands. Band shapes are being increasingly realized as a difficult problem. Straightforward application of symmetric functions to resolve absorption bands must either be justified or recognized as a simplistic approach.

## References and Notes

- (1) V. M. Csizmadia, S. A. Houlden, G. J. Kaves, J. M. Boggs, and I. G. Csizmadia, *J. Org. Chem.*, **38**, 2281 (1973).
- (2) S. A. Houlden, O. Meresz, and I. G. Csizmadia, *Physiol. Chem. Phys.*, **2**, 403 (1970).
- (3) D. B. Siano and D. E. Metzler, *J. Chem. Phys.*, **51**, 1856 (1969).

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**J. L. Isidor and R. L. McKee\*:** Synthesis of 2-Methylene-4-thiazolidinones.

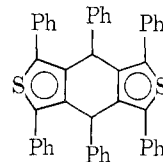
Page 3615. It is regretted that the following important references were overlooked: Satzinger, *Justus Liebigs Ann. Chem.*, **665**, 151 (1963); P. J. Taylor, *Spectrochim. Acta*, **26A**, 153, 164 (1970).

**Shinichi Motoki\* and Hiraku Satsumabayashi:** The Preparation of Diacyl Dithiosulfites.

Page 3654. Add the following to ref 2. Recently several dithiosulfites have been prepared by treatment of thiols with thionyl chloride in the presence of pyridine [L. Field and W. B. Laceyfield, *J. Org. Chem.*, **31**, 3555 (1966)].

**M. P. Cava\* and M. A. Sprecker:** Nonclassical Condensed Thiophenes. III. Studies in the Benzo[1,2-*c*:4,5-*c'*]dithiophene System.

Page 3976. In column 2, The structure for 20 should be



**S. K. Gupta:** An Exceptionally Facile Reaction of  $\alpha,\alpha$ -Dichloro- $\beta$ -keto Esters with Bases.

Page 4081. Column 2, line 22. Add the following to ref 1. The cleavage of diethyl  $\alpha$ -fluoro- $\alpha$ -carboxy succinate by  $\text{KHCO}_3$  has been recorded: F. H. Dean and F. L. M. Pattison, *Can. J. Chem.*, **41**, 1833 (1963)

**Louis de Vries:** Thermal Transformations of an Aminoalnonitrile and of an Aminocyanoketenimine. Evidence for Homolysis and Heterolysis and for Aminocyanocarbenes.

Page 4357. In the abstract, the fourth line from the bottom now reads: "Also obtained was an enaminoimine 23 which formally corresponds to the product of elimination of hydrogen cyanide from the dimer, but which may originate from insertion of the aminocyanocarbene 11 in the C-H bond of 1." The latter part of this sen-