Table 3. *Atomic co-ordinates*

Hydrocarbon chains

	x/a	z/c		x/a	z/c		x/a	z/c
C_1	0·1792	0·0260	C_{13}	0·5425	0·4464	C_{25}	0·7728	0·5766
C_2	0·1824	0·0554	C_{14}	0·5393	0·4170	C_{26}	0·7760	0·6060
C_3	0·1251	0·0950	C_{15}	0·5966	0·3774	C_{27}	0·7187	0·6456
C_4	0·1283	0·1244	C_{16}	0·5934	0·3480	C_{28}	0·7219	0·6750
C_5	0·0710	0·1640	C_{17}	0·6507	0·3084	C_{29}	0·6646	0·7146
C_6	0·0742	0·1934	C_{18}	0·6475	0·2790	C_{30}	0·6678	0·7440
C_7	0·0169	0·2330	C_{19}	0·7048	0·2394	C_{31}	0·6105	0·7836
C_8	0·0200	0·2624	C_{20}	0·7016	0·2100	C_{32}	0·6137	0·8130
C_9	0·9628	0·3020	C_{21}	0·7589	0·1704	C_{33}	0·5564	0·8526
C_{10}	0·9660	0·3314	C_{22}	0·7557	0·1410	C_{34}	0·5596	0·8820
C_{11}	0·9087	0·3710	C_{23}	0·8130	0·1014	C_{35}	0·5023	0·9216
C_{12}	0·9119	0·4004	C_{24}	0·8098	0·0720	C_{36}	0·5055	0·9410

References

Clarkson, C. E. & Malkin, T. (1934). *J. Chem. Soc.* p. 666.

Clarkson, C. E. & Malkin, T. (1948). *J. Chem. Soc.* p. 985.

Lange, J. J. de, Robertson, J. M. & Woodward, I. (1939). *Proc. Roy. Soc.* A, **171**, 398.

Müller, A. & Lonsdale, K. (1948). *Acta Cryst.* **1**, 129.

Vand, V. (1948). *J. Appl. Phys.* **19**, 852.

Vand, V. (1949). *Nature, Lond.*, **163**, 129.

Vand, V. (1951). *Acta Cryst.* **4**, 104.

Vand, V., Aitken, A. & Campbell, R. K. (1949). *Acta Cryst.* **2**, 398.

Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

Acta Cryst. (1951). **4**, 469

The positions of the barium atoms in hollandite.

By Anders Byström and Ann Marie Byström. *Institute of Inorganic and Physical Chemistry, University of Stockholm, and Geological Survey of Sweden, Stockholm 50, Sweden*

(*Received* 28 *April* 1951)

In a previous paper in this journal (Byström & Byström, 1950) a determination of the crystal structure of hollandite was reported. In the suggested structure, which is tetragonal or pseudotetragonal, the barium atoms occupy the positions $0, 0, 0$; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. However, there are only about 1·0 barium atoms per unit cell, and so only 50 % of the positions are filled with barium atoms. Because of the length of the c axis (2·86 A.) some of the Ba–Ba distances will be very short. A statistical distribution of the barium atoms over all positions requires that on the average every fourth barium atom has another barium atom at the distance of 2·86 A., which is only a little more than twice the ionic radius.

Prof. A. Westgren has suggested to us that the barium atoms may be arranged over the same atomic sites in another way. On each tetragonal axis only every other position is occupied by barium atoms. However, the positions on one tetragonal axis are independent of the positions on the other tetragonal axes, and thus a one-dimensionally ordered but two-dimensionally disordered arrangement of the barium is obtained. This arrangement will give the same intensity distribution as that previously suggested, but as no close Ba–Ba distances are obtained in this case it is obviously preferable.

This modification of the arrangement of the barium atoms may have the consequence that the objections against water molecules in the vacant positions are less convincing (see Byström & Byström, 1950, p. 155). It is in fact possible that some of the water, which is always present in these minerals, is placed between the barium atoms (and probably forming hydrogen bonds with the surrounding oxygen atoms). The observed densities are in some cases somewhat higher than those calculated with all the water molecules among the oxygen atoms in sixteen atomic sites. This may be an indication that some part of the water lies in the positions on the fourfold axes, and leads to a modification of the general formula, thus:

$$(\mathrm{Ba, K, Pb})_{2-y}(\mathrm{H_2O})_u(\mathrm{Mn, Fe})_{8-z}(\mathrm{O, OH})_{16};$$

y is always close to unity, but may be somewhat less in the coronadites; u is probably always small and cannot possibly exceed unity; z is equal to or close to zero ($< 0·5$) in minerals hitherto analysed.

An interesting consequence of the suggested arrangement of barium atoms and vacant sites or water molecules on the fourfold axes is that atomic sites belonging to the same point position are not equivalent, as there occurs a further one-dimensional order of a period twice that of the unit cell.

Reference

Byström, A. & Byström, A. M. (1950). *Acta Cryst.* **3**, 146.