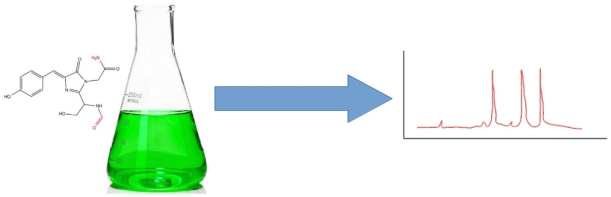
A computational protocol for calculation of IR and Raman spectra for solvated systems

Karen Oda Hjorth Dundas[a], Maarten Beerepoot[a], Magnus Ringholm[a,b], Simen Reine[c], Bin Gao[a], Radovan Bast[d], Kenneth Ruud[a] and Jógvan Magnus Haugaard Olsen[a]

[a]*Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, UiT - The Arctic University of Norway,* [b]*Department of Theoretical Chemistry and Biology at KTH Royal Institute of Technology* [c]*Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, University of Oslo*, [d]UiT - The Arctic University of Norway
karen.o.dundas@uit.no

The combination of focused polarizable embedding methods[1] with purely analytical solutions of quasi-energy derivatives[2] is a powerful tool for accurately calculating spectroscopic properties of molecules embedded in large and complex molecular environments. It thus opens a path for determining a wide range of properties for both biomolecules and general solutions. We here present a protocol for how to determine IR and Raman spectra for molecules in solution, with main emphasis on the quantum chemistry program LSDalton[3, 4] and software libraries FraME[5], which handles the polarizable embedding part, and OpenRSP[6, 7], which determines the analytical quasi-energy derivatives.



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