SHORT COMMUNICATIONS

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Erratum to *Kinetics of dehydration of single crystals of copper formate tetrahydrate* by Fichte and Flanagan.

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Abstract

An error has been detected in the title paper [Fichte & Flanagan (1971). *Trans. Faraday Soc.* **67**, 1467–1479] concerning the use of X-ray powder data to infer structural information. The nature of the error is discussed and the corrected information given.

In the paper by Fichte & Flanagan (1971), the authors correctly ascribe the strong 6·23 Å line in copper formate tetrahydrate (CFT) to $(001)_{CFT}$, based on the well known argument that in lamellar structures strong, low-angle reflexions correspond to interplanar spacings between layers (Grim, 1953). Besides, the assignment was corroborated by single-crystal data, available at the time. After dehydration into copper formate anhydride (CFA), they assigned the strongest peak in the X-ray diagram (5·24 Å) to the corresponding $(001)_{CFA}$, based on the same qualitative arguments. They thus inferred a 15·9% interplanar contraction in good agreement with the 16·0% they measured in the bulk. As no single-crystal work was attempted at the time, this was as far as they could go.

Recently, a thorough crystallographic report has appeared (Günter, 1980) on the topotactically dehydrated pseudomorph CFA. The powder data presented therein show that the strong 5·24 Å line in fact corresponds to $(110)_{CFA}$, $(001)_{CFA}$ being 3·06 Å and with only a medium intensity. The collapse of $(001)_{CFT}$ planes is thus much more severe (51% shrinkage) than reported by Fichte & Flanagan. Measured values in the bulk, however, are usually very low, due perhaps to some splitting taking place at a submicroscopic level along CFT cleavage planes. Figures as low as a few per cent are not uncommon, even under very careful working conditions. It was certainly an unfortunate coincidence, then, for the authors to have such a misleading match between their measured and expected values.

The reason why a well established, general rule failed to provide the right answer should be attributed to the fact that it was applied too loosely: although CFT is a perfectly suitable (as far as the rule is concerned) layered structure, CFA is not, being distinctly three dimensional in nature. The rule, then, was not applicable from the onset.

References

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On the aplanarity of the CO_3 group in buetschliite, dipotassium calcium dicarbonate, $K_2Ca(CO_3)_2$: a further refinement of the atomic arrangement.

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Abstract

$M_r = 238·3$, rhombohedral, $R\bar{3}m$, $a = 5·3822$ (4), $c = 18·156$ (2) Å, $V = 455·48$ Å^3, $Z = 3$, $D_x = 2·607$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0·710688$ Å, $\mu = 2·321$ mm^{-1}, $F(000) = 354$, room temperature, $R = 0·017$ for 171 observed reflections up to $\sin\theta/\lambda = 0·70$ Å^{-1}. The carbonate group is slightly pyramidal with a deviation of the C atom from the plane defined by the three O atoms of $d = 0·014$ (2) Å. This new value for d agrees with the values found in related compounds.

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Introduction

The crystal structure of buetschliite was determined by Pabst (1974) and refined by Knobloch, Pertlik & Zemann (1980). Although the refinement was very accurate, a relatively large deviation of the carbon atom from the plane defined by the three oxygen atoms of the carbonate group was found [$d = 0·038$ (9) Å]. Because a two-circle diffractometer had been used for data collection with the rotation axis parallel to the direction of the distance d, this value especially seemed open to discussion. In connection with studies of the

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