

Whitten J L. Gaussian lobe function expansions of Hartree-Fock solutions for the first-row atoms and ethylene. *J. Chem. Phys.* 44:359-64, 1966.  
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Gaussian expansions of ground-state Hartree-Fock solutions for the first-row atoms and the ethylene molecule are constructed from a basis designed primarily for molecular calculations which consists only of groups of functions of the form  $\exp(-ar^2)$ . Angular dependence is achieved by defining origins at different points in space. [The SCI® indicates that this paper has been cited in over 385 publications since 1966.]

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"The work has a curious history and it was only by the barest of margins that the article was even published. It had the simplest of beginnings. When I was a graduate student at Georgia Tech I read a footnote in a book on quantum chemistry by Daudel, Lefebvre, and Moser commenting negatively on a theoretical method of using Gaussian functions to construct electronic wavefunctions.<sup>1</sup> From the references, however, I could see that there were other ways of proceeding that had not been tried. I was working on a thesis project at the time, but my adviser, William H. Eberhardt, encouraged me to take up the wavefunction investigation as a sideline. With his help and constructive criticism, in a short time the work resulted in my first publication.<sup>2</sup> Partly on the promise of this research, I obtained a postdoctoral position at Princeton University with Leland Allen. Allen urged me to continue the Gaussian work and provided valuable suggestions on what it would take to make the Gaussian lobe function approach, as I called it, competitive with other methods.

"Another postdoctoral fellow, Allen Wasserman, and I were given the choice of a crowded room in the Frick Chemical Laboratory or moving in with the crystallographers in an old wooden building resembling an auto repair shop. We chose the lat-

ter with its redeeming features of individual offices, flowering vines, a Ping-Pong table, and a talkative janitor. In about a year I wrote my second paper, the reference cited.

"The paper was not an overwhelming success. The reviewer, who was clearly knowledgeable, listed five objections and wrote in summary, [The paper] adopts a useless point of view in molecular calculations. It should be compressed as a "curiosity note." Do not publish as a paper.' I responded instead by adding an applications section, and sending the paper back. This time there was no objection to the paper (by a different reviewer), but the reviewer left blank the category concerning the possible significance of the work.

"The paper was accepted and published by the *Journal of Chemical Physics*, computer programs were written, and a period of intensive activity began at Princeton. Allen, Bob Buenker, and Sigrid Peyerimhoff all contributed significantly to this stage of the work, and independently carried out an impressive series of molecular studies.<sup>3</sup>

"Why were people interested in this paper? Its significance was that it allowed the rapid development of electronic structure programs by persons independent of the established centers which were Slater function and diatomic molecule oriented. There is a pleasing simplicity to the idea of using only spherical Gaussians, recognized in some respects even earlier by Preuss in Germany.<sup>4</sup> In computer terms it is the question of a simple algorithm vs. a more complicated but possibly more efficient one. Also of interest was the selection of sets of Gaussian functions as the conceptual entities as opposed to the use of individual Gaussians or large-size atomic orbital expansions. This idea also met with objections at the time, but it is now common in Gaussian expansion work. In 1982, Gaussian lobe functions offer advantages primarily for developmental work in new directions; for standard molecular applications Cartesian Gaussians have proved more efficient.<sup>5</sup> A resurgence in the use of lobe functions must await specialized algorithm circuits for electronic computers."

1. Daudel R, Lefebvre R & Moser C. *Quantum chemistry: methods and applications*. New York: Interscience, 1959. 572 p.

2. Whitten J L. Gaussian expansion of hydrogen-atom wavefunctions. *J. Chem. Phys.* 39:349-52, 1963.

3. Peyerimhoff S D, Buenker R J & Allen L C. Geometry of molecules. I. Wavefunctions for some six- and eight-electron polyhydrides. *J. Chem. Phys.* 45:734-49, 1966.

4. Preuss H. Bemerkungen zum Self-consistent-field-Verfahren und zur Methode der Konfigurationenwechselwirkung in der Quantenchemie. *Z. Naturforsch.* 11:823-31, 1956.

5. Schaefer H F, III, ed. *Methods of electronic structure theory*. New York: Plenum Press, 1977. 462 p.