

# 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.

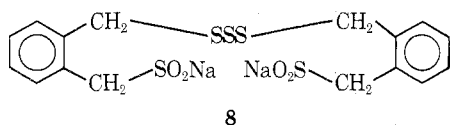
Vol. 37, 1972

**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.

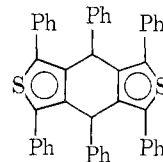
Page 3615. It is regretted that the following important references were overlooked: Satzinger, *Justus Liebigs Ann. Chem.*, **665**, 151 (1963); P. J. Taylor, *Spectrochim. Acta*, **26A**, 153, 164 (1970).

**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-

tence should read but which may originate from addition of the aminocyanocarbene 11 to the tautomeric aminocyanoketenimine form of 1.

Page 4360. In the text, column 2, the fourth paragraph now reads "The enaminoimine 23 may originate from insertion of the carbene 11 into the C-H bond of 1, as proposed earlier<sup>1</sup> for formation of 23 from 1 in triethylamine." This paragraph should read "The enaminoimine 23 may originate from addition of the carbene 11 to 2—the tautomeric aminocyanoketenimine form of 1—as proposed earlier for formation of 23 from 1 in triethylamine."

**Y. Sato,\* Y. Ban, and H. Shira:** Synthesis of *N*-(2-Triphenylsilyl)ethylamines and Their Reactivities.

Page 4376. In Table III, sixth entry, replace "Bz" by C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub> in second and fifth columns

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**M. J. Robins\* and R. A. Jones:** Nucleic Acid Related Compounds. 9. The Synthesis of 6-Amino-9-(2-deoxy-D-erythro-pent-1-enofuranosyl)purine, the First 1',2'-Unsaturated Purine Nucleoside.

Page 115. Column 1, paragraph 2, line 4. "9-(5-methyl-2-furyl)adenine<sup>3a</sup>" should read 9-(5-hydroxymethyl-2-furyl)adenine.

**W. E. Truce,\* D. L. Heuring, and G. C. Wolf:** Addition of Sulfonyl Iodides to Allenes.

Page 241. Column 1, Scheme II. The one pair of bracketed formulas in scheme II should be interchanged with the other pair.

**George L. Hardgrove, Jr.,\* J. Stuart Bratholdt, and Mary M. Lien:** The Crystal Structure of *cis*-2,4-Diphenylthietane *trans*-1-Monoxide.

Page 246. Line 3. Third author's name should read Lien (not Lein).

**Kenneth L. Marsi:** Phenylsilane Reduction of Phosphine Oxides with Complete Stereospecificity.

Page 267. Column 1, line 28. The compound used was (-)-(*S*)-menthyl methylphenylphosphinate.

Page 267. Column 1. Reference 2b should be H. Christol and H.-J. Cristau, *Ann. Chim.*, 6, 191 (1971).

**Donald J. Hart and Warren T. Ford\*:** Carbon-13 Nuclear Magnetic Resonance Spectra of Tetraalkylammonium Tetraalkylborides.

Page 365. Column 2, Table IV. Below the title and above the data in the table should be the equation  $\delta_{C^X} = A(\delta_{C^{alkane}}) + B$ .

**Joseph San Filippo, Jr.,\* and G. M. Anderson:** The Reduction of 2-Substituted 2-Halonorbornanes by Tri-*n*-butyltin Hydride.

Page 474. Table I. Footnote g should be as follows. <sup>g</sup> Taken from ref 38.

**M. P. Cava,\* H. Firouzabadi, and M. Krieger:** 1,2-Diphenylanthra[b]cyclobutadiene.

Page 480. In structure 13, the lower four-membered ring is incorrectly drawn. It should be the same as the upper four-membered ring, *i.e.*, an exomethylenecyclobutenone.

**N. C. Deno,\* K. A. Eisenhardt, D. G. Pohl, H. J. Spinnelli, and R. C. White:** Photochlorination of Alcohols.

Page 520. We wish to call specific attention here to the work of Dr. Kollonitsch and coworkers, comprising the first synthesis of chloro alcohols from alcohols by free-radical chlorination in acid media [J. Kollonitsch, G. A. Doldouras, and V. F. Verdi, *J. Chem. Soc., B*, 1093 (1967), ref 11 in our paper].

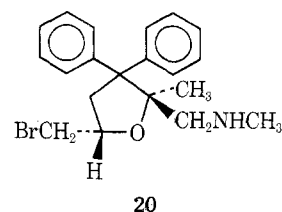
**I. Angres and H. E. Zieger:** The Reaction of Lithium Naphthalenide with Quaternary Ammonium Salts.

