



Supporting Information

© Wiley-VCH 2007

69451 Weinheim, Germany

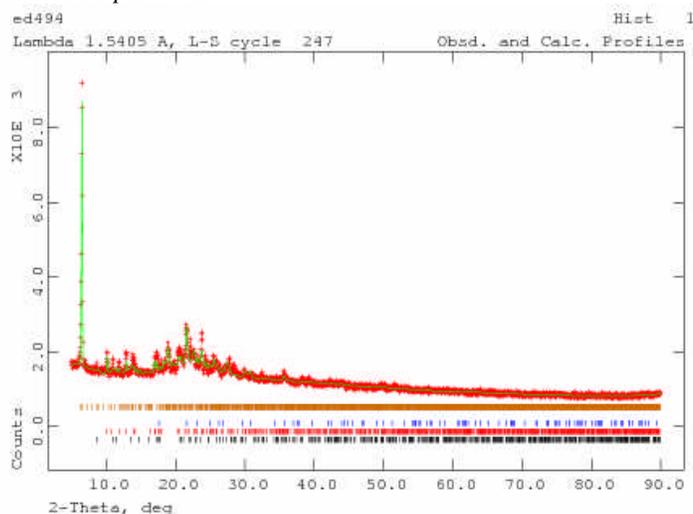
# Ionothermal Synthesis of Choline-Templated Metal Aluminophosphate Materials with Unusual Chemistry

Ewan A. Drylie, David S. Wragg, Emily R. Parnham, Paul S. Wheatley, Alexandra M.Z. Slawin, John E. Warren & Russell E. Morris\*

## Rietveld refinement of SIZ-13

The crystal data for SIZ-13 collected on the in house diffractometer (Bruker SMART diffractometer with graphite-monochromated Cu  $K_{\alpha}$  radiation) is not good due to the small size and weak x-ray scattering of the crystals. Unfortunately better data was not obtained at the SRS so a Reitveld refinement on the powder data was attempted, although this was complicated as the sample was not phase pure or highly crystalline. The powder x-ray pattern was collected from 5 to 90 °C on a STOE stadip diffractometer using Cu  $K_{\alpha 1}$  radiation. Reitveld fitting of the pattern in triclinic P-1 did not satisfactorily model all the observed peaks. This was expected as it was known that there were additional phases in the sample. Addition of the two other aluminium cobalt phosphate phases (SIZ-14 and SIZ-15) as minor impurities gave a much more reasonable fit ( $wRp = 4.99\%$ ,  $\chi^2 = 2.958$ ). The liveplot is shown in Figure S1. This confirms that the crystalline material in the sample is mostly SIZ-13 and that the structure is consistent with the single crystal XRD structure.

**Figure S1** Plot of the Reitveld refinement of the PXRD Pattern of SIZ-13. The red crosses are of the observed powder pattern and the green line is the calculated powder pattern. The purple line shows the difference between the observed and calculated patterns.



[\*] E.A. Drylie, Dr. D.S. Wragg, E.R. Parnham, Dr. P.S. Wheatley, Prof. R.E. Morris.

EaStChem School of Chemistry  
University of St Andrews  
Purdie Building, St Andrews KY16 9ST, UK  
Fax: (+) 44 1334 463808  
E-mail: rem1@st-and.ac.uk

J.E. Warren

Synchrotron Radiation Source  
CCLRC Daresbury Laboratory  
Warrington WA4 4AD, UK

[\*\*] REM thanks the Royal Society for the provision of a University Research Fellowship. We thank the CCLRC and John Warren for access to the Synchrotron Radiation Source (Daresbury) and the EPSRC for funding

Supporting information for this article is available on the WWW under <http://www.angewandte.org> or from the author.