Methods in Computational Chemistry, Volume 2: Relativistic Effects in Atoms and Molecules. Edited by Stephen Wilson. Plenum Press, New York, 1988, xiv + 291 pp., $55.

This book is the second in a series of specialist reviews of methods and algorithms and aims to "provide a broad-ranging yet detailed analysis of contemporary theories, algorithms and computational techniques." This volume on relativistic effects is uneven in its fulfillment of these aims. The review is written from the standpoint of a knowledgeable quantum chemist, but one whose area of expertise is not relativistic effects.

The book has chapters on atomic, molecular, effective core potential, semiempirical, and many-body perturbation calculations and methods. A very useful chapter on semiempirical molecular methods (Pekka Pyykko, University of Helsinki) comes with an MS-DOS floppy disk and listing for Extended Huckel calculations. Although the discussion concentrates on EH, the low-reliability method is put in its proper context with respect to other semiempirical techniques, with a large number of references.

Odd Gropen (University of Tromso) contributed the chapter on relativistic effective core potentials, with a general discussion of the methods proposed for their calculation and a cursory review of the literature. The discussion is fairly complete and, as such, makes a useful introduction to the topic and to method selection, but it is not detailed enough to go beyond that level. There is no discussion of codes available for these methods.

Harry Quiney's (Oxford University) chapter on relativistic many-body perturbation is a solid disucssion of the theory and its implementation concerns and strategies. The chapter should prove useful to chemists interested in understanding computational results.

Ian P. Grant's (Oxford University) contribution on atomic calculations is, to my mind, the best chapter in the book. It has a thorough description of the methods in use and, most important, their implementation. The chapter comes with a large number of references, despite the fact that it does not attempt to review the extensive literature on relativistic atomic results.

Stephen Wilson's (Oxford University) discussion of molecular calculations is too general to be of use to either specialists or readers interested in understanding the topic. In particular, its treatment of the methods available for introducing electron correlation effects in molecular calculations is disappointing in that it concentrates on many-body perturbation theory (which has a better chapter of its own) and does not present it in a satisfactory context. It would have been useful to see a discussion of electron correlation methods and their implementation bottlenecks.

In all, the book may be a useful addition to the library of researchers and graduate students interested in relativistic atomic, Extended Huckel, and molecular many-body perturbation calculations, and less so (or in conjunction with other reviews) for those interested in relativistic effective core potential calculations.

Nora H. Sabelli
University of Illinois at Urbana-Champaign
Urbana, Illinois 61801

Addendum

Dr. P. Macheras' name was inadvertently omitted from the list of Reviewers for *Pharmaceutical Research* (1989).