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An electron spin, ENDOR, and TRIPLE resonance and INDO study of fluorine-substituted N,N'-diphenyl-4,4'-bipyridylium radical cations
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Abstract
E.s.r., ENDOR, and TRIPLE resonance results are reported for the radical cation of N,N'-diphenyl-4,4'bipyridylium dichloride and a series of its fluorophenyl analogues. The effect of ortho-, meta-, and parasubstitution on the spin density distribution within the molecule is discussed and the observed coupling constants for the fluorine-substituted phenyl derivatives are analysed with the aid of INDO molecular orbital calculations. The magnitude of the spin delocalised into the phenyl rings when ortho-substituted suggests that these rings are substantially twisted with respect to the plane of the bipyridylium rings.