The ^1H Nuclear Magnetic Resonance Spectra and Conformations of *cis*- and *trans*-Decahydroquinoline

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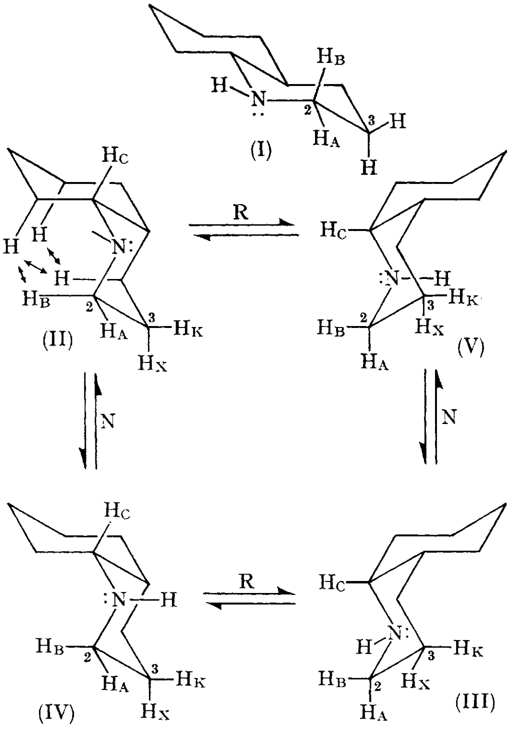
trans-DECAHYDROQUINOLINE is expected to exist entirely in conformation (I). *cis*-Decahydroquinoline, however, can assume two conformations, (II) and (III), related by ring inversion (R) and nitrogen inversion (N) as shown.

If a hydrogen atom is more space-demanding than the nitrogen lone pair,[1] the order of stability of these conformations is (III) > (II) > (IV) ≡ (V), since the 1,4-repulsions, illustrated only in (II), dominate the situation as far as nonbonded interactions are concerned.

The ^1H n.m.r. spectrum of *trans*-decahydroquinoline (I) (C_6H_6, CCl_4, or $CHCl_3$) consists largely of an ill-defined resonance from τ 7·9—9·2, but signals due to the protons H_A and H_B at position 2 are well separated at low field. The signal at τ 7·15 is due to the equatorial proton H_A, as it is a doublet ($J \simeq 12$ c./sec.), each component being a quartet (separations ~ 3 c./sec.). The signal at τ 7·55 is due to the axial proton H_B, as it is a triplet ($J \simeq 12$ c./sec.), each part being a doublet (separation *ca.* 4 c./sec.). This low-field pattern is simplified to an AB quartet ($J = 11{\cdot}8$ c./sec.) by strong irradiation at τ 8·44.

In the ^1H n.m.r. spectrum of *cis*-decahydroquinoline (C_6H_6 or CCl_4), the signals of H_A, H_B, and H_C are well separated at low field from a broad resonance between 7·9 and 9·1. In addition, decoupling experiments which will be described in the full paper, located the *axial* proton at position 3 (H_K) at τ 8·32 and the *equatorial* proton at position 3 (H_X) at τ 8·74. The following features were noted:



(a) H_C appears at τ 7·35 as a narrow signal (half band-width 8 c./sec.; one-third band-width 11 c./sec.), consistent with (III) or (V), but not with (II) or (IV); (b) the unusual deshielding of the axial proton H_K relative to the equatorial proton H_X is expected[2] for (III) or (V), but not for (II) or (IV); (c) the chemical shifts of the equatorial (H_A) and axial (H_B) protons at position 2 are τ 7·12 and 7·52, respectively, values which are almost identical to those of the corresponding protons in (I). This is consistent with either (III) or (V), but not with (II) or (IV), as in the latter case H_B would be abnormally deshielded.[2]

These arguments clearly demonstrate that *cis*-decahydroquinoline consists largely of (III) or (V) or a mixture of both. However, (V) cannot be involved to an appreciable extent, because this would imply an equal involvement of (IV), since (IV) and (V) are energetically equivalent. It is concluded that *cis*-decahydroquinoline exists largely, or exclusively, in conformation (III), and that a hydrogen atom is appreciably more space-demanding than the nitrogen lone-pair.

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[1] *Cf.* E. L. Eliel and Sr. M. Carmeline Knoeber, *J. Amer. Chem. Soc.*, 1966, **88**, 5347, and references therein.

[2] H. Booth, *Tetrahedron*, 1966, **22**, 615.