

MS16-P13 | HOW DIFFERENT DO DIFFRACTION PATTERNS OF THE SAME SUBSTANCE HAVE TO BE TO INDICATE POLYMORPHISM?

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Theoretically, any difference in a crystal of the compound results in changes in its diffraction pattern (diffractogram in the powder sample). The differences may be related either to the arrangement of atoms within a crystal (called structure) or to experimental conditions. Some experimental conditions also change the structure, i.e. temperature.

The basic relations between the structure and diffraction patterns are as follows:

1. Bragg's angles of diffraction maxima depend on averaged dimensions of all unit cells within the studied crystal;
2. The intensities of maxima depend on the electron density of respective diffracted hkl family planes;
3. The width of maxima depends on experimental conditions and on the structure itself.

It has to be mentioned that the X-rays wave "see" atoms frozen in their accidental positions as atoms' vibrations have much lower frequencies. As a result, the diffraction pattern reflects "space-averaged" structure, which is presented as the "time-averaged" one. In practice, there are no two identical diffraction patterns, not only of the same substance but even of the same sample. So, if one of the main methods to distinguish polymorphs is diffraction, when are we allowed to "discover" a new polymorph basing on comparison of diffractograms as we usually do?

In the case of API (Active Pharmaceutical Ingredient) the discovery of a new polymorph may be rewarded by a patent. Therefore, the title question is a very serious one and in the presentation I will demonstrate, how difficult the answer is.