

Table 5. *The standardized structure data for LiSn based on the values given by Müller & Schäfer (1973)*

$mP6$ ,  $P12/m1$ ,  $a = 5.17 \pm 0.02$ ,  $b = 3.18 \pm 0.02$ ,  $c = 7.74 \pm 0.02$  Å,  
 $\beta = 104.5 \pm 0.3^\circ$ .

			x	y	z
Li(1)	in	2(n)	0.263	$\frac{1}{2}$	0.336
Sn(1)	in	2(m)	0.234	0	0.660
Li(2)	in	1(e)	$\frac{1}{2}$	$\frac{1}{2}$	0
Sn(2)	in	1(a)	0	0	0

Note that LiSn had to be transformed from setting  $P112/m$  to standard setting  $P12/m1$ . This was obviously also intended in *Structure Reports* Vol. 39A, p. 82, but while the atom coordinates were transformed to the setting with  $b$  axis unique, the cell parameters given correspond to the original setting with  $c$  axis unique.

shown in the lower part of Fig. 1, are rectangular and have plane groups  $p2mm$  and  $p2mg$ , respectively. Four  $AB$  structure types can be interpreted as different stackings of the rectangular  $p2mm$  layer: MgCd [(h)<sub>2</sub>], LiSn [(h<sub>h</sub>c)<sub>3</sub>],  $\alpha$ -TaRh [(h<sub>h</sub>c)<sub>2</sub>] and TiAl [(c)<sub>3</sub>]. The UPb [(c)<sub>3</sub>] type is the only  $AB$  type known where  $p2mg$  layers are stacked. The LiSn type is built up of 9 rectangular  $AB$  layers without a glide line which are stacked in the sequence (h<sub>h</sub>c)<sub>3</sub>.

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## Structure Determination of Ba(OD)Br.2D<sub>2</sub>O by Neutron Powder Diffraction

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**Abstract.** Barium hydroxide bromide dihydrate ( $d$ -5), Ba(OD)Br.2D<sub>2</sub>O,  $M_r = 275.32$ , tetragonal,  $P4/nmm$ ,  $Z = 2$ , neutron radiation,  $\lambda = 1.09$  Å,  $\mu_{\text{calc}} = 0.065$  cm<sup>-1</sup>,  $F(000) = 126.62$  fm,  $[(\sin\theta)/\lambda]_{\text{max}} = 0.632$  Å<sup>-1</sup>,  $T_1 = 300$  K,  $a = 4.5825$  (4),  $c = 11.791$  (2) Å,  $V = 247.60$  (3) Å<sup>3</sup>,  $D_x = 3.693$  Mg m<sup>-3</sup>,  $R_{\text{profile}} = 0.0208$ ;  $T_2 = 16$  K,  $a = 4.5567$  (2),  $c = 11.718$  (1) Å,  $V = 243.30$  (1) Å<sup>3</sup>,  $D_x = 3.758$  Mg m<sup>-3</sup>,  $R_{\text{profile}} = 0.0209$ . The structure is related to the PbFCl type with ninefold coordination of the Ba atoms. The OD<sup>-</sup> ions are not coordinated to the Ba

atoms, but are acceptors of four very strong hydrogen bonds. The OD distances are 0.992 (5) [0.994 (4)] Å for D<sub>2</sub>O, 0.956 (13) [0.951 (9)] Å for OD<sup>-</sup> and 1.639 (5) [1.622 (4)] Å for DOD...OD<sup>-</sup>.

**Introduction.** Recently we reported the crystal structure of Ba(OH)Cl.2H<sub>2</sub>O, which is the first representative of a new structure type (Lutz, Kellersohn & Beckenkamp, 1989). From vibrational spectra and X-ray powder photographs it was inferred that Ba(OH)Br.2H<sub>2</sub>O is isotypic. Because single crystals of sufficient quality for an X-ray structure determination could not be grown, we performed a neu-

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iron powder diffraction study on the fully deuterated compound, especially to obtain precise data on the hydrogen bond geometry.

