Analysis of Structure Factors of 2D-connected Crystal Structures Jordi Rius, Inmaculada Peral, Carles Miravitlles, Departament de Cristallografia i Química de l'Estat Sòlid, Institut de Ciència de Materials de Barcelona-CSIC, Catalunya, Spain. E-mail: jordi.rius@icmab.es

The solution of complex inorganic structures from powder diffraction data is much easier when dominant scatterers are present. Due to the small X-ray scattering contrast between Si and O, solution of complex zeolitic materials is still difficult. One characteristic of the latter is their 3D connectivity and the known tetrahedral coordination that means that once the positions of the Si are located, the positions of the O atoms can be interpolated. In other words, the positions of the O atoms are not independent from the Si positions. The ideal situation for solving crystal structures from powder data at moderate resolution (d>2Å) by direct methods would be to have at one's disposal structure factor moduli with the contributions of the O atoms removed [1], [2].

In order to better analyse this possibility, the modulus C and the phase angle δ of group structure factor of one triangular O polyhedron around a central Si atom have been plotted as a function of its orientation. The respective variation coefficients of C are 9.1 and 21.5% at 2 and at 1.85 Å resolution, respectively, while the corresponding standard deviations of δ are 27° and 12°. These values are used to estimate the accuracy of the structure factors of an hypothetical planar 2D connected model built of such triangular polyhedra after removal of the average O contribution.

[1] Rius J., Acta Cryst., 1993, A49, 406. [2] Rius J., Z. Kristallogr., 2004, 219, 826.

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