NMR SPECTRAL ASSIGNMENT OF 6,13-DIHYDRO-5-OXO-5H-ISOQUINOLINO[1,2-b][1,3]BENZOXAZINE

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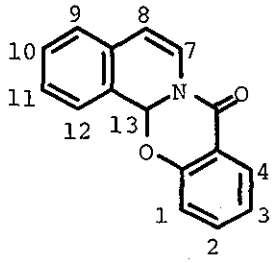
A revision of nmr spectral assignment of the title compound is described.

We have recently reported the synthesis of 6,13-dihydro-5-oxo-5H-isoquinolino[1,2-b][1,3]benzoxazine (1)[1] by a condensation of isoquinoline with salicyl chloride. On the basis of the coupling constant (J = 7.0 Hz) the signal at 7.95 δ was assigned as the low field doublets arising from proton C_7-H.[1] Comparison of this assignment with that reported by Uff[2] (2) for a proton in a similar environment; C_3-H, 6.65 δ (the Reissert compound 2) suggested that the assignment for 1 was too low.

Therefore careful reinvestigation of the nmr spectrum of 1 revealed that the resonance at 7.95 δ showed a double doublet having J = 2 and 7.0 Hz which suggested this resonance should be assigned

as C_4-H. This was confirmed by irradiation of the upfield part of the doublet at 5.85 δ (J = 7.0 Hz) when part of the aromatic multiplet at 7.42 δ collapsed to a singlet. No effect was discernible on the low field doublet at 7.95 δ. Thus a doublet at 7.95 δ reported earlier should be assigned as C_4-H.



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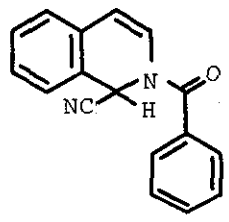

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Received, 9th May, 1978