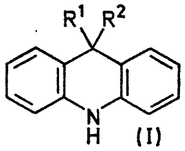
The Conformation of 9,10-Dihydroacridines

By G. A. TAYLOR*
(*Department of Chemistry, University of Sheffield, Sheffield* S3 7HF)
and S. A. PROCTER
(*Department of Pure and Applied Science, Doncaster College of Technology, Doncaster, Yorks.*)

Summary The n.m.r. spectra of a series of 9-substituted 9,10-dihydroacridines are consistent with a preferred conformation having a boat-shaped central ring with the more bulky 9-substituent in a ψ-axial orientation.

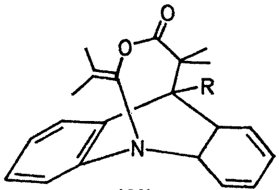
RECENT interest[1] in the conformation of 9,10-dihydroanthracenes prompts us to report our results in a study of 9-substituted 9,10-dihydroacridines (I). A series of these containing all combinations of the substituents H, Me, Et, Pr^i, and Bu^t (except for $R^1 = Pr^i$, $R^2 = Bu^t$, and $R^1 = R^2 = Bu^t$) has been prepared and the n.m.r. spectra measured for deuteriochloroform solutions. In all cases where $R^1 = R^2$ the two substituent groups are magnetically equivalent, indicating a planar time-average structure. Models suggest that the lowest energy conformation of (I; $R^1 = R^2 = H$) has a flattened, boat-shaped central ring with a very low barrier to inversion.

Comparison of the n.m.r. spectra of a series of these compounds, in which R^1 remains constant and R^2 varies from H to Bu^t, shows interesting trends in the τ values of R^1. For the series $R^1 = Me$, the signal due to R^1 moves steadily downfield from τ 8·66 to 8·25 as R^2 progresses from H to Bu^t. Likewise, the signal due to the CH_2 group in the series $R^1 = Et$ moves from τ 8·37 to 7·66 whereas the CH_3 signal of the ethyl group varies in an irregular fashion between τ 9·40 and 9·25. For $R^1 = Pr^i$ the methine proton signal decreases from τ 8·23 when $R^2 = H$ to τ 7·48 when $R^2 = Pr^i$. These variations are taken to indicate an increasing population of a preferred conformation as R^2 changes from a small to a bulky group. Models suggest that the preferred conformation will be that in which the larger substituent at the 9-position is in a ψ-axial orientation and confirmation for this comes from a comparison of the spectra of (Ia) and (Ib) with the bridged compounds (IIa) and (IIb).[2] Chemical shifts for the relevant groups are given beside the diagrams.



(I)

a; R^1 = Me (τ 8·25) R^2 = Bu^t (τ 9·23)
b; R^1 = Et (τ 7·66, 9·33) R^2 = Bu^t (τ 9·22)



(II)

a: R = Me (τ 8·26)
b: R = Et (τ 7·71, 9·31)

Surprisingly, for the series $R^1 = H$, $R^2 = H—Bu^t$ the signal due to R^1 moves steadily upfield from τ 5·95 to 6·37 as R^2 increases in size. This behaviour must be due to the different position of the H atom with respect to the boundary between the shielding and deshielding zones of the aromatic systems.

(*Received, October 2nd,* 1969; *Com.* 1490.)

---

[1] A. L. Ternay, A. W. Brinkmann, S. Evans, and J. Herrmann, *Chem. Comm.*, 1969, 654, and references therein; J. MacMillan and E. R. H. Walker, *Chem. Comm.*, 1969, 1031.

[2] S. A. Procter and G. A. Taylor, *J. Chem. Soc.* (*C*), 1967, 1937.