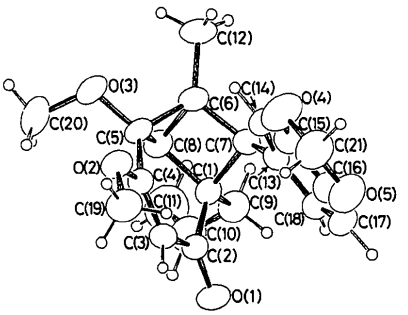
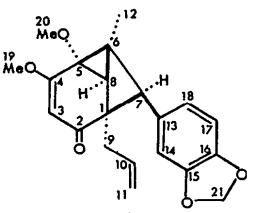


Fig. 1. An *ORTEP* drawing (Johnson, 1965) of the molecule with thermal ellipsoids scaled at the 50% probability level. H atoms are represented by circles of radius 0·08 Å.

map and the remaining from Fourier synthesis; block-diagonal least-squares refinement with anisotropic thermal parameters ($R = 0{\cdot}080$) using *UNICS*-III computation program system (Sakurai & Kobayashi, 1979). All H atoms found from difference synthesis and refined with isotropic thermal parameters. $\sum w||F_o| - |F_c||^2$ minimized, $w^{-1} = \sigma^2(|F_o|) + (0{\cdot}015\,|F_o|)^2$. Final $R = 0{\cdot}040$, $wR = 0{\cdot}048$, $S = 2{\cdot}2$.* Reflection/parameter (refined) ratio 7·2, $\Delta/\sigma < 0{\cdot}5$, $-0{\cdot}23 < \Delta\rho < 0{\cdot}14$ e Å^{-3}. Complex neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974). Atomic parameters in Table 1. Bond lengths and bond angles in Table 2. Molecular structure in Fig. 1.

* Lists of structure factors, anisotropic thermal parameters, atomic parameters for H atoms, bond lengths and bond angles involving H atoms, torsion angles, and a projection of the crystal structure have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43321 (29 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Related literature. Title compound (I) having anti-feedant activity against insects was totally synthesized (Shizuri, Nakamura, Yamamura, Ohba, Yamashita & Saito, 1986). The elongation of the C(6)–C(7) bond length results from the strain in the 3–4–6 fused ring structure, which seems larger than that in 5–5–5 fused ring structures (Luyten, Luef, Beck & Buergi, 1986; Iball, Motherwell, Barnes & Golnazarians, 1986).



(I)

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SHORT COMMUNICATION

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1987). C**43**, 173–174

Structure of barium germanium hydroxide oxide: erratum.

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Abstract

In the paper by Ozima [*Acta Cryst.* (1986). C**42**, 513–515], the space group of $BaGe_3O_6(OH)_2$ was reported to be *Cc*. Further calculation revealed that the correct space group is *C*2/*c*. Refinement based on the correct space group gave an *R* value of 0·042 for 843 independent reflections.

0108-2701/87/010173-02$01.50

Table 1. *Fractional coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^2$), *with e.s.d.'s in parentheses, for* $BaGe_3O_6(OH)_2$

$$B_{eq} = \tfrac{8}{3}\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j .$$

Old	New	x	y	z	B_{eq}
Ba	Ba	0	6622 (2)	−2500	63 (2)
Ge(1)	Ge(1)	2500	2500	0	43 (3)
Ge(2)(3)	Ge(2)	1922 (1)	7341 (2)	1215 (1)	41 (2)
O(1)(5)	O(1)	2294 (5)	4359 (14)	−1915 (7)	63 (13)
O(2)(6)	O(2)	1269 (5)	4231 (14)	255 (7)	51 (13)
O(3)(4)	O(3)	3193 (5)	5819 (13)	703 (7)	40 (12)
OH(1)(2)	OH	4375 (5)	6337 (15)	−1392 (8)	95 (15)

The $C2/c$ model can be obtained by subtracting about 0·25 from the x and z coordinates in Table 1 of the previous paper. Full-matrix least-squares refinement with no absorption or extinction corrections gave $R = 0{\cdot}042$, $wR = 0{\cdot}046$, $S = 1{\cdot}3319$, $w = 1$, max. $\Delta/\sigma = 0{\cdot}53$, max. and min. $\Delta\rho$ in final difference map 1·3 and −1·4 e $Å^{-3}$. Refined atomic parameters for the $C2/c$ model are given in Table 1,* where the old and new names of the atoms are correlated. Bond lengths and angles are listed in Table 2. Other descriptions and discussions are not essentially changed by this correction.

Table 2. *Interatomic distances* (Å) *and interbond angles* (°) *with e.s.d.'s in parentheses for* $BaGe_3O_6(OH)_2$

		Distance	Angle O–*M*–O
Ge(1) octahedron			
Ge(1)–O(1)	(×2)	1·975 (6)	
–O(2)	(×2)	1·851 (7)	
–O(3)	(×2)	1·885 (6)	
O(1)–O(2)	(×2)	2·701 (10)	89·8 (3)
–O(2^{vi})	(×2)	2·712 (9)	90·2 (3)
–O(3)	(×2)	2·529 (8)	81·8 (3)
–O(3^{vi})	(×2)	2·918 (9)	98·2 (3)
O(3)–O(2)	(×2)	2·492 (9)	83·7 (3)
–O(2^{vi})	(×2)	2·783 (9)	96·3 (3)
Ba polyhedron			
Ba–O(1)	(×2)	3·029 (7)	
–O(2)	(×2)	2·911 (6)	
–O(2^{ii})	(×2)	3·010 (7)	
–O(3^{iii})	(×2)	2·764 (6)	
–OH^{iv}	(×2)	2·740 (8)	
–OH^{v}	(×2)	2·980 (7)	

		Distance	Angle O–*M*–O
Ge(2) octahedron			
Ge(2)–O(1^{i})		1·891 (6)	
–O(1^{iii})		1·922 (7)	
–O(2)		1·853 (6)	
–O(3)		1·952 (7)	
–O(3^{iii})		1·990 (6)	
–OH^{iii}		1·819 (7)	
O(1^{i})–O(1^{iii})		2·794 (14)	94·3 (3)
–O(2)		2·726 (8)	93·4 (3)
–O(3)		2·776 (10)	92·5 (3)
–OH^{iii}		2·726 (9)	94·6 (3)
O(3^{iii})–O(1^{iii})		2·529 (8)	80·5 (3)
–O(2)		2·740 (9)	90·9 (3)
–O(3)		2·515 (12)	79·3 (3)
–OH^{iii}		2·792 (11)	94·2 (3)
O(1^{iii})–O(3)		2·766 (10)	91·2 (3)
–OH^{iii}		2·734 (9)	93·9 (3)
O(2)–O(3)		2·492 (9)	81·8 (3)
–OH^{iii}		2·647 (10)	92·2 (3)

Symmetry code: (i) $+x$, $1-y$, $\frac{1}{2}+z$; (ii) $+x$, $1-y$, $-\frac{1}{2}+z$; (iii) $\frac{1}{2}-x$, $1\frac{1}{2}-y$, $-z$; (iv) $\frac{1}{2}-x$, $\frac{1}{2}+y$, $-\frac{1}{2}-z$; (v) $\frac{1}{2}-x$, $-\frac{1}{2}+y$, $-\frac{1}{2}-z$; (vi) $\frac{1}{2}-x$, $\frac{1}{2}-y$, $-z$.

The author is indebted to Dr R. E. Marsh of the California Institute of Technology for the correction of the space group.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43305 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.