References:

Sánchez-Muñoz, L.; Sanz, J.; Sobrados, I. & Gan Z.H. (2013) Am. Mineral., 98, 2115-2131

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Application of the full-symmetry Patterson sum-function to the solution of complex cluster-based minerals from powder diffraction data

Jordi rius[1]

1. Institut de Ciència de Materials de Barcelona (CSIC), 08193 Bellaterra, Catalonia, Spain

email: jordi.rius@icmab.es

Often, poorly growing minerals are based on self-assembly of metal clusters e.g. via H bond networks [1]. If the unit cell and the space group symmetry of these compounds can be estimated from the powder diffraction pattern, then this information can be used 1) to extract the cluster intensities from the pattern 2) to strengthen the Patterson sum-function application (S_P) [2] by reducing the number of phases to be refined (the S_P -FT algorithm is implemented in the XLENS_PD6 code retrievable from https://departments.icmab.es/crystallography/software). Unlike direct-space structure solution methods, the S_P -FT algorithm is especially well-suited for crystal structures containing cations with irregular or unpredictable coordination polyhedra or when some structural disorder is present. Although this algorithm was initially developed for organic compounds, it will be shown that it is also suitable for the location of light atoms in the presence of a large number of heavy atoms.

In those cases where the unit cell cannot be found directly from the powder pattern, electron diffraction tomography (EDT) constitutes an alternative way of solving the crystal structure.. However, its efficiency decreases if the sample is sensitive to vacuum induced dehydration. It will be shown that even in such unfavorable circumstances the information provided by EDT is complementary to that of PD and can be used to advantage by the S_P-FT algorithm. This will be illustrated on the solution of the unknown crystal structure of decrespignyite-(Y), a new complex copper yttrium rare-earth carbonate chloride hydrate from Paratoo (South Australia) [3].

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References:

[1] León-Reina, L., Cabeza, A., Rius, J., Maireles-Torres, P.J., Alba-Rubio, A.C., López-Granados, M. (2013) Journal of Catalysis, 300, 30.

[2] Rius, J. (2014) IUCrJ , 1, 291.

[3] Wallwork K., Kolitsch U., Pring A., Nasdala L. Mineralogical Magazine, 2002, 66, 181.

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