**Experimental.** Polycrystalline samples of Ba(OD)-Br.2D<sub>2</sub>O were prepared by fusing stoichiometric amounts of Ba(OD)<sub>2</sub> and BaBr<sub>2</sub> in glass carbon crucibles (SIGRADUR®) at 823 K in a vacuum and subsequent rehydration of the resulting Ba(OD)Br with gaseous D<sub>2</sub>O at room temperature. The deuterium content was > 99% as shown by IR spectroscopy. The product was finely ground under argon and transferred to a vanadium container.

The neutron diffraction intensities were measured in four separate blocks in the SV7 powder diffractometer, equipped with a linear position-sensitive scintillation detector (Schäfer, Jansen, Elf & Will, 1984), of the Mineralogisches Institut der Universität Bonn at the FRJ2 of the Kernforschungsanlage Jülich. Measuring temperatures were 300 K (16 K), measuring times were 24 h in each case. After rescaling, successive refinement of profile, positional and isotropic displacement parameters with the fractional coordinates of Ba(OH)Cl.2H<sub>2</sub>O as starting values was performed with a modified Rietveld program (Wiles & Young, 1981), yielding final *R* values of *R*<sub>profile</sub> = 0.0208 (0.0209), *R*<sub>expected</sub> = 0.0113 (0.0162), *R*<sub>bragg</sub> = 0.0731 (0.0598). The maximum ratios of least-squares shift to e.s.d. in the final cycles were less than 0.01. Scattering lengths for all atoms were taken from Sears (1986). The final profile parameters are given in Table 1 and the structural parameters in Table 2.\*

**Discussion.** Ba(OD)Br.2D<sub>2</sub>O is confirmed to be isostructural with Ba(OD)Cl.2D<sub>2</sub>O. No phase transition is observed between 16 and 300 K. The actual lattice constants of Ba(OD)Br.2D<sub>2</sub>O (neutron data) differ from those obtained for Ba(OH)Br.2H<sub>2</sub>O by X-ray powder photographs (Lutz, Kellersohn & Beckenkamp, 1989), but this is not owing to an H/D isotopic effect. Some general features of this structure type have been described by Lutz, Kellersohn & Beckenkamp (1989). Therefore the following discussion is limited to some additional aspects.

*Relation to the PbFCl structure.* The layered structure (see Fig. 1) is closely related to the PbFCl type, but in a different way to the one that would be expected from the chemical formula alone.

Thus, Ba<sup>2+</sup> occupy the Pb<sup>2+</sup> positions with a regular (4mm) monocapped quadratic antiprismatic environment, Br<sup>-</sup> the Cl<sup>-</sup> positions, and the water O

Table 1. *Refined profile parameters [defined according to Rietveld (1969)] for Ba(OD)Br.2D<sub>2</sub>O; e.s.d.'s are given in parentheses*

	300 K	16 K
Scale factor	0.01570 (8)	0.0079 (4)
<i>u</i>	1.05 (5)	0.75 (3)
<i>v</i>	-0.65 (3)	-0.55 (2)
<i>w</i>	0.199 (2)	0.188 (2)
Zero point	-0.178 (2)	-0.217 (2)
Asymmetry parameter	0.011 (6)	0.006 (11)

Table 2. *Structural parameters of Ba(OD)Br.2D<sub>2</sub>O; data for 300 and 16 K are given in the first and second line, respectively; e.s.d.'s are given in parentheses*

	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>iso</sub> (× 10 <sup>2</sup> Å <sup>2</sup> )
Ba	2(c)	0.25	0.25	0.1914 (7)	0.6 (2)
		0.25	0.25	0.1895 (6)	0.21 (15)
Br	2(c)	0.75	0.75	0.0944 (5)	0.9 (2)
		0.75	0.75	0.0947 (4)	0.17 (12)
O(1)	4(f)	0.75	0.25	0.3221 (5)	1.0 (1)
		0.75	0.25	0.3238 (4)	0.13 (8)
O(2)	2(c)	0.75	0.75	0.4294 (7)	1.4 (2)
		0.75	0.75	0.4315 (5)	0.50 (14)
D(1)	8(i)	0.75	0.4242 (8)	0.3721 (3)	1.9 (1)
		0.75	0.4271 (6)	0.3733 (3)	0.98 (6)
D(2)	2(c)	0.75	0.75	0.5105 (9)	4.3 (3)
		0.75	0.75	0.5127 (6)	2.3 (2)

