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Simulations of the Raman Optical Activity of Peptides

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Raman optical activity (ROA) provides important information about molecular structure, stereochemistry and conformation. Thus peptides are natural target molecules for this technique. However, the interpretation of the spectra is almost entirely dependent on *ab initio* simulations, which imposes limits on molecular size and overall accuracy.

Computation of ROA is a difficult and complex process. Molecular force fields and polarizability tensors have to be calculated accurately. Currently only a slow finite difference methods can be used for evaluation of the tensors. Moreover, an origin dependence of magnetic perturbation involved in ROA has to be overcome. For peptides, another complication arises from their strong interaction with the solvent. Thus the usual vacuum-based procedures are inadequate.

Nevertheless, many of these obstacles can be overcome using suitable models and approximations. These include simplified models of the polarizabilities[1-2] and transfer of molecular tensors.[3] Currently we explore the potential of the continuum solvent models for the simulations.

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