



STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 73 (2017)

Supporting information for article:

Accurate charge densities from powder X-ray diffraction – a new version of the Aarhus vacuum imaging-plate diffractometer

Kasper Tolborg, Mads R. V. Jørgensen, Sebastian Christensen, Hidetaka Kasai, Jacob Becker, Peter Walter, Ann-Christin Dippel, Jens Als-Nielsen and Bo B. Iversen

Table S1 Gaussian and Lorentzian FWHM parameters from Rietveld refinement with a Pseudo Voigt profile for the new and the old diffractometer.

	Old Diffractometer	New Diffractometer
GW	2.333(6)	0.1609(9)
LX	0.695(5)	0.336(2)
LY	2.37(6)	1.84(2)

The Gaussian and Lorentzian FWHM are given from the parameters as $FWHM_G^2 = 8 \ln 2 GW$ and $FWHM_L = LX/\cos \theta + LY \tan \theta$. The total FWHM is given from equation 3 of Thompson *et al.* (1987). Lorentzian parameters are in units of 0.01 degrees and the Gaussian parameter is in units of 0.0001 squared degrees.