

### FIGURE B.1

Prof. Clemens Roothaan (1918) was born in the Netherlands but came to the University of Chicago in the United States in 1949. His 1951 paper in *Rev. Mod. Phys.* **23**, 69–89 (1951) deriving the self-consistent-field equations in a LCAO basis set was the most highly cited paper between 1945 and 1954. He was director of the Computation Center of the University of Chicago from 1962 to 1968; this photo was taken in October of 1962. In the 1970s, he remained far ahead of others in writing an efficient MCSCF (multi-configurational-SCF; simultaneously optimizing more than one determinant) program with his student John Detrich and other students so that his group was at least 10 years ahead of other developments. Prof. Roothaan's many honors include a Guggenheim Fellowship in Physics (Cambridge University, 1957); election to The International Academy of Quantum Molecular Science in 1967; named the Louis Block Professor of Physics and Chemistry, the University of Chicago (still Emeritus Title); and honored by a special session in honor of Clemens' 70th birthday in 1988 at the International Symposium on the Electronic Structures and Properties of Molecules and Crystals, Rudor Boskovic Institute Zagreb, Cavtat, Yugoslavia. Today he continues to serve as a consultant to IBM in the development of the Itanium processor. See also <http://pubs.acs.org/cen/science/science2001.html> for an interview.



