Two new anharmonic forms for the Debye-Waller factor, aimed at modelling curvilinear and asymmetric motion, will be introduced.[1] They permit the refinement of crystallographic data for structures that contain these types of motion using only a small number of additional parameters over what is currently used in the thermal ellipsoid model. In this presentation the two forms will be assessed using numerical atomic probability density functions derived from molecular dynamics simulations.


Keywords: anharmonicity, Debye-Waller factors.