Page 1013. The premise "... the mole percentage of unreacted salt (Table I) is a measure of the maximum amount of carbanion formed by path B ..." cannot possibly be correct. It may be a measure of the amount of carbanion that escaped dimer formation and appeared as % RH in Table I. Consequently, the conclusion that dimer forms by both path A and path B is not supported by the data. The only evidence available indicates path B, and path A remains an undemonstrated possibility.

The % (CH<sub>3</sub>)<sub>3</sub>N for compound 3 in Table I is 81 not 18.

**Henry Wong, Jacques Chapuis, and Ivo Monkovic\*:** Stereochemical Course of Bromocyclizations of  $\gamma,\delta$ -Unsaturated Alcohols. II. Approaches to Various Oxaazabicyclooctane and -nonane Systems.

Page 1043. The structure given for 20 is erroneous; the correct structure is shown below.



20

**R. B. Nelson and G. W. Gribble\*:** Reduction of Aryl Iodides with Sodium Hydride.

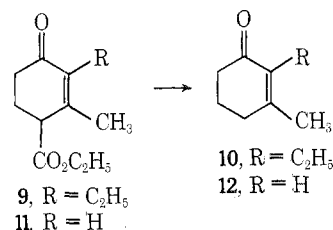
Page 1425. Column 3, Table I. The yield for conversion of *o*-iodobenzoic acid to benzoic acid should read 95%.

**Dwain M. White:** 2,5-Dicarbomethoxy-3,4-diphenylcyclopentadienone. Synthesis and Reaction with Acetylenes.

Page 1951. Reference should be made to the synthesis and characterization of the title compound and its precursor 2,5-dicarbomethoxy-4-hydroxy-3,4-diphenylcyclopenten-2-one by R. C. Cookson, J. B. Henstock, J. Hudec, and B. R. D. Whitear, *J. Chem. Soc.* 1989 (1967), and B. Eistert and A. J. Thommen, *Chem. Ber.*, 104, 3048 (1971).

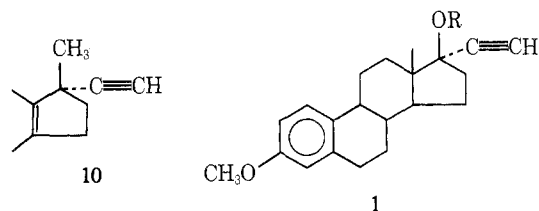
**Edward J. Parish, Naresh V. Mody, Paul A. Hedin, and D. Howard Miles\*:** Cleavage of  $\delta$ -Keto  $\beta,\alpha$ -Unsaturated Esters by 1,4-Diazabicyclo[2.2.2]octane.

Page 1593. Column 1, Scheme I. For structures 9-12 the R group was not located. Structures 9-12 should be as follows.



**Ramesh M. Kanojia,\* Linda Yarmchuck, and Irving Scheer:** Epimerization of Mestrand Acetate on Alumina.

Page 2304. Column 2. The formulas for the structures 10 and 11 are in error showing an extra methyl group at C<sub>13</sub> in 10 and at C<sub>10</sub> in 11 and should be correctly represented as follows.



**C. Wong and W. W. Paudler\*:** Synthesis and Conformation of [2.2](2,5)Furano(2,5)pyridinophane.

Page 2570. In the abstract, "C<sub>3</sub>-C<sub>4</sub>" should be N-C<sub>6</sub>, and "N-C<sub>6</sub>" should be C<sub>3</sub>-C<sub>4</sub>.

Page 2570. Column 2, Table I. The first entry should be 2 (opposite 48%); the second entry should be 1a instead of "21a" (opposite 18%).

**R. A. Hites:** Phytadienes from the Pyrolysis of Pheophytin a.

Page 2634. In our paper we indicated "It is possible that the phytadienes reported to be present in zooplankton (Blumer and Thomas, *Science*, 1965) may have been an artifact." Dr. Blumer has provided the following additional information to indicate that the zooplankton phytadienes are not artifacts: "They were isolated and resolved after cold pentane extraction from zooplankton by chromatography over deactivated silica gel, under conditions demonstrated neither to dehydrate phytol to phytadienes nor to isomerize the olefins. Thus, the proof of their presence does not hinge on exposure to gc temperatures. Where gc was used to determine amounts or to trap the olefins, it was applied to chromatographed fractions that contained neither phytol nor pheophytin or other chlorophyll derivatives. Injector temperature was at or below 200° and it was demonstrated that isomerization of the olefins did not take place."