The Molecular Structure of Bis[di(trimethylsilyl)amino]beryllium

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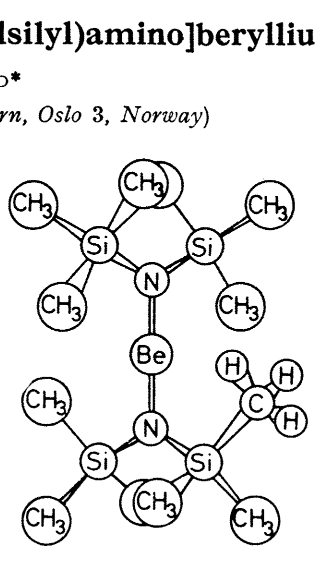
Summary The molecular structure of $[(Me_3Si)_2N]_2Be$ has been determined by gas-phase electron diffraction.

BIS[DI(TRIMETHYLSILYL)AMINO]BERYLLIUM, $[(Me_3Si)_2N]_2$-Be, first prepared by Bürger, Forker, and Goubeau,[1] is monomeric in organic solvents and forms no adducts even with strong complexing agents.[1] We have determined the molecular structure of this unusual beryllium derivative which, with its 55 atoms, is the largest molecule successfully studied by gas phase electron diffraction till now.

The sample of bis[di(trimethylsilyl)amino]beryllium was a gift from Dr. H. Bürger. The electron scattering pattern from s = 3·50—38·00 Å^{-1} was recorded on the Oslo electron diffraction unit[2] with a nozzle temperature of 120 ± 15°. The molecular structure was initially refined under the assumption that the molecular symmetry was D_{2d}. It became clear, however, that a model of this symmetry would lead to prohibitively short distances between methyl groups bonded to different Si atoms and that it was incapable of yielding a satisfactory fit between experimental and calculated intensities. The model was therefore deformed in the following way: the D_{2d} symmetry of the $Si_2NBeNSi_2$ skeleton was retained, but the trimethylsilyl groups were allowed to rotate about the Si–N bonds in such a way that the distance between the methyl groups increased. The molecular symmetry was thus lowered to D_2. (See Figure.)



The four bond distances, the three valence angles, the torsional angle of the trimethylsilyl groups and the vibrational amplitudes of the 13 most important atom pairs were refined by least-squares calculations on the intensity data, using a diagonal weight matrix.[3] The refinement converged to give the bond distances and angles listed in the Table. The estimated standard deviations listed have

TABLE

Bond distances and valence angles of bis[di(trimethylsilyl)amino]-beryllium with estimated standard deviations

Be–N ..	..	1·566(17) Å
N–Si ..	..	1·726(6) Å
Si–C ..	..	1·880(4) Å
C–H ..	..	1·094(7) Å
∠ SiNSi	..	129·3(0·5)°
∠ NSiC	..	110·0(0·6)°
∠ SiCH	..	114·1 (1·4)°
Me_3Si twist	..	7·8(2·1)°

been obtained in the following way: the standard deviations obtained by the least-squares calculations were multiplied by a factor of three to compensate for correlation in our data[4] and further expanded to take into account the uncertainty of 1·4 p.p.t. in the electron wavelength.

The Be–N and N–Si bond distances and the allene-like structure of the $Si_2NBeNSi_2$ skeleton are consistent with dative p_π–p_π Be–N bonding[5] and dative p_π–d_π N–Si bonding.[6] It should not be concluded, however, that dative π-bonding is the reason for the monomeric nature of the compound or its inertness to complexing agents. A molecular model makes it clear that the bulk of the amino group is sufficient to prevent the formation of a trimeric structure like that of bis(dimethylamino)beryllium[5] or the approach of complexing agents. Dative Be–N π-bonding probably only becomes operative when valence saturation of the beryllium atom through polymerization is impossible.

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