

## The crystal structure of högbomite-8H

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## Abstract

Högbomite-8H from Central Australia has hexagonal symmetry,  $P6_3mc$  with unit-cell parameters of  $a = 5.734(3)\text{\AA}$  and  $c = 18.389(8)\text{\AA}$ . Its unit-cell composition, as determined from microprobe analysis (combined with information from the structure determination), is  $\text{Fe}_{2.84}^{2+}\text{Fe}_{1.44}^{3+}\text{Mg}_{1.40}\text{Ti}_{1.00}\text{Zn}_{0.60}(\text{Ga},\text{Mn},\text{Na})_{0.11}\text{O}_{30}(\text{OH})_2$ . The correct structural model was predicted with the aid of geometric principles previously derived from a structure determination for the related mineral, nigerite-24R. The structure was refined to an  $R$  value of 0.032 ( $R_w = 0.031$ ) for 1425 observed reflections, with  $F \geq 6\sigma(F)$ , collected using  $\text{MoK}\alpha$  radiation. The model is based on a closest-packed anion framework with an 8-layer mixed stacking sequence along  $c$  given by ABCABACB, *i.e.* (ccchccch), and with cations ordered into 6 tetrahedral and 16 octahedral sites per unit cell. The structure may be described as a 1:1 intergrowth of a spinel-like structure with composition  $2(\text{Fe},\text{Zn},\text{Mg})_2^{[4]}\text{Al}_4^{[6]}\text{O}_8$  and a nolanite-like structure with composition  $2(\text{Mg},\text{Al},\text{Fe})^{[4]}(\text{Al},\text{Fe},\text{Ti})_4^{[6]}\text{O}_7(\text{OH})$ .

## Introduction

The minerals högbomite, nigerite, and taaffeite form a series of polytypes that have similar X-ray diffraction patterns and that have been considered to have closely related structures, based on various stacking sequences of closest-packed oxygen layers with interstitial cations on octahedral and tetrahedral sites (McKie, 1955). Their diffraction patterns have in common a spinel-like subcell grouping of strong reflections, as well as extra reflections that can be indexed using hexagonal (H) or rhombohedral (R) lattices, with hexagonal cell dimensions  $a_h \approx 5.7\text{\AA}$ ,  $c_h \approx 2.3 \times n\text{\AA}$ . Using Peacor's (1967) nomenclature, the various polytypes are then designated as  $n\text{H}$  or  $n\text{R}$ , where  $n$  is the number of closest-packed oxygen layers.

We recently reported the structure determination for a 24-layer rhombohedral nigerite polytype, nigerite-24R, from which the geometric principles relating the structures of various polytypes were established (Grey and Gatehouse, 1979). These principles were used to predict the structures of some simple polytypes such as nigerite-6H, högbomite-8H, and taaffeite-8H. We subsequently com-

pleted a structure refinement for högbomite-8H that confirmed the model predicted, and the results of that refinement are the subject of this paper.

## Experimental

A sample of zincian högbomite from the Strangways Range, Central Australia (Wilson, 1977), was kindly supplied by Ian M. Threadgold. It was in the form of a hexagonal column, rounded at the edges, so that it closely approximated a cylinder 0.25 mm in diameter and 0.19 mm long. Precession photographs showed that it was predominantly an 8H polytype with a few weak reflections from a 10H polytype. The large crystal was broken, and a fragment measuring  $0.17 \times 0.14 \times 0.13$  mm was found for which the precession photographs showed reflections only from an 8H polytype. The only systematic absence observed was  $(hh2hl)$ ,  $l = 2n + 1$ , consistent with space groups  $P6_3mc$ ,  $P6_2c$ , or  $P6_3/mmc$ .

For the collection of intensity data, the crystal fragment was remounted on a Philips PW1100 4-circle automatic diffractometer in an arbitrary orientation. Lattice parameters were obtained from

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR HOGBOMITE ABSORR/HK-L/HKL DATA UNDO PA

PAGE 1

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0	0	2-34	15	15	-1	6	30	11	11	0	1	26	35	35	0	3	24	11	10	-1	3	22	10	10
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PAGE 2

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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR HOGBOMITE ABCORR/HK-L/HKL DATA UNDO PA

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
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-1	9	0	8	7	0	4	2	62	60	-1	7	3	8	9	0	9	4	36	36	-1	3	6	100	104
0	9	0	27	27	-2	5	2	22	22	0	7	3	9	8	-5	10	4	36	37	-2	4	6	16	15
-5	10	0	43	44	-1	5	2	15	15	-3	8	3	10	10	-3	10	4	11	11	-1	4	6	77	78
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-4	11	0	24	26	0	6	2	5	4	-1	9	3	7	7	0	2	5	84	86	-2	6	6	31	31
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0	5	15	21	20	-4	9	16	18	17	-1	4	18	20	20	-2	8	19	8	8	-1	3	21	23	23
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-2	6	16	12	13	0	8	17	16	17	0	3	19	10	11	0	7	20	13	13	0	4	22	37	38



OBSERVED AND CALCULATED STRUCTURE FACTORS FOR HCBOMITE ABCORR/HK-L/HKL DATA UNDO PA

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-2	5	22	19	19	0	0	24	18	18	-2	8	25	9	8	-1	7	27	12	11	0	5	30	11	13
-1	5	22	17	17	0	1	24	19	20	0	0	28	20	20	0	0	28	14	14	-3	6	30	15	14
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