

flipping and symmetry determination by analysis of phased reflections on the other hand. The comparison is done on more than 500 structures of variable size and composition and diffraction data of intermediate to excellent quality using default parameters for all data sets, i.e. without any intermediate human intervention, with the aim to determine success rates in automatic structure solution using widely available and free crystallographic software.

[1] L. Palatinus & A. van der Lee : *J. Appl. Cryst.*, **2008**, 41, 975-984.

**Keywords: structure solution; software**

#### FA4-MS12-O4

**Intensity Statistics of Friedel Opposites and Classification of Reflections.** Uri Shmueli<sup>a</sup>, Howard D. Flack<sup>b</sup>. <sup>a</sup>*School of Chemistry, Tel Aviv University, Israel.* <sup>b</sup>*Faculté des Sciences, University of Geneva, Switzerland.*

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An extensive analysis of intensity differences of Friedel opposites [1] carried out by algebraic and, in part, probabilistic methods showed that the mean-square intensity difference of Friedel opposites is independent of space-group symmetry. A recent study [2] arrived at the previous results by purely statistical methods and also showed that the experimentally important Bijvoet ratio depends only on the composition of the unit-cell content and the wavelength of the radiation. This work [2] also provided a complete classification of the reflections based on the above intensity statistics, for all the non-centrosymmetric point groups and relevant axial systems. Such a full classification enables one to decide which reflections should or should not be considered as candidates for Friedel opposites, and effectively for any non-centrosymmetric space group.

This presentation summarizes concisely the main results of the intensity statistics of Friedel opposites, provides several examples of classifications of point groups and explains their relations to the statistics discussed.

[1] Shmueli U., Schiltz M., Flack H. D., *Acta Cryst.* A64, **2008**, 476-483. [2] Shmueli U., Flack H. D., *Acta Cryst.* A65, **2009**. In the press.

**Keywords: resonant scattering; moments; intensity statistics**

#### FA4-MS12-O5

**What is the Cause of Ghost Peaks Close to Heavy Atoms?** Regine Herbst-Irmer<sup>a</sup>, Julian Henn<sup>a</sup>, Daniel Kratzert<sup>a</sup>, Daniel Stern<sup>a</sup>, Dietmar Stalke<sup>a</sup>. <sup>a</sup>*Department of Structural Chemistry, University of Göttingen, Göttingen, Germany.*

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Ghost peaks close to heavy atoms are a common problem in crystal structure determinations, and data of charge density quality and resolution even accentuate this problem.

There are a number of possible explanations, for example absorption or Fourier series termination errors. Here we describe a convenient way of eliminating this problem, although we are not quite sure why it works!

Two high resolution datasets for 9-Diphenylthiophosphinoyl-anthracene were measured, one at 15 and one at 100 K. First the structure was refined with SHELXL [1]. Then the aspherical atom approach of Hansen and Coppens [2] was applied for the description of the overall electron density distribution, including the density deformation due to bonding [3]. In the refinement process residual density peaks close to the sulfur atom appeared and could not be explained. These peaks disappeared only when Gram-Charlier anharmonic coefficients were introduced and the residual density became flat and featureless. The refinement process could nicely be followed by plotting the fractal dimension distribution of the residual density analysis [4]. The refinement procedure will be explained in detail and a comparison of the refinement against the different data sets will be shown. The properties of the structure will be discussed. The molecules absorb UV and emit visible light and so are interesting as photoluminescent materials.

[1] Sheldrick, G.M., *Acta Crystallogr.* **2008**, A64, 112. [2] Hansen, N. K., Coppens, P., *Acta Crystallogr.* **1978**, A34, 909. [3] Volkov, A., Macchi, P., Farrugia, L.J., Gatti, C., Mallinson, P.R., Richter, T., Koritsanszky, T., *XD2006*, **2006**. [4] Meindl, K., Henn, J., *Acta Crystallogr.* **2008**, A64, 404.

**Keywords: charge density; anharmonic refinement; residual electron density**