atoms occupy the F<sup>-</sup> positions. For the sake of stoichiometry, this latter layer has to be doubled with different orientations of the water molecules. The two water layers thus obtained are separated by two intermediate hydroxide (OD<sup>-</sup>) layers, see Fig. 2. It should be noted that this 'extended PbFCl type' structure has the same space group as PbFCl itself. It represents one of the very few examples where the structure of a hydrate can directly be related to the structure of a typical ionic compound. In this context, it should be mentioned that the anhydrous salts, Ba(OD)Cl and Ba(OD)Br, do not adopt the PbFCl structure, but crystallize as the laurionite [Pb(OH)Cl] type (Lutz, Kellersohn & Beckenkamp, 1990).

The seemingly more straightforward alternative structure, namely that the OD<sup>-</sup> ions occupy the F<sup>-</sup> positions and the water molecules build up the intermediate layers, would satisfy electrostatic requirements better than the actual structure, but it is obviously less favourable, because hydrogen bonds formed in such a case are less efficient. Thus, for the compound under study, hydrogen bonds are determinative for the structure and overcome ionic interactions.

*Water molecules and hydroxide ions.* The water (D<sub>2</sub>O) molecules with site symmetry 2mm act as donors for strong, nearly linear hydrogen bonds. This is revealed by the short DOD...OD<sup>-</sup> distance (see Table 3) and the low-energy H<sub>2</sub>O stretching modes of ≈ 2700 cm<sup>-1</sup> in the IR spectra. The coordination of the water molecules is tetrahedral (see Fig. 1), type

\* Lists of observed and calculated profile intensities have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53497 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

*B* according to Chidambaram, Sequeira & Sikka (1964).

As already pointed out (Lutz, Kellersohn & Beckenkamp, 1989), the hydroxide ( $\text{OD}^-$ ) ions are *not* coordinated to the metal ions, a feature which is very unusual for solid hydroxides. The hydroxide ions by themselves do not act as hydrogen bond donors. The  $\text{OD}^-$  stretching modes (isotopically dilute samples) possess very high wavenumbers, 2698 and 2706 (IR), and 2694 and 2698  $\text{cm}^{-1}$  (Raman) at 300 and 90 K, respectively, compared to that of 2625.33  $\text{cm}^{-1}$  for free  $\text{OD}^-$  ions (Rehffuss, Crofton & Oka, 1986). There are two possible explanations for this increased intramolecular bond strength, (i) the fact that the hydroxide ( $\text{OD}^-$ ) ions serve as acceptors for four very strong hydrogen bonds obviously acts in a similar manner to metal–oxygen interactions (Lutz, Henning & Haeuseler, 1987), and (ii) repulsive interactions between adjacent H atoms. In contrast to the vibrational frequencies, the intramolecular O–D distances are a less sensitive measure of the OD bond strength because of the relatively large standard deviations and systematic errors arising from librational motions *etc.*

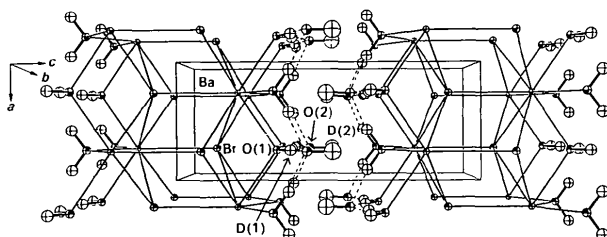


Fig. 1. Structure of  $\text{Ba}(\text{OD})\text{Br}\cdot 2\text{D}_2\text{O}$ , 16 K data, view along  $[010]$ , drawn at the 50% level (Johnson, 1976). Dashed lines represent hydrogen bonds.

