

MS22-P02 | EVALUATION OF COVALENT BOND DENSITY IN MOLECULAR CRYSTALS USING SIMPLIFIED VIRTUAL SCATTERING CENTERS

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Here we address a 'gray area' of good quality structures with 0.5-0.8 Å resolution, which show visible deviation from IAM but are not satisfactory for experimental charge density calculations. The suggested methodology follows the well-known virtual atom method. Virtual scattering centers (VSC) are placed at fixed calculated positions between C, N, and O atoms with 'occupancies' being different for single, double, aromatic, and triple bonds. Scattering is approximated by a single Gaussian which can be justified by a small value of correction. VSCs are treated as isotropic; multiplication of scattering Gaussian by Debye-Waller factor yields one Gaussian function to describe both effects (no deconvolution of vibrations and charge density). The number of introduced parameters can be as low as one (for overall occupancy of the VSC part of the structure). Alternatively, each bond can be treated separately (number of additional parameters is roughly equal to the number of bonds). An attempt was made to handle S-C, S-O, and C-H bonds and various types of lone pairs. A number of organic and element-organic molecules were tested. When it was possible, charge density calculations (MoPro) and/or HART calculations (Tonto) were performed using the same experimental data. Visible improvement of fitting characteristics was achieved, especially for the molecules with aromatic fragments. After removing residual bond density from the Fourier difference map, other sources of deviation such as disorder and experimental and data processing errors can be addressed.