This Week's Citation Classic

CC/NUMBER 23
JUNE 4, 1979

Johnson C E, Jr. & Bovey F A. Calculation of nuclear magnetic resonance spectra of aromatic hydrocarbons. *J. Chem. Phys.* **29**:1012-4, 1958.
[Minnesota Mining and Manufacturing Co., Central Research Lab., St. Paul, MN]

Pauling's free electron model is used to calculate the magnetic field around a benzene ring which is tumbling rapidly about all axes in a magnetic field. It is assumed that the electrons precess in two circular paths, one on each side of the benzene ring, with radii equal to the C-C distance in a benzene ring. Separation of these rings is taken at 1.28 A, which gives a calculated value for the nuclear magnetic resonance shielding for benzene protons equal to the observed. [The *SCI*® indicates that this paper has been cited over 805 times since 1961.]

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July 25, 1978

"Both Dr. Frank A. Bovey and I are honored to be most-cited authors.' This paper was an anomaly for me since I am a magnetics physicist. Bovey, my co-author, suggested the analysis and, particularly, to make available a complete set of tables for future investigators.

"Two interesting incidents occurred with this paper. First of all, the 3M Company had, at the time of the research work, only an IBM 705 computer which was geared strictly for accounting use. We "bootlegged' time on this computer during evenings and weekends after all of its accounting duties were completed. We used an assembly language called PRINT-1, which IBM had generated for this machine. Remember, this was back in the days before FORTRAN. The execution times of this computer seem incredibly lethargic when compared to presentday computers. For example, a multiplication instruction took something on the order of 25 milliseconds! Nonetheless, we were able to generate the tables over a period of several weeks because of a paper by Bartky which presented a rapidly converging iterative method of evaluating elliptic integrals.[1] Using 'standard' iterative techniques for these integrals would have made the project impossibly time consuming.

"We had another interesting experience after publication of this paper in comparing our results with those of Waugh and Fessenden.[2] In the paper an error crept in, evidently, as I remember it, from the confusion between rationalized MKS units and CGS units. This mathematical error was later corrected by Waugh.[3]

"All in all, this paper was an interesting experience in the use of a large digital computer designed for business accounting purposes to solve a physical problem using iterative techniques, the thing that digital computers are especially well suited to do. While others had addressed the problem before, we, evidently, were the first to make detailed tables and graphs available. It is probably the availability of the shielding tables which make this paper so useful. Bovey, who is now at Bell Telephone Laboratories in Murray Hill, New Jersey, tells me that our tables are 'still in wide use.' "

1. **Bartky W.** Numerical calculation of a generalized complete elliptic integral. *Rev. Mod. Phys.* **10**:264-9, 1938.
2. **Waugh J S & Fessenden R W.** Nuclear resonance spectra of hydrocarbons: the free electron model. *J. Amer. Chem. Soc.* **79**:846-9, 1957.
3. **Waugh J S & Fessenden R W.** Nuclear resonance spectra of hydrocarbons: the free electron model. *J. Amer. Chem. Soc.* **80**:6697-99, 1958. Correction submitted by J.S. Waugh (3 June 1958).