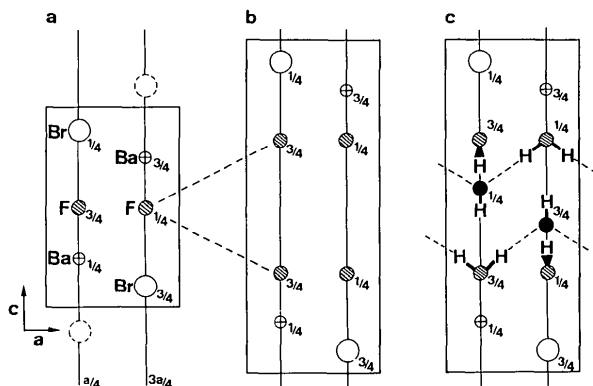


Fig. 2. Formal development of the structure of  $\text{Ba}(\text{OD})\text{Br}\cdot 2\text{D}_2\text{O}$  from  $\text{PbFCl}$  type  $\text{BaFBr}$  (a) with doubling of the  $\text{F}^-$  layer (b) and replacement of  $\text{F}^-$  by  $\text{D}_2\text{O}$  and insertion of two  $\text{OD}^-$  layers (c); figures ( $\frac{1}{4}$  and  $\frac{3}{4}$ ) indicate fractional  $y$  coordinates of the respective atoms.

Table 3. Selected interatomic distances ( $\text{\AA}$ ) and angles ( $^\circ$ ) for  $\text{Ba}(\text{OD})\text{Br}\cdot 2\text{D}_2\text{O}$ ; *e.s.d.*'s are given in parentheses

	300 K	16 K	
<b><math>\text{BaBr}_5(\text{D}_2\text{O})_4</math> polyhedron</b>			
Ba—Br	3.436 (3)	3.408 (3)	(o-o, o-i, o-ii, o-iii)
Ba—Br	3.370 (10)	3.330 (8)	(o-iv)
Ba—O(1)	2.761 (6)	2.769 (5)	(o-o, o-ii, o-v, o-vi)
Br—Ba—Br	83.64 (9)	83.90 (8)	(4x, e.g. o-o-i)
Br—Ba—Br	70.56 (16)	70.98 (13)	(4x, e.g. o-o-iv)
Br—Ba—O(1)	68.44 (10)	68.60 (8)	(8x, e.g. o-o-o)
O(1)—Ba—O(1)	71.85 (16)	71.16 (13)	(4x, e.g. o-o-v)
<b><math>\text{D}_2\text{O}</math> molecules and <math>\text{OD}^-</math> ions</b>			
O(1)—D(1)	0.992 (5)	0.994 (4)	(o-o, o-ix)
D(1)—O(1)—D(1)	107.1 (6)	108.6 (5)	(o-o-ix)
D(1)—D(1)	159.7 (7)	161.4 (5)	(o-ix)
O(2)—D(2)	0.956 (13)	0.951 (9)	(o-o)
<b>Hydrogen bonding</b>			
D(1)···O(2)	1.639 (5)	1.622 (4)	(o-o)
D(1)···O(2)···D(1)	80.2 (2)	84.8 (1)	(4x, e.g. o-o-vi)
D(1)···O(2)···D(1)	131.3 (6)	130.3 (3)	(2x, e.g. o-o-x)
D(1)···O(2)···D(2)	114.4 (3)	114.9 (2)	(4x, e.g. o-o-o)
O(1)···O(2)	2.617 (5)	2.605 (3)	(o-o, o-i)
O(1)—D(1)···O(2)	167.9 (5)	169.2 (4)	(o-o-o)
<b>Interlayer distances</b>			
D(2)···O(2)	3.317 (3)	3.282 (2)	(4x, e.g. o-viii)
D(2)···D(2)	3.250 (2)	3.236 (2)	(4x, e.g. o-viii)

Symmetry operations (consistent with Lutz, Kellersohn & Beckenkamp, 1989): (o)  $x, y, z$ ; (i)  $x, y-1, z$ ; (ii)  $x-1, y, z$ ; (iii)  $x-1, y-1, z$ ; (iv)  $1-x, 1-y, -z$ ; (v)  $y, x, z$ ; (vi)  $y, x-1, z$ ; (vii)  $x, y+1, z$ ; (viii)  $1-x, 1-y, 1-z$ ; (ix)  $x, \frac{1}{2}-y, z$ ; (x)  $x, \frac{3}{2}-y, z$ .

