# Application of Raman and IR Spectroscopy in Pharmaceutical Development

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Fourier Transformed Infrared (IR) and Raman Spectroscopy are important tools for the solid state characterization of pharmaceutical solids and for the identification of their chemical structures. We apply both methods always in combination with other methods for solid state characterization of pharmaceutical solids (e.g. X- ray powder diffraction, DSC, TG). But today we would like to focus only on Raman and IR spectroscopy. Five examples are shown which illustrate the advantages and disadvantages of both methods and also some limitations for the characterization of polymorphism and the detection in drug product.
The 1st example shows the identification of three different polymorphs of a drug substance by IR and Raman in comparable quality since this compound is highly active for IR and Raman spectroscopy. Both methods are also suitable for the detection of the polymorphic form in the tablet.
The 2nd example shows limits of the detection of hydrates by Raman spectroscopy whereas by IR spectroscopy the hydrate can nicely be differentiate from the anhydrous form.
The 3rd example shows how important spectroscopic methods during the polymorph screening are. A new crystalline form found during crystallization experiments at about 50°C could be identified as a chemically different substance, namely the precursor of the synthesis by IR spectroscopy.
The 4th and 5th example show the advantage of Raman spectroscopy for the identification of toxic substances by measurements through glass bottles, for the identification of very low quantities in a drug product (0.4 % and 1%), and for the identification of metastable forms by direct measurements in suspensions or crystallization vials.

Based on the obtained results we conclude that only a single method is not sufficient for polymorph screening and solid state characterization. Based on the chemical structure of the compound, the molecular interaction and differences between polymorphs and pseudopolymorphs and the scope of the respective task and the most appropriate method has to be chosen.