

This Week's Citation Classic

Huzinaga S. Gaussian-type functions for polyatomic systems. I. *J. Chem. Phys.* **42**:1293-1302, 1965.

[IBM San Jose Research Lab., San Jose, CA]

This paper reported the first comprehensive compilation of the Gaussian-type orbitals (GTO) to be used for polyatomic molecular calculations. Assessment of relative merit of Slater-type orbitals (STO) and GTO was attempted and a cautious optimism for GTO was expressed, which has been substantiated far beyond the original expectation. [The **SCI**[®] indicates that this paper has been cited over 1,065 times since 1965.]

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"In 1959 I was invited to join the so-called Chicago group (or Chicago gang?) under R.S. Mulliken and C.C.J. Roothaan. On my way from Japan to Chicago, I attended the Boulder Conference on Molecular Quantum Mechanics (held at the University of Colorado, June 21-27, 1959), one of the most memorable conferences on quantum chemistry. During my two year (1959-1961) stay at the physics department of the University of Chicago, I was lucky enough to witness, on the spot, the monumental outburst of computational quantum chemistry. Upon my arrival, I inherited kitchen utensils from W. Kolos who was about to leave Chicago after finishing his work on H₂ with Roothaan. S. Fraga and B. Ransil were working on their diatomic molecule calculations using minimum STO basis sets. D. McLean and M. Yoshimine were senior students and C. Wahl and W. Huo joined as young students. I shared a small room with R. Moccia and E. Clementi. The whole atmosphere was almost toxic when it came to the excitement and the bubbling enthusiasm at the dawn of an era of real *ab initio* molecular calculations.

"Mulliken seemed never to be interested in that infectious fascination (love and hate) of computer programming which trapped everybody else including, of course, Roothaan. It was, however, Mulliken who urged me to explore the future potential of GTO as an alternative to then-prevalent STO. Quite possibly, he foresaw the serious difficulty of computing three- and four-center molecular integrals over STO which are necessary for non-linear polyatomic molecules.

"My work on GTO which is described in the present paper came into fruition during my one-year stay at the IBM San Jose Laboratory in 1963-1964. E. Clementi was building a computational quantum chemistry group, and he was engaging in his gigantic effort of preparing analytic Hartree-Fock-Roothaan solutions for atoms covering He through Xe. Compared to Clementi's STO project, my atomic calculation project based on GTO was miniature in size, but it would have been impossible to complete without Clementi's substantial support, both moral and financial. The presence of R.K. Nesbet at the IBM San Jose Laboratory was also a source of encouragement for my work. Nesbet is one of the pioneers in the use of GTO for molecular calculations.¹

"At the time of the publication of the present paper, the *ab initio* molecular calculation was still in its infancy. It was difficult to predict precisely the future status of GTO in relation to STO. During these 15 years, however, GTO has established an overwhelmingly superior position to STO as far as *ab initio* calculations on non-linear polyatomic molecules are concerned.^{2,3}

"Frequent citations to the present paper merely reflect the spectacular growth of activities in the field of computational quantum chemistry."

1. Nesbet R K. Ground state electronic wave function of methane. *J. Chem. Phys.* **32**:1114-22, 1960.
2. Richards W G, Walker T E H, Farnell L & Scott P R, eds. *Bibliography of ab initio molecular wave functions. Supplement for 1970-1973.* Oxford: Clarendon Press, 1974. 358 p.
3. Richards W G, Scott P R, Colbourn E A & Marchington A F, eds. *Bibliography of ah initio molecular wave functions. Supplement for 1974-1977.* Oxford: Clarendon Press, 1978. 526 p.