Additions and Corrections

Determination of the Heat of Reaction for the Formation of Diphenylcarbene from Diphenyldiazomethane Using Photoacoustic Calorimetry [*J. Am. Chem. Soc.* **1983**, *105*, 5156]. JOHN D. SIMON and KEVIN S. PETERS*

In this publication we reported that the enthalpy change for the reaction $Ph_2CN_2 \rightarrow {}^3Ph_2C: + N_2$ is $\Delta H = -12 \pm 2$ kcal/mol. This number is in error due to reaction of diphenylcarbene with oxygen. Using time-resolved photoacoustic calorimetry (Rudzki, J. E.; Goodman, J. L.; Peters, K. S. *J. Am. Chem. Soc.* **1985**, *107*, 7849) we have been able to resolve the kinetics of triplet carbene formation from triplet carbene reaction with oxygen. The enthalpy change for $Ph_2CN_2 \rightarrow {}^3Ph_2C: + N_2$ in benzene is $\Delta H = 0 \pm 1.7$ kcal/mol. This value represents a lower limit as the volume of expansion due to dissociation has not been taken into account.

Computer Software Reviews

NBS Mass Spectral Database. PC Version 1.02 (Database 1-A). Program by Dr. Stephen E. Stein, National Bureau of Standards, Office of Standard Reference Data, Building 221, Room A-325, Gaithersburg, MD 20899. List Price $750.00.

In the fall of 1973 the first version of the Mass Spectral Search System (MSSS) was made publicly available to the scientific community on the General Electric Mark III computer network.[1] At that time it consisted of slightly under 9000 non-unique spectra and required a large timesharing system to store the database and programs. Now, some 15 years later, the database has increased to about 44 000 unique spectra, and the entire system can be searched almost as quickly and flexibly on an IBM PC as it was searchable on that million dollar computer system.

The National Bureau of Standards (NBS), Office of Standard Reference Data (OSRD) has created an excellent and inexpensive source of mass spectral data and search software for the scientific community. The NBS MS system is well designed to serve the researcher who needs access to a large mass spectral database for spectral identification or as an aid in structure determination of an unknown from mass spectral data. It is also a very useful tool for the classroom, both for a course on mass spectrometry or spectral interpretation as well as for any course in organic chemistry.

The details of the database have been described previously[2-4] and consist of about 44 000 EI (electron impact) only spectra. Each spectrum has a complete list of masses (m/z values) and intensities, a chemical name (only the first 25 characters) for searching as well as a display option for showing synonyms, molecular formula (and partial formula), molecular weight, CAS Registry Number, source of the spectrum, and a Quality Index (QI) assigned to the spectrum.[5] Regular updates of the database, which will consist of additional spectra as well as replacing existing spectra with higher quality data are planned. At present users cannot add their own spectra to the database.

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Species. 1-DECENE, Formula  C10H20
Contributor: CONTINENTAL OIL CO., PONCA CITY, OKLA, USA

ID# 5834  CAS# 872059     EPA# 34716   Source APM  MW 140   Qual Index 673

Ten Largest Masses and Abundances
41      56      55      43      70      57      29      69      27      39
999     821     807     769     691     616     571     525     495     428

65  Masses and Abundances
26  34    51  25    68  100   86  3     141 11
27  495   52  15    69  525   88  1
28  113   53  100   70  691   91  3
29  571   54  138   71  97    95  4
30  13    55  807   72  4     96  24
37  6     56  821   77  14    97  213
38  18    57  616   78  4     98  169
39  428   58  27    79  13    99  13
40  70    62  1     80  3     110 7
41  999   63  4     81  25    111 83
42  353   64  1     82  66    112 65
43  769   65  14    83  378   113 5
44  26    66  9     84  270   125 2
50  10    67  85    85  50    140 103
                    Press any key to return to list
```

Figure 1.

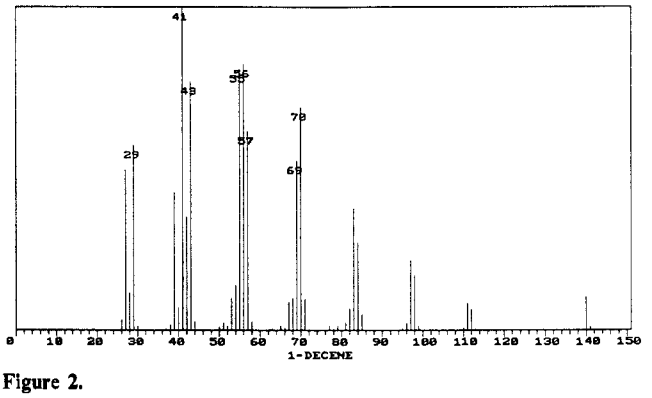

Figure 2.

The search software, written in C (although that is really irrelevant as the user never gets near the actual source code), is almost as flexible and extensive as the same database and search system which is currently available on a number of commercial timesharing systems. The menus are easy to use, and the help messages are indeed helpful. One can search the database by ID number (an internal numbering system code found on each spectrum), by the CAS Registry Number, by the chemical name (using only the first 25 characters, but since very few of us can type more than 25 characters of a chemical without making an error this does not

(1) Heller, S. R.; McGuire, J. M.; Budde, W. L. *Environ. Sci. Technol.* **1975**, *9*, 210.

(2) Heller, S. R.; Milne, G. W. A. *EPA/NIH Mass Spectral Data Base*, in five volumes, part of the National Standard Reference Data Series of Critical Data Compilations (GPO SN 003-003-01987-9, NSRDS-NBS 63, 4634 pages, U.S. Government Printing Office: Washington, 1978 and reprinted in 1980).

(3) Heller, S. R.; Milne, G. W. A. *EPA/NIH Mass Spectral Data Base*; Supplement Number One, in two volumes, part of the National Standard Reference Data Series of Critical Data Compilations (GPO SN 003-003-02268-3, NSRDS-NBS 63, Suppl. 1, 2151 pages, US Government Printing Office: Washington, December 1980).

(4) Heller, S. R.; Milne, G. W. A.; Gevantman, L. H. *EPA/NIH Mass Spectral Data Base*; Supplement Number Two, in two volumes, part of the National Standard Reference Data Series of Critical Data Compilations (GPO SN 003-003-02268-3, NSRDS-NBS 63, Suppl. 2, 1110 pages, U.S. Government Printing Office: Washington, 1983).

(5) Dillard, J. G.; Heller, S. R.; McLafferty, F. W.; Milne, G. W. A.; Venkataraghavan, R. *Org. Mass Spectrom.* **1981**, *16*, 48-49.