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CONFORMATIONAL BEHAVIOR OF FLUOROCARBONYL TRIAFULVENES

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4-Fluorocarbonyl-4-trifluoromethyltriafulvenes were synthesized by cycloaddition reactions of F-dimethylketene and cyclopropenones followed by elimination of COF_2 (I. Agranat et al., Tetrahedron 31, 1163 (1975)). A dynamic ^{19}F NMR investigation of the conformational behavior of these fluorocarbonyltriafulvenes indicated high energy barriers ($\Delta G_c^{\ddagger}$) about the fluorocarbonyl - triafulvene bonds. For 4-fluorocarbonyl-4-trifluoromethyl-1,2-diphenyltriafulvene, $\Delta G^{\ddagger}_{240\ K}$ = 11.0 Kcal/mole. For comparison, the free energy barrier in benzoyl fluoride is 7.0 Kcal/mole (F.A.L. Anet and M. Ghiaci, J.C.S. Chem. Comm 588 (1979)). For (E)- and (Z)-1-ferrocenyl-4-fluorocarbonyl-4-trifluoromethyl-2-phenyltriafulvene $\Delta G_c^{\ddagger}$ = 11.9 and 11.0 cal/mole. The barriers for E,Z-isomerizations in these triafulvene derivatives are >23 Kcal/mole.