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Li₂C₂ 4 Feb 2014 -XRD Analysis

Discussion

The sample of Li₂C₂ from 4 February 2014 is 92.0(2) wt% Li₂C₂ and 8.0(2) wt% LiOH (Figure 1). The Li₂C₂ crystallizes in *Immm* with $a = 3.649(2)$ and $c = 5.440(4)$ Å. The Li is at 0,1/4,0 and the C at 0,0,0.376. The average crystallite size is 60(1) Å. Even though the crystallites are small, I had to include a small preferred orientation correction to obtain a good fit to the pattern (Figure 2). The texture index was 1.046.

The average crystallite size of the LiOH is ~165 Å, but I had difficulty in refining the profile coefficient. The broad low angle feature and the sharp peak at 13.0° arise from removing the anti-scatter screen, and do not come from the air-sensitive cell itself.

Experimental

Data collected by you from a specimen packed in the air-sensitive sample cell was processed. The X-ray powder pattern was measured (5-100° 2θ, 0.0202144° steps, 0.5 sec/step, 0.6 mm divergence slit, 2.5° Soller slits, 3 mm scatter screen height) on a Bruker D2 Phaser diffractometer equipped with a LynxEye position-sensitive detector. Quantitative phase analysis of the crystalline phases was carried out by the Rietveld method using GSAS [1].

James A. Kaduk

References

1. A. C. Larson and R. B. Von Dreele, "General Structure Analysis System, (GSAS)", Los Alamos National Laboratory Report LAUR 86-784 (2004).

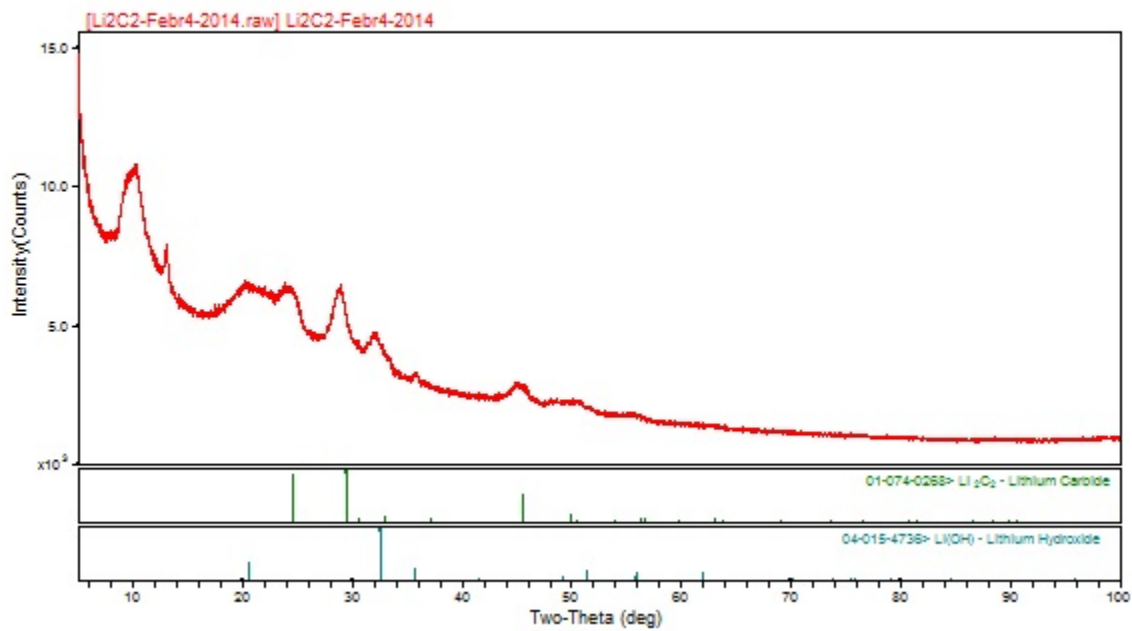


Figure 1

Li2 C2 4 Feb 2014 (LI2C2040214)

Hist 1

Lambda 1.5406 A, L-S cycle 153

Obsd. and Diff. Profiles

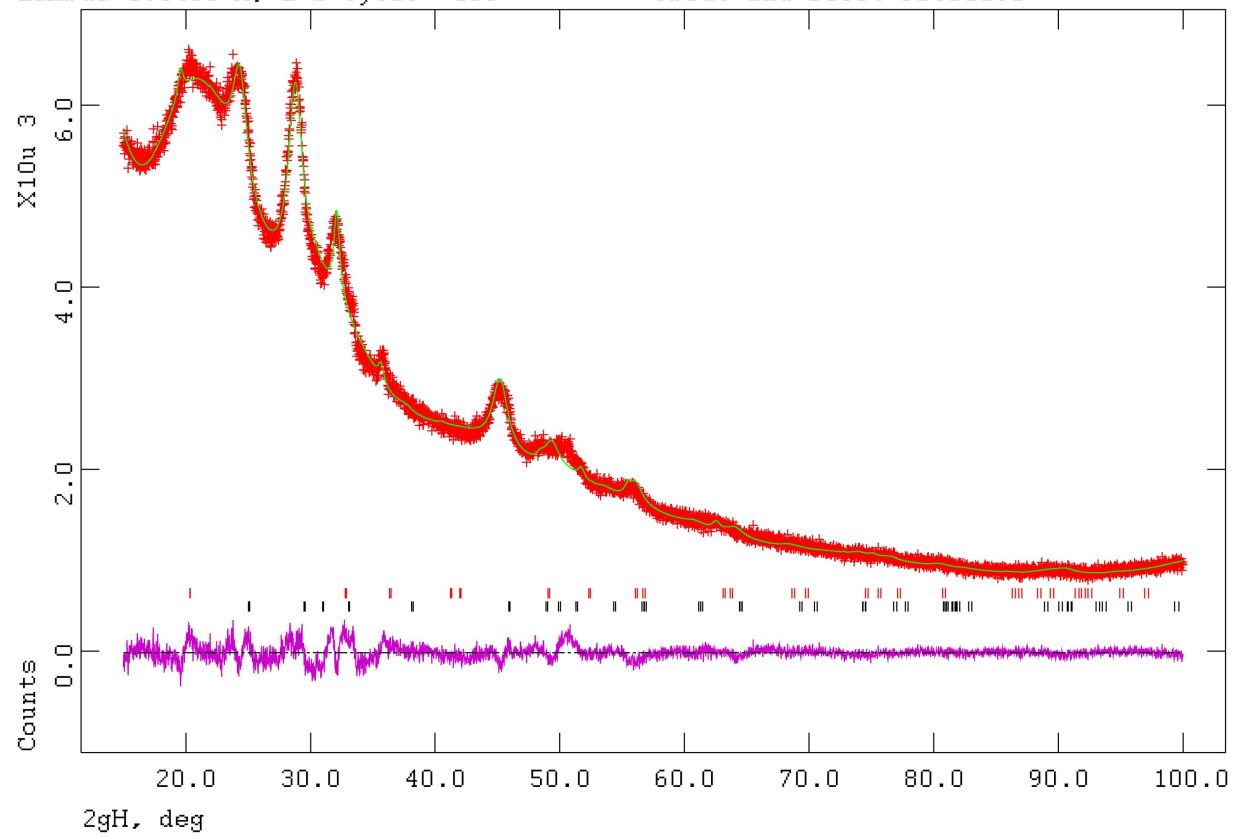


Figure 2