**The hydrogen bond system.** The actual  $\text{D}\cdots\text{OD}^-$  and  $\text{O}_w\cdots\text{OD}^-$  distances of 1.639 (5) and 2.617 (5)  $\text{\AA}$ , respectively, and those of the isostructural chloride [1.60 (2) and 2.60 (2)  $\text{\AA}$  (Lutz, Kellersohn & Beckenkamp, 1989)] are significantly shorter than for other hydroxide hydrates. Thus, in most cases  $\text{D}\cdots\text{OD}^-$  distances  $> 1.65$   $\text{\AA}$  and  $\text{O}_w\cdots\text{OD}^-$  distances  $> 2.60$   $\text{\AA}$  (Beckenkamp, 1990; Seidel, 1988) are observed. These findings are possibly due to the 'free' hydroxide ions which are stronger hydrogen bond acceptor groups than those with reduced negative charge owing to the adjacent metal ions. This (and the synergetic effect, see below) corresponds also to the bond valences for  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, which should increase in such a case as discussed by Ferraris, Fuess & Joswig (1986) and Ferraris & Ivaldi (1988).

The so-called synergetic effect, *i.e.* the increase of the hydrogen bond donor strength of water molecules due to metal–oxygen interaction (Lutz & Henning, 1987a; Lutz, 1988), should be larger for  $\text{Ba}(\text{OD})\text{Br}\cdot 2\text{D}_2\text{O}$  than for  $\text{Ba}(\text{OD})\text{Cl}\cdot 2\text{D}_2\text{O}$ , as inferred from the shorter  $\text{Ba}\cdots\text{O}(1)$  distance of 2.761 (6) compared to 2.79 (1)  $\text{\AA}$ , and, hence, the hydrogen bonds of the bromide should be stronger than those of the chloride. However, the opposite is observed when the  $\text{D}\cdots\text{OD}^-$  distances (see above) are considered. Unfortunately, the water bands in the IR

spectra (Lutz, Kellersohn & Beckenkamp, 1989) are too broad to determine accurate mode energies, and therefore a clear comparison between the bromide and the chloride is not possible.

The observed hydrogen bond lengths of the hydroxides under investigation, however, are influenced additionally by constraints due to the symmetry of the structure and the dimensions of the unit cells. This means that the most favourable bond distance of the hydrogen bond donor-acceptor pair DOD...OD<sup>-</sup> is modified, e.g. enlarged in the case of the bromide, due to packing effects (Lutz & Henning, 1987b; Henning, 1988). This might explain the discrepancies in hydrogen bond strength outlined above.

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## Structure of Trisilylphosphine, P(SiH<sub>3</sub>)<sub>3</sub>, at 100 K

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**Abstract.** H<sub>9</sub>PSi<sub>3</sub>, *M<sub>r</sub>* = 124.30, monoclinic, *P*2<sub>1</sub>/*c*, *a* = 6.0631 (16), *b* = 12.734 (3), *c* = 9.6784 (20) Å, β = 93.872 (16)°, *V* = 742.2 Å<sup>3</sup>, *Z* = 4, *D<sub>x</sub>* = 1.112 Mg m<sup>-3</sup>, λ(Mo Kα) = 0.71073 Å, μ = 0.714 mm<sup>-1</sup>, *F*(000) = 264, *T* = 100 K, *R* = 0.0287 for 1778 unique observed reflections. Individual molecules have approximate, non-crystallographic C<sub>3v</sub> symmetry: they are linked by P...Si intermolecular contacts to give a corrugated sheet structure with P—Si...P angles close to linear and [3 + 2] coordination at phosphorus.

**Introduction.** We have previously determined the crystal structures of several simple compounds con-

taining Si—N bonds, such as trisilylamine (Barrow & Ebsworth, 1984) and dimethylsilylamine (Blake, Ebsworth & Welch, 1984a). These two compounds may be taken as representing two extremes: the former shows little if any difference between its gas-phase and solid-state structures, while the latter is monomeric in the vapour (Gundersen, Mayo, Rankin & Robertson, 1984) but forms a unique cyclic pentamer in the crystal. Although IR and Raman spectroscopic results (Davidson, Ebsworth, Sheldrick & Woodward, 1966) were consistent with trisilylphosphine being similar to trisilylamine in that the central atom was surrounded by a trigonal planar arrangement of Si atoms, electron diffraction studies (Beagley, Robiette & Sheldrick, 1968) established pyramidal geometry in the gas phase. The purpose of the present work was to discover the precise structure of trisilylphosphine in the solid state

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