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The assignment of the hyperfine coupling constants for the pyridyl protons in aryl and alkyl n-substituted bipyridylium radical cations (1983) *Tetrahedron*, 39 (21), pp. 3615-3620. Cited 1 time.

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Abstract

The coupling constants for the pyridyl protons of the radical cations of N,N'-dimethyl-4,4'-bipyridylium dichloride PQ⁺ and N,N'-diphenyl-4,4'-bipyridylium dichloride DPQ⁺ have been unambiguously assigned from an ENDOR study of selectively deuterated compounds. The experimental results confirm the early theoretical assignments for PQ⁺ made by Johnson and Gutowsky; however subsequent assignments for DPQ⁺ based on this work have now been revised. The revision of the assignments and the difference between the two compounds are discussed using INDO molecular orbital calculations. © 1983.