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Bilbao Crystallographic Server: Computer Determination of Non-characteristic Orbits. <u>Mois I. Aroyo</u>[a], Danel Orobengoa[a], Massimo Nespolo[b].

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A crystallographic orbit is called *characteristic* if its intrinsic symmetry (given by the so-called *eigensymmetry group* E) is that of the original or *generating* space group G. The orbit is called *non-characteristic* if it displays higher symmetry. The interest in the determination of non-characteristic orbits and their eigensymmetry groups is based on their importance in crystal structure determination, crystal physics and structural chemistry. Both theoretical discussions and tabulations of non-crystallographic orbits and their eigensymmetry groups can be found in the literature (*e.g.* see Engel *et al.* [1], and the literature therein).

The aim of this contribution is to report on the development of an algorithmic procedure for the determination of the non-characteristic orbits of the space groups and their eigensymmetry groups. The procedure is based on the following basic arguments:

(*a*) Consider a non-characteristic orbit of a point X of the space group G with an eigensymmetry group E. In the eigensymmetry group, the point X belongs to the orbit that does not split during the symmetry reduction from E to G, only its site symmetry group is reduced. The crystallographic orbits in E that satisfy this non-splitting condition are possible solutions for the non-characteristic orbits of G.

(*b*) The number *n* of points per primitive unit cell of a non-characteristic orbit limits the index of the translation lattices of E and G. Thus, the eigensymmetry group of an orbit of G could be only among the supergroups of G with a reduction of the primitive unit cell that is smaller than *n*.

(*c*) Consider a space group Z intermediate between G and the eigensymmetry group E of a non-characteristic orbit of point X. The orbit of X does not split neither for the symmetry reduction from E to G, nor for the reduction from Z to G, *i.e.* non-characteristic orbits may appear as solutions for several supergroups of G. Obviously, these supergroups are group-subgroup related, and the eigensymmetry group is the supergroup of highest index with respect to G.

The algorithmic procedure is implemented in the computing program NONCHAR that is available on the Bilbao Crystallographic Server (www.cryst.ehu.es) [2] The method for the determination of the non-characteristic orbits and their eigensymmetry groups is based on the crystallographic databases and computer tools available on the Bilbao Crystallographic Server. The efficiency of the program is increased taking into account the close relationships between the concepts of lattice complexes and limiting complexes, and those of non-characteristic orbits [3].

[1]. Engel P., Matsumoto T., Steinmann G., Wondratschek H. The Non-characteristic Orbits of the Space Groups. *Z. Kristallogr.*, Suppl. Issue No.1, Oldenbourg, Muenchen, **1984**. [2] Aroyo M.I., Perez-Mato J.M., Capillas C., Kroumova E., Ivantchev S., Madariaga G., Kirov A., Wondratschek H., *Z. Kristallog.* **2006**, 221, 15-27. [3]. Koch E., Fischer W. *Acta Cryst.* A **1985**, 41, 421-426.

Keywords: bilbao crystallographic server; non-characteristic orbits; eigensymmetry groups

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van der Waals Contacts Retrieved from CSD. Should the Histograms be Weighted? <u>Åke Oskarsson</u>[a], Christian Hansson[a]. *[a]Organic Chemistry, Lund University, PO Box 124, SE-221 00 Lund, Sweden.*
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Previously we have studied intermolecular distances Cl--Cl in Pt(II)-Cl complexes and observed a frequency maximum in the interval 3.8-3.9 Å [1]. However, the maximum is not very pronounced and for larger distances, the frequency of distances in the intervals start to increase. This is to be expected since the sphere, or sphere segment, on which the neighboring Cl is located will increase proportional to the square of the Cl--Cl distance. In order to find a non-biased frequency maximum we suggest that histograms for studying van der Waals contacts should be weighted with the inverse square of the midpoint distance in the interval. Examples from Pt(II)-halogen complexes retrieved from CSD [2] will be shown on the Poster.

[1] Hansson, C., Carlson, S., Giveen, D., Johansson, M., Yong, S. and Oskarsson, Å., *Acta Cryst.*,**2006**, B62, 474. [2] Allen, F.H., *Acta Cryst.*,**2002**, B58, 380.

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Regularized Reference Intensity Ratio Method. <u>Igor S. Yakimov</u>. *Institute of Non-Ferrous Metals and Materials, Siberian Federal University, Krasnoyarsk, Russian Federation.*
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Tikhonov's regularization theory of solving of ill-posed problems [1] had been applied to qualitative X-ray phase analysis of powder patterns successfully [2]. The application of Tikhonov's regularization to reference intensity ratio method (RIR) of standardless X-ray quantitative phase analysis (QPA) is reported in this paper. Reference intensity ratios (I/Ic) are extracted from PDF2/PDF4 ICDD database after a search-match for the best matching reference patterns calculated from crystal structure data. A mathematical model of the multi-peaks RIR with addition of element balance equations for chemical analysis data is constructed and common least square functional is regularized. An algorithm of automatic search of regularization parameters and QPA by regularized RIR is described. Applications of new regularized reference intensity ratio (RRIR) method are demonstrated on CPD data of Round Robin on Quantitative

Phase Analysis [3]. The RRIR standard deviation without using of chemical data is 1.1 % mass per phase and with using of some XRF analysis data is 0.7 % mass per phase. The RRIR method was integrated into the search-match system [4].

[1] Tikhonov, A. N., Arsenin, V. Ya., *Methods of Solution of Ill-Posed Problems [in Russian],* Nauka, Moscow, **1979**. [2] Burova, E.M., Shchedrin, B.M., *Computational Mathematics and Modeling,* **2006**, 1, 45. [3] Scarlett, N.V.Y., Madsen, I.C., Cranswick, L.M.D., Lwin, T., Groleau, E., Stephenson, G., Aylmore, M., Agron-Olshina, N., *J. Appl. Cryst*., **2002**, 35, 383. [4] Yakimov, I.S., *Inorganic Materials*, **2008**, 14, 1531.

Keywords: reference intensity ratio; quantitative phase analysis; powder diffraction