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AB INITIO CD SPECTRA CALCULATIONS

It's clearly not the job of hardware specialists to talk about structural information obtained by CD (or ORD), since only the experimental aspects are our duties.
However we cannot neglect the theoretical studies to assign molecular absolute configuration which always played a relevant role; while many groups have been involved in this fascinating area, the current trends clearly indicate a substantial expansion in these activities.
While the practical measurement extension to NIR and IR ranges is further stimulating this sort of research (VCD and ROA spectra are in this sense ideal since rich of many sharp bands) computer technology and software development have been by sure faster and more impressive than any instrumental progress in these years.

When we talk of small or relatively small molecules (the *classical* organic chemistry favorite old field for chiral techniques), computational methods are now supported by a few software packages which make life somehow easier:

- Gaussian 03 which is available also under Windows environment and it's moderately priced for academia (www.gaussian.com)
- Dalton a free of charge package running under Linux (www.kjemi.uio.no/software/dalton)
- Turbomole from Univ. of Kalsruhe, under Linux (www.turbomole.com)
- Cadpac from Univ. of Cambridge (www-theor.ch.cam.ac.uk/software/cadpac.html)

Groups involved are many: names as Prof. Stephens[1] [2] [3] (Southern California Univ.), Polavarapu[4] [5] (Vanderbilt Univ.), Beratan[6] (Duke Univ.), Rosini[7] (Potenza Univ.), …… are well known.

Most of the practical applications of CD are however related to large biomolecules such as peptides and proteins. The interpretation of protein CD UV spectra is still mainly based on empirical methods[8] [9], here too however *ab initio* calculations start to play a relevant role, often combined with more classical methods, such as the classical Schellman matrix method[10]. A program based on the dipole interaction model of Applequist[11] [12] [13] can be downloaded from www.public.iastate.edu/jba . This program (CaPPS) enables to calculate the UV absorption and CD spectra and runs on a Unix system with f90 Fortran compiler.
Several other groups are involved in this field[14] [15] [16] [17] [18] [19] [20] and good news have to be expected.

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