

The Triplet State of Ethylene

D. P. Craig

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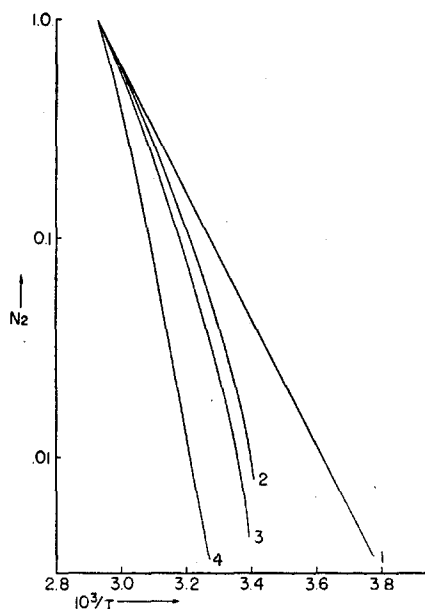


Fig. 2. Solubility of stearic acid in various organic solvents (from data of reference 8) compared with ideal solubility, curve (1).

- (1) Ideal solubility
- (2) Cyclohexane
- (3) *n*-butyl alcohol
- (4) Methyl alcohol

manner shown in Fig. 1 simplifies the discussion of these complicated systems, it leaves many phenomena still unexplained.

The writer was unable to find any solubility data of simpler compounds undergoing phase transition in the solid state, such as camphor, C_2Cl_6 , and the like, to compare with the apparently more thoroughly studied soap systems.

The writer wishes to acknowledge discussions with Professor J. W. McBain and Dr. O. Redlich, which led to this work.

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² C. W. Leggett, Jr., R. D. Vold, and J. W. McBain, *J. Phys. Chem.* **46**, 429 (1942).

³ G. H. Smith, Ph.D. Thesis, Stanford, 1946.

⁴ J. H. Hildebrand, *Solubility of Non-Electrolytes* (Reinhold Publishing Corporation, New York, 1936).

⁵ A. Bondi, *J. Phys. Chem.* **51**, 891 (1947).

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The Triplet State of Ethylene

D. P. CRAIG

University College, London, England
December 9, 1947

IN dealing with the separation between the ground and triplet states of ethylene, Laidler¹ has drawn attention to the remarkable agreement existing between the experimental value of 74 kcal. obtained by Lewis and Kasha,² and the calculated value of 72 kcal. found by Hartmann³ by the method of antisymmetrical molecular orbitals.

It is not, however, indicated in Hartmann's paper what

values were used for the various integrals that occur, and in treating the same problem by the same approximation during the course of other work, the writer has obtained a considerably greater value for the singlet-triplet separation. Using values for the integrals obtained by interpolation between the values given by Sklar and Lyddane,⁴ the singlet-triplet separation comes out to be 95 kcal. or greater, the exact value depending on the assumptions made about the configuration of the triplet state. Therefore, there is probably not the good agreement between calculated and experimental values that Hartmann's value suggests. Hartmann's value for the excited singlet state, given in the same paper, appears to be in error due to the use of a wrong wave function, and the corrected value again proves to be considerably greater than the experimental.

The values for the integrals used in these calculations are so closely in agreement with those given recently by Griffing⁵ that there is no need to quote them here.

¹ K. J. Laidler, *J. Chem. Phys.* **15**, 712 (1947).

² G. N. Lewis and M. Kasha, *J. Am. Chem. Soc.* **66**, 2100 (1944). These authors commented that Hartmann's value was improbably low.

³ H. Hartmann, *Zeits. physik. Chemie* **B53**, 96 (1943).

⁴ A. L. Sklar and R. H. Lyddane, *J. Chem. Phys.* **7**, 374 (1939).

⁵ V. Griffing, *J. Chem. Phys.* **15**, 421 (1947).

Erratum: Infra-Red Spectrum and Depolarization Factors of the Raman Lines of Spiropentane and the Raman and Infra-Red Spectra of 1,1-Dimethylcyclopropane, 1-Methylcyclobutene, and Methylene cyclobutane

FORREST F. CLEVELAND

Department of Physics, Illinois Institute of Technology,
Chicago 16, Illinois

AND

M. J. MURRAY AND W. S. GALLAWAY
Universal Oil Products Company, Chicago, Illinois

[*J. Chem. Phys.* **15**, 742 (1947)]

DUE to a faulty distillation and an oversight, the infrared spectrum of methylenecyclobutane reported in Table IV of the above paper contains spurious bands at 782, 990, 1051, and 1155 cm^{-1} , which correspond to the prominent bands of spiropentane. If these are deleted, the remaining bands are those of methylenecyclobutane. (It should also be noted that the strongest band of spiropentane is nearly coincident with the 877- cm^{-1} band of methylenecyclobutane.) The Raman data, however, were obtained with another sample which was pure enough not to show the strongest line of the spiropentane.

This correction of the experimental data necessitates the following changes in the assignments for eight of the weak bands: the combination or overtone frequencies whose values are given in the last column of Table IV as 801, 1509 or 1510, 1883, 2013, 2061 or 2063, 2118 or 2109, 2177 or 2188, 2310, and 2416 should be deleted; they may be replaced by the combination frequencies 1167-373=794, 354+1167=1521, 728+1167=1895, 954+1070=2024, 895+1167=2062, 954+1167=2121, 1029+1167=2196, and 1029+1395=2424. Thus eight of the nine carbon skeleton frequencies and eighteen of the twenty-four C-H frequencies are now tentatively assigned.