Preferred Conformation of Bicyclo[3,3,2]decane:- Crystal Structure of 7,8,9,10-Tetrahydro-6,10-propano-6*H*-cyclohepta[*b*]quinoxaline

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Summary The crystal structure of the quinoxaline derivative of bicyclo[3,3,2]decan-9,10-dione has been determined by *X*-ray analysis and shows that the molecule has a boat–chair conformation.

Considerable interest has been shown recently in the preferred conformation of the bicyclo[3,3,2]decane system. Evidence has been presented in favour of both the boat–chair[1] and twin-chair[2,3] conformations, while calculations[4] have suggested that these are of similar energy content whereas the twin-twist–boat conformation is less stable than either. Two of the authors have already suggested[3] that the twin-chair conformation is preferred when there is a flexible sp^3 system around C(9), C(10), but that the boat–chair conformation is preferred when there is a rigid sp^2 system at C(9), C(10).

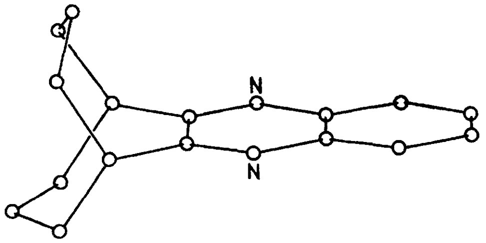

Figure. *Conformation of the molecule.*

The title compound was synthesised by the method described for the homoadamantane analogue by Schlatmann *et al.*[5] *Crystal data:* $C_{16}N_2H_{18}$; space group $P2_12_12_1$; $Z = 4$; $a = 710(1)$, $b = 722(1)$, $c = 2561(2)$ pm; $D_m = 1{\cdot}23$; $D_c = 1{\cdot}22$ g cm^{-3}.

Data were collected on a Hilger–Watts linear diffractometer and the structure was solved by direct methods. Refinement by full matrix least squares with anisotropic temperature factors but not hydrogen atoms gives an R factor of 0·086.

The conformation of the molecule is of the boat–chair type shown in the Figure. The bond lengths (e.s.d. = 1 pm) are all within the expected limits [C–C (sat) = 154(2), C–N(arom) = 135(2), C–C(arom) = 141(2) pm] and the angles (e.s.d. = 0·5°) in the aromatic moiety are normal. The bridgehead atoms lie in the plane of the aromatic system which constrains the molecule to have almost exact mirror symmetry perpendicular to this plane. As twisting is impossible the molecule must relieve the strain in the bridged system by distortion of bond, torsional, and dihedral angles and these are 5—10° different from those calculated from a Dreiding model. All the differences can be described as a pronounced 'flattening' of the two halves of the cyclo-octane ring which is necessary to relieve the serious non-bonded H---H interactions.

It would appear from this evidence, and Russell's e.s.r. measurements[1] that the boat–chair conformation is preferred whenever C(9), C(10) are held in a rigid coplanar configuration. However, if there is a flexible two-carbon bridge, the twin-chair form may well be more stable, and a derivative of this type is being investigated.

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