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Citation Classics

Stewart R F, Davidson E R & Simpson W T. Coherent x-ray scattering for the hydrogen atom in the hydrogen molecule. *Journal of Chemical Physics* **42**: 3175-87, 1965.

The authors calculate the x-ray form factors for a bonded hydrogen in the hydrogen molecule for a spherical approximation to the bonded atom. [The *SCI*® indicates that this paper was cited 1879 times in the period 1965-1975.]

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"This particular paper was written in response to a recognized need. It contains a table of X-ray scattering factors appropriate for a bonded hydrogen atom. This table has been incorporated in most standard X-ray crystallography computer packages and generates an 'automatic' citation each time a new crystal structure containing a hydrogen atom is solved. The popularity of this table was greatly enhanced by the fact that R.F. Stewart is a crystallographer who at that time had a joint post-doctoral appointment with W.T. Simpson and L. Jensen. Consequently the table was generated in a format which could be readily incorporated in the standard crystal programs, and it was put to immediate use at the University of Washington.

"This paper was, in a sense, a finishing touch to a sequence of more fundamental papers. A few years previously Kolos and Roothaan[1] had generated an improved James and Coolidge-type wavefunction for the hydrogen molecule. Also Löwdin[2] had introduced the concept of natural orbitals and Shull and Löwdin[3] had showed their utility for understanding simpler wavefunctions for the hydrogen molecule. Finally Davidson[4] had developed a method for converting the James and Coolidge-type wavefunctions to natural orbital form and Davidson and Jones[5] had published the natural orbital expansion of the Kolos and Roothaan wavefunction. From the natural orbital expansion an accurate charge density for the molecule could be constructed. The fundamental conceptual problem remaining in calculating the X-ray scattering factors was how to partition the molecular charge density into the sum of two 'atomic' charge densities. In addition there was the difficult numerical problem of performing the Fourier transform of the atomic density in confocal elliptical co ordinates, which was solved by R.F. Stewart following suggestions of Dr. George Hufford. After many false starts, the partitioning problem was finally solved in an elegant manner by showing the connection between a best least-squares fit to the density in coordinate and momentum space."

1. **Kolos W & Roothaan C C J.** Accurate electronic wave functions for the H_2 molecule. *Reviews of Modern Physics* **32**:219-32, 1960.
2. **Löwdin P O.** Quantum theory of many-particle systems. I. Physical interpretations by means of density matrices, natural spin-orbitals, and convergence problems in the method of configurational interaction. *Physical Review* **97**: 1474-89, 1955.
3. **Löwdin PO & Shull H.** Natural orbitals in the quantum theory of two- electron systems. *Physical Review* **101**:1730-9, 1956.
4. **Davidson E R.** Natural expansions of exact wave functions. I. Method. *Journal of Chemical Physics* **37**:577-81, 1962.
5. **Davidson E R & Jones L L.** Natural expansion of exact wave-functions. II. The hydrogen molecule ground state. *Journal of Chemical Physics* **37**:2966-71, 1962.