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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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. Some, however, represent still the best available data for the hydrogen molecule.