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THE CRYSTAL STRUCTURE OF TRIBENZOTALARENE

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The compound tribenzotalarene was first reported by Dewar, Dougherty, and Fleischer[1] and has the empirical formula $C_8H_{11}BNO$. On the basis of chemical and spectral evidence a trimeric strain-free cage structure was proposed by these authors. We now report the molecular structure of tribenzotalarene as determined by a three dimensional X-ray diffraction study. This structure was proposed for study to confirm the proposed molecular structure and as a test to the direct phase determining methods for equal-atom noncentric structures.

Tribenzotalarene crystallizes in the orthorhombic space group $P2_12_12_1$ with cell constants a=26.97, b=8.07, c=10.02 Å and has an observed density of 1.31 gm/cm^3 and a calculated density of 1.30 gm/cm^3 with four molecules per unit cell.

The structure was solved by direct methods[2] using the program MAGIA[3] and refined by least-squares with isotropic temperature factors yielding an R-factor of 0.064 for the 1065 observed reflections. The structure as shown in the drawing confirms the original proposed structure.[1] The structure has two features of special interest: one is that the $(B\text{-}O)_3$ six membered ring is nearly planar(all atoms are within .13 Å of the "best plane" of the six atoms); the second is the B-N bond length is 2.00 (± .02)Å which is about .5 Å longer than an expected B-N single bond length. This long bond length is probably due to the steric constraints imposed by the multicyclic nature of the molecule.

All other bond lengths and angles are in the expected range.

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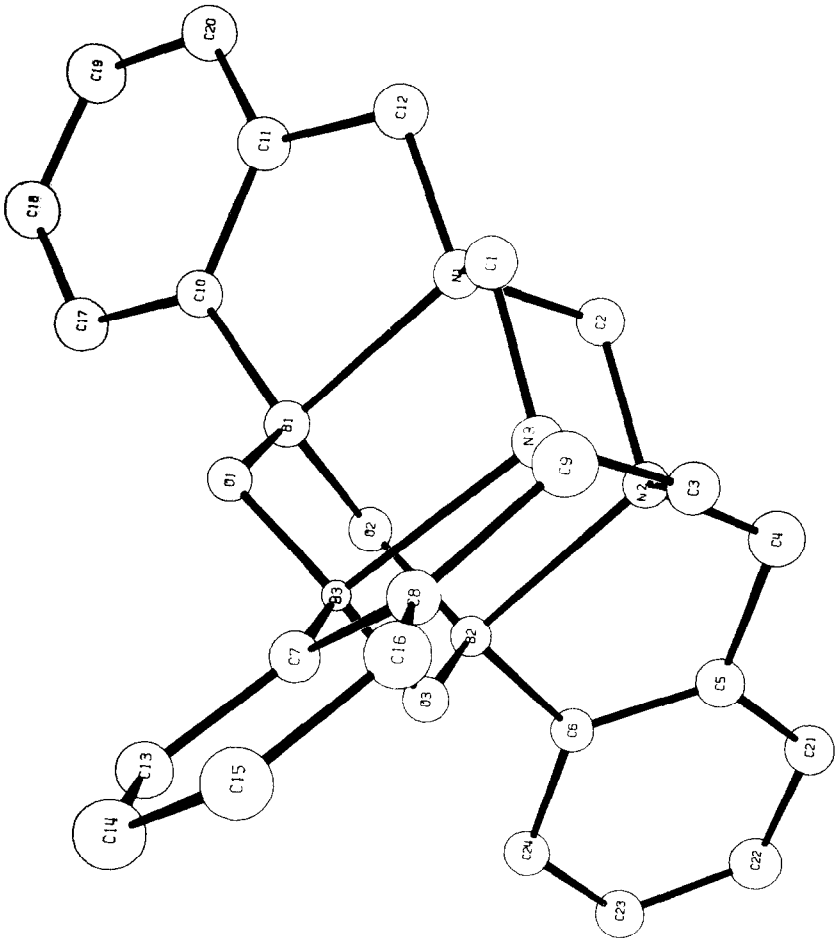

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