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This Week's Citation Classic

Kolos W & Wolniewicz L. Potential-energy curves for the $X\ ^1\Sigma_g^+$ + $b^3\Sigma_u^+$, and $C^1\Pi_u$ states of the hydrogen molecule. *J. Chem. Phys.* **43:**2429-41, 1965.
[Lab. Molecular Structure and Spectra, Dept. Physics, Univ. Chicago, Chicago, IL]

Accurate potential energy curves have been computed for the ground state and for two excited states of the hydrogen molecule including the region of the van der Waals interaction. For the ground state, accurate expectation values of several operators have also been calculated as functions of the interatomic distance. [The ***SCI***® indicates that this paper has been cited over 480 times since 1965.]

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"In December 1957 I joined, for the first time, the famous Laboratory of Molecular Structure and Spectra (LMSS) at the University of Chicago, directed by R.S. Mulliken and C.C.J. Roothaan. It was just the beginning of the computer era and two important projects were under way in LMSS: one aimed at very accurate results for simple atoms, and another at Hartree-Fock, i.e., approximate, results for diatomic molecules. It was under these circumstances that I decided to start a new project which would be a hybrid of those two. It was meant to compete in accuracy with the first, and to take the object of the study, the hydrogen molecule, from the second. Two papers[1,2] containing the first results obtained within this project were soon followed by many papers dealing with excited states of H_2, reporting values of various properties of the molecule, or increasing the accuracy of previous results. A large part of the whole project was carried out in collaboration with L. Wolniewicz whose contributions to the development of the theory, to programming, and to computations were most essential. On the nonhuman level very essential for the completion of the work were the excellent, at the time, computing facilities offered by the University of Chicago.

"Why has this particular paper become a *Citation Classic?* I see several reasons which could have had a cumulative effect. The hydrogen molecule is *per se* an interesting object frequently studied experimentally in many laboratories. It also represents a favourite testing ground for new theoretical methods. In addition, the paper deals with two very important states, viz., those that arise from two ground state hydrogen atoms. The most essential factor, however, that promoted our work to a classic paper was definitely our following Roothaan's principle: 'If something is worth doing, it should be done right.' Therefore, like our colleagues at LMSS, we tried to push the theory, the programs, and the computations to the limit, and this apparently extended the lifetime of our results. Some of the numbers and curves published in the paper have been improved.[3-5] Some, however, represent still the best available data for the hydrogen molecule."

1. **Kolos W & Roothaan C C J.** Correlated orbitals for the ground state of the hydrogen molecule. *Rev. Mod. Phys.* **32**:205-10, 1960.
2. .....Accurate electronic wave functions for the H2 molecule. *Rev. Mod. Phys.* 32:219-32, 1960.
3. **Kolos W & Wolniewicz L.** Variational calculation of the long-range interaction between two ground state hydrogen atoms. *Chem. Phys. Lett.* **24:**457-60, 1974.
4. .....Improved potential energy curve and vibrational energies for the electronic ground of the hydrogen molecule. *J. Mol. Spectrosc.* **54**:303-11, 1975.
5. **Kolos W & Rychlewski J.** *Ab initio* potential energy curves and vibrational levels for the C and D states of the hydrogen molecule. *J. Mol. Spectrosc.* **62**:109-21, 1976.