THE DEVELOPMENT OF QUANTUM CHEMISTRY CODES

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The Cambridge Analytic Derivatives Package (CADPAC) has continued to be developed as a Computational Chemistry Package, in line with the grant proposal. During the period of this report the following extensions have been made.

(i) Evaluation of third and fourth derivatives of the SCF energy.

(ii) Evaluation of fourth order force constants for MP2 theory.

(iii) The development of the theoretical spectroscopy package SPECTRO.

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Full Period of Grant June 1 1990 - August 31 1993
Title of Grant "The Development of Quantum Chemistry Codes"

Over the entire period of the grant, we have continued to develop our Quantum Chemistry Code, CADPAC.

The specific advances for the period 1 March 1991 - 31 October 1992 are concerned with theoretical spectroscopy.

(i) The development of a code which calculates analytically the third and fourth derivatives of the Self Consistent Field Energy. This is the first such code.

(ii) The development of a code which calculates by central finite differences third and fourth order force constants for the correlated Møller-Plesset second order MP2 method.

(iii) The development of a code, SPECTRO, which accepts the force fields generated in (i) and (ii), and delivers spectroscopic constants such as anharmonic constants, fundamental frequencies and vibration-rotation interaction constants.

Dr. A. Willets, partially funded by this AFOSR grant, have been actively involved with all aspects of this project. Attached is a list of scientific papers which have been published in connection with these developments of CADPAC.

150. SPECTRO - a program for the derivation of spectroscopic constants from provided quartic force fields and cubic dipole fields. J F Gaw, A Willetts, W H Green and N C Handy, Advances in Molecular Vibrations and Collision Dynamics. ed. J M Bowman, JAI, Greenwich CT, 1B,169-185 (1991).

153. Higher Analytic Derivatives. (1) A new implementation for the third derivative of the SCF energy. S M Colwell, D Jayatilaka, P E Maslen, R D Amos and N C Handy. Int J Quant Chem. 40, 179 (1991).

168. Anharmonic Vibrational Properties of CH_2F_2: A comparison of theory and experiment. R.D. Amos, N.C. Handy, W.H. Green, D. Jayatilaka, A. Willetts and P. Palmieri. J.Chem. Phys. 95, 8323 (1991)

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179. Higher Analytic Derivatives (3) Geometrical Derivatives of the Dipole and Dipole Polarisabilities. D. Jayatilaka, P. E. Maslen, R. D. Amos, and N. C. Handy. Molec. Phys. 75, 271 (1992)

186. Higher Analytic Derivatives IV. Anharmonic Effects in the Benzene Spectrum. P. E. Maslen, N. C. Handy, R. D. Amos and D. Jayatilaka . J. Chem. Phys. 97, 4233 (1992)