Crystal Structure of Potassium Amidoberyllate

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Summary The $[Be(NH_2)_3]^-$ anion is monomeric with approximate D_{3h} symmetry; the mean Be–N distance is 1·592 Å.

POTASSIUM AMIDOBERYLLATE was prepared by the reaction of metallic beryllium with a solution of potassium in liquid ammonia.[1] An i.r. study indicated the presence of (NH_2) groups,[2,3] and two structures were considered possible; either polymeric tetrahedral beryllium (as in the structure of $CsBeF_3$)[4] or monomeric trigonal beryllium. An *X*-ray study has resolved this ambiguity.

Crystal data: H_6N_3BeK, $M = 96{\cdot}19$, orthorhombic, $a = 12{\cdot}880(9)$, $b = 11{\cdot}213(9)$, $c = 13{\cdot}195(10)$ Å, $U = 1905{\cdot}5$ Å^3, $D_c = 1{\cdot}34$, $D_m = 1{\cdot}33$, $Z = 16$, space group *Pbca*.

The intensities of 881 independent reflections above background ($2\theta < 45°$) were measured on an G.E. XRD 5 manual diffractometer by the stationary-crystal stationary-counter technique. The structure was solved by Patterson and Fourier methods and refined (K, N, Be anisotropic, H isotropic) to R 0·040. The asymmetric unit contains two potassium cations and two $[Be(NH_2)_3]^-$ anions. The anions are monomeric and have approximate D_{3h} symmetry with the amide groups acting as terminal ligands. The deviations from D_{3h} symmetry are small but significant; *e.g.* the N–Be–N angles range between 118·3(5) and 121·6(5)° and the average deviation of a hydrogen atom from a N,N,N plane is 0·21(5) Å, but such deviations follow no distinct pattern and can be ascribed to intermolecular packing, there being several H···H contacts of *ca.*

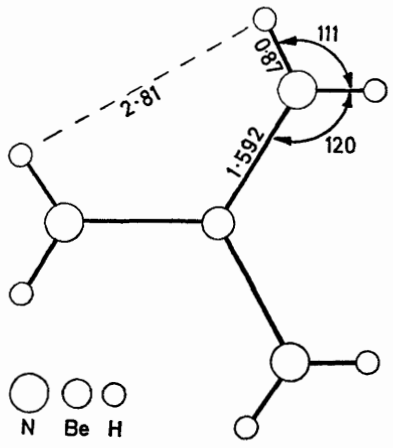

FIGURE. *Mean dimensions in the* $[Be(NH_2)_3]^-$ *anion.*

2·50 Å. The mean dimensions are shown in the Figure. Those concerning the NH_2 groups are in good agreement with those found in $Mg(NH_2)_2$.[5]

The individual Be–N bond lengths are 1·598(8), 1·584(8), 1·607(8), 1·576(8), 1·587(8), and 1·600(8) Å. These values are similar to those found in the two-co-ordinate bis(trimethylsilylamino)beryllium [1·566(17) Å][6] and to the terminal Be–N distances [1·573(11) Å][7] found in the trimeric bis(dimethylamino)beryllium, and are thus consistent with dative p_π–p_π Be ← N bonding. All lengths quoted are considerably shorter than those found for a Be–N single bond [1·76(1) Å] in the trimer[7] in which both atoms are in polymeric tetrahedral environments. It has been suggested that π bonding (Be ← N) only occurs when valence saturation of the beryllium atom through polymerisation is impossible: as, for example, in the sterically crowded molecules mentioned in refs. 6 and 7. This is not true for the present anion as an alternative polymeric tetrahedral structure would be sterically stable.

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