

Methods in Computational Molecular Physics

edited by

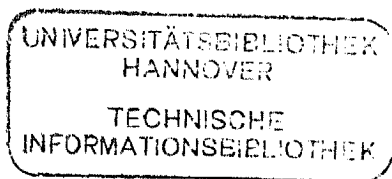
G. H. F. Diercksen

Max-Planck-Institute for Physics and Astrophysics,
Garching, West Germany

and

S. Wilson

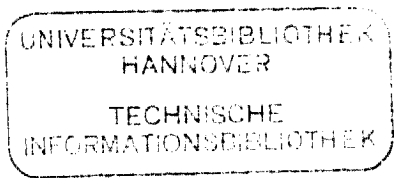
University of Oxford, Theoretical Chemistry Department,
Oxford, U.K.



D. Reidel Publishing Company

Dordrecht / Boston / Lancaster

Published in cooperation with NATO Scientific Affairs Division



RN 2937 (113)

CONTENTS

Preface	vii
MOLECULAR INTEGRALS FOR GAUSSIAN TYPE FUNCTIONS V.R. Saunders	1
ON THE EVALUATION OF EXPONENTIAL (SLATER) TYPE INTEGRALS E. Otto Steinborn	37
BASIS SETS S. Wilson	71
MATRIX EIGENVECTOR METHODS Ernest R. Davidson	95
GROUP THEORY APPLIED TO CI METHODS B.T. Sutcliffe	115
THE MULTICONFIGURATIONAL (MC) SCF METHOD Björn O. Roos	161
THE DIRECT CI METHOD Per E.M. Siegbahn	189
PAIR CORRELATION THEORIES R. Ahlrichs	209
ON A GREEN'S FUNCTION METHOD FOR THE CALCULATION OF IONIZATION SPECTRA IN THE OUTER AND INNER VALENCE REGION W. von Niessen, J. Schirmer, and L.S. Cederbaum	227
INTRODUCTORY POLARIZATION PROPAGATOR THEORY Jens Oddershede	249
DIAGRAMMATIC MANY-BODY PERTURBATION THEORY S. Wilson	273
SCHRÖDINGER SPECTRA P.W. Langhoff	299

COMPUTERS AND COMPUTATION IN MOLECULAR PHYSICS G.H.F. Diercksen, N.E. Grüner, and J. Steuerwald	335
PARTICIPANTS	351
INDEX	361