The Crystal Structure of the Etherate of Sodium Hydridodiethylberyllate

By G. W. ADAMSON and H. M. M. SHEARER

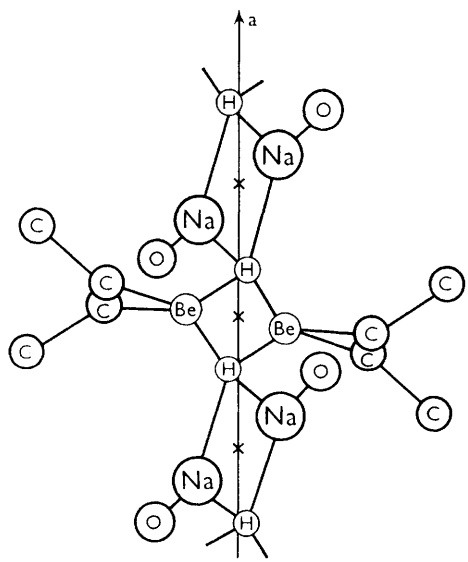
(*Chemistry Department, University of Durham*)

ALKYLBERYLLIUM hydride derivatives, of the formula $Na_2(R_4Be_2H_2)$ have recently been prepared[1] and shown to have the beryllium atoms linked by hydrogen bridges.[2] When R = Et, the compound crystallises from diethyl ether with one molecule of ether per sodium atom.

An *X*-ray examination shows that the monoclinic unit cell contains two units of $(NaOEt_2)_2$-$(Et_4Be_2H_2)$ with $a = 5{\cdot}04$, $b = 11{\cdot}17$, $c = 20{\cdot}90$ Å, $\beta = 101°\ 15'$ and space group $P2_{1/c}$. The three-dimensional intensity data were recorded using precession and equi-inclination Weissenberg techniques and were estimated visually. The structure was elucidated by calculation of the Patterson function and application of superposition methods. The positions of the atoms, other than hydrogen, were refined by Fourier and least-squares methods first with isotropic and then anisotropic temperature parameters. The reliability index *R* for the 1124 independent reflections is now 0·16.

The Figure shows schematically the arrangement of atoms along the *a* axis. The beryllium atoms are related by the centre of symmetry at $(\frac{1}{2}00)$, giving rise to centrosymmetric $Et_4Be_2H_2$ units with the berylliums linked by hydrogen bridges as expected. The mean beryllium–carbon bond length is 1·80 Å, compared with the value of 1·83 Å obtained by the addition of covalent radii.[3] The beryllium atom and the adjoining methylene carbons lie within experimental error on the mean plane passing through the centre at $(\frac{1}{2}00)$. Above and below this plane lie pairs of sodiums, related by the centres of symmetry at (000) and its equivalent positions. Attached to each sodium is an ether oxygen, the sodium–oxygen distance being 2·35 Å and the sodium–sodium–oxygen angle 167°. The ether carbon atoms were found to have large temperature parameters and are not shown in the Figure, although their positions are known.

A difference electron-density distribution, with the atoms other than hydrogen subtracted out, indicated the positions of the hydrogens in the ethyl groups attached to beryllium. It also showed a well-defined peak in the region expected for the bridging hydrogen, with two sodiums and two berylliums around it in a distorted tetrahedral arrangement. The beryllium–hydrogen distance of 1·4 Å compares with an average value of 1·33 Å found for bridging boron–hydrogens in a number of boron hydrides and the sodium–hydrogen distance is 2·4 Å, equal to that in sodium hydride. The sodium–sodium separation of 3·62 Å is less than in the metal (3·72 Å) but greater than in sodium hydride (3·45 Å) where each sodium is surrounded by six hydrogens. The beryllium–beryllium separation of 2·20 Å is very similar to that in the free metal. The structure may be regarded as built up of $(NaOEt_2)^+$ cations and $(Et_4Be_2H_2)^{2-}$ anions but the similarity in the positions of the sodiums and the berylliums with respect to the bridging hydrogens suggests that it may be unrealistic to differentiate too markedly between the two kinds of metal–hydrogen bonding.



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[1] G. E. Coates and G. F. Cox, *Chem. and Ind.*, 1962, 229.
[2] N. A. Bell and G. E. Coates, *J. Chem. Soc.*, 1965, 692.
[3] L. Pauling, "The Nature of the Chemical Bond," Cornell Univ. Press, Ithaca, 1960.

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