Different Approaches to Absorption Corrections for Charge Density Analyses

Jozef Kožíšek[a], Martin Breza[a], Hartmut Fuess[b], Robert H. Blessing[c], [a]*Department of Physical Chemistry, Slovak University of Technology, Bratislava, Slovakia.* [b]*Materials Science, Darmstadt University of Technology, Darmstadt, Germany*. [c]*Hauptman-Woodward Medical Research Institute, Buffalo, New York, U.S.A.* E-mail: jozef.kozisek@stuba.sk

In order to increase the accuracy of high-angle diffraction data for multipole refinement with XD, crystals with diameters of up to 0.5 mm were measured. Bigger crystals give intensity data with higher signal-to-noise ratios, especially for high-angle reflections, but large crystals also make accurate absorption and extinction corrections a necessity, especially for crystals of *3d*-coordination compounds. Extinction corrections require values of TBAR, the absorption-weighted mean sum of incident and diffracted beam path lengths through the crystal, and anisotropic extinction corrections require also the direction cosines of the incident and diffracted beams [1].

Several absorption correction methods were compared based on crystallographic R-values, maximum and minimum values of residual densities, and the *d*-orbital populations from the experimental electron density studies of several *3d*-coordination compounds [2-3]. Valuable additional information was obtained from quantum chemical calculations and subsequent topological analysis of both experimental and theoretical electron densities [4].

[1] Blessing R. H., *J. Appl. Crystallogr*., 1997, **30**, 421. [2] Kožíšek J., Fronc M., Skubák P., Popkov A., Breza M., Fuess H., Paulmann C., *Acta Cryst*., 2004, **A60**, 510. [3] Kožíšek J., Hansen N.K., Fuess H., *Acta Cryst.*, 2002, **B58**, 463. [4] Májek P., Brudíková K., Breza M., *J. Mol.Struct. (Theochem)*, 2004, **711**, 115.

Keywords: charge density, organometallic copper compounds, properties