BM: a python code for modelling physically based background for XRD

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Abstract. A python code and a graphic interphase using TKinter have been developed to run a program to calculate a physically based background in XRD patterns. The calculation takes into account correction factors for absorption and air scattering under a symmetrical reflection geometry with a given sample thickness, divergence and receiving slit width, scale factor, average temperature factor and specimen density of packing. Then the whole diffraction pattern was evaluated on a physical basis, considering the Bragg and the diffuse scattering (Thermal Diffuse Scattering plus static disorder, Compton and air scattering) using a Python code. Compton scattering was also corrected for the bandpass function of the monochromator. The program has been applied for different organic materials as ciprofloxacin (Figure 1), sildenafil citrate, ampicillin, acetylsalicylic acid and sucrose. To made the code accessible to the users, a graphic interphase has been codified in TKinter. The program asks for the diffraction pattern, a run in the diffractometer without sample, a run with sample holder (zero-background holder) and other equipment parameters.

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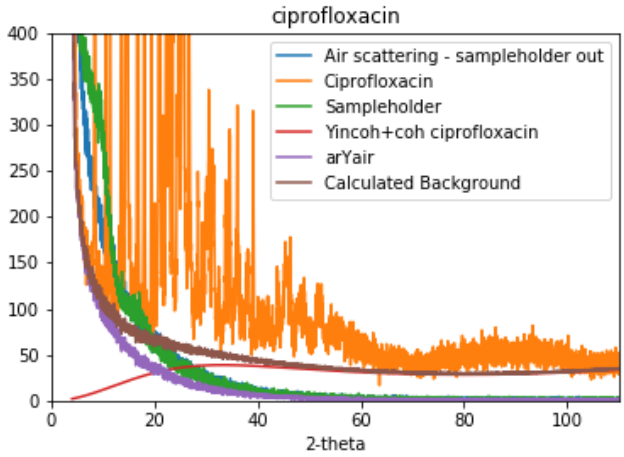

Figure1: Ciprofloxacin diffraction pattern with physical background.