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Vibrational Circular Dichroism as a probe of the structure of crystals

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Vibrational circular dichroism (VCD) is the tiny difference in absorption between right- and left-circular polarised light in the infrared range for a chiral molecule. Besides its use for determining absolute configurations of chiral molecules,(1) it is a very subtle probe of molecular conformations, aggregation, and interactions with the solvent.(2-3)

Although VCD has been mostly applied so far to species in solution, recent theoretical advances now allow obtaining reliable spectra also in the solid phase.(4-5) There, the sensitivity of VCD to structural factors makes it a good probe of the crystal structure, in particular polymorphism that plays a major role in pharmaceutical sciences. We present here recent results on the interpretation of VCD spectra crystal of alcohols or diols in the solid state. We show that the crystal symmetry influences the non-local contributions to the VCD spectrum, which strongly modify its shape. Finally, we will show how VCD spectra can be taken as a signature of the formation of co-crystals between a chiral anti inflammatory drug, Naproxen, and an amino-acid.

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