conference abstracts

s10.m1.p5 **Advances in automatic powder indexing: An enhanced 32-bit version of the Crysfire suite.** R. Shirley. *School of Human Sciences, University of Surrey, Guildford, Surrey, GU2 7XH.*
Keywords: indexing, powder diffraction, computing.

A new 32-bit Windows version of Crysfire automatic powder-indexing suite will be demonstrated.

The Crysfire software suite under MSDOS has become established as a convenient way for users of powder-indexing programs, particularly if non-specialists, to run most of the available, mature automatic-indexing programs on their data, conveniently and within a single, integrated operating environment.

Indexing programs supported within Crysfire include better known ones like ITO12, DICVOL91 and TREOR90, and also others previously less accessible, such as Taupin's POWDER (TAUP), Kohlbeck's TMO (KOHL), FJZN6, and the heuristic combination-strategy programs LZON and LOSH

Useful features of Crysfire include log and summary files. The log file provides a concise sequential record of all Crysfire runs for that dataset, while the corresponding cumulative summary file displays the proposed solutions found by the indexing programs, sorted into descending order of quality. The versions of the indexing programs used within the suite have been modified where necessary to support these functions. The new state of the summary file is displayed after each indexing run.

In this new Windows release, the existing 16-bit versions of the indexing programs are replaced by optimised 32-bit code. This runs up to 50% faster, and frees the programs from constraints of available base memory and from segment-size limitations.

Although only 32-bit Microsoft Windows is expected to be supported at ECM-19, it is hoped that this may be followed by a Linux version. The difficulty is that much code in the indexing programs is mainframe Fortran IV with proprietary extensions, often dating back over 20 years. These extensions are still supported by commercial 32-bit Windows compilers, but not by Linux f77.

It is hoped that this new 32-bit system will make it easier to accommodate indexing programs that use newer approaches such as genetic algorithms, which require extenders to run under DOS and so could not be supported within DOS Crysfire, and also to integrate Crysfire more closely with profile-oriented powder diffraction software.

Crysfire and its constituent programs are distributed free for non-commercial use via the CCP14 web site (see http://www.ccp14.ac.uk/tutorial/crys/index.html).

s10.m1.p6 **X-Ray Powder Diffraction Study of Tetragonal Rare Earth Oxybromides, REOBr.** J. Hölsä[1], M. Lahtinen[2], M. Lastusaari[1,3], J. Niittykoski[1,3], J. Valkonen[2], [1]*University of Turku, Department of Chemistry, FIN-20014 Turku, Finland,* [2]*University of Jyväskylä, Department of Chemistry, P.O. Box 35, FIN-40351 Jyväskylä, Finland,* [3]*Graduate School of Materials Research, Turku Finland.*
Keywords: powder diffraction, advanced methods, structure determination.

The rare earth (RE) oxybromides (REOBr) are - together with the RE oxides and oxysulfides - the most efficient materials used for many luminescent applications[1]. The RE oxybromides belong to a quite large family of compounds, the RE oxycompounds, the structure of which is characterized by alternating layers of the $[REO]^+$ complex cations and the anions. Since the anion can be either very simple (F^-, Cl^-) or complex ($[NO_3]^-$, $[SO_4]^{2-}$, $[UO_6]^{6-}$) it may be assumed with good reason that the stable and structurally rigid $[REO]^+$ complex cation is responsible for the excellent luminescence properties of the RE oxycompounds. However, no detailed study of the structure-luminescence relationship has yet been carried out to explain the exact role of the $[REO]^+$ cation.

In this contribution we report the results on the Rietveld structure refinement based on the X-ray powder diffraction data for the complete - excluding promethium - isomorphous series of the tetragonal phase of RE oxybromides, REOBr (RE = La - Pr, Nd - Lu, and Y). At room temperature the whole REOBr series crystallizes in the P4/nmm (Z = 2) space group as found previously[2].

All structural parameters were found to behave regularly with the ionic radius of the RE host cation - but only when the microabsorption and preferred orientation corrections were applied. The stability of the tetragonal REOBr phase was assessed by using the bond valence model. The main contribution to the decreasing stability in the REOBr series with decreasing ionic radius of the RE host cation arises from the repulsions in the bromide layer perpendicular to the c-axis. These repulsions finally lead to a structural transformation from the tetragonal phase to a hexagonal, more efficiently packed SmSI-type REOBr form[3]. This phase was found only for the LuOBr compound and was obtained at elevated temperature (above 800 K) but is, however, stable also at ambient condition when quenched.

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