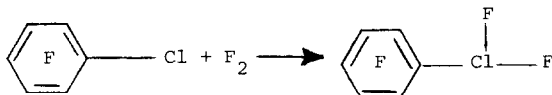


PENTAFLUOROPHENYLCHLORINE(III) DIFLUORIDE

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The title compound has been synthesized by oxidation of pentafluorophenyl chloride with elemental fluorine.



Pentafluorophenylchlorine(III) difluoride was a colorless liquid (Boiling Point $96-98^\circ\text{C}$) which fumed when exposed to air. It oxidized 2.0 equivalents of iodide ion and did not decolorize a 0.1 M potassium permanganate solution. Anal. calcd. for $\text{C}_6\text{F}_5\text{ClF}_2$: C, 29.96; F, 55.29; Cl, 14.74. Found: C, 29.79; F, 55.07; Cl, 14.90. The ^{19}F nuclear magnetic resonance spectrum at 25°C consists of a doublet at 141.63, a triplet at 157.05, and a triplet at 162.25 ppm (CFCl_3). The liquid phase infrared spectrum contains absorption bands as 703 (s), 640 (vs), 621 (vs), 553 (vs), 530 (s), 502 (w), 459 (s), 425 (s), 395 (m), 370 (m), 334 (m), 315 (vs), 301 (m), 278 (m), 242 (vw), and 220 (vw) cm^{-1} .

Molecular ions at m/e 240 and 242 accompanied by supporting fragmentation patterns, were present in the mass spectrum along with the isotopic ratio of approximately 3:1 as expected for the ^{35}Cl and ^{37}Cl . The mass spectrum of $\text{C}_6\text{F}_5\text{ClF}_2$ consists of peaks assigned to $\text{C}_6\text{F}_5\text{ClF}_2^+$ (13), $\text{C}_6\text{F}_5\text{ClF}^+$ (0.71), $\text{C}_6\text{F}_5\text{Cl}^+$ (26), $\text{C}_6\text{F}_4\text{Cl}^+$ (0.92), C_6F_6^+ (6.7), C_6F_5^+ (29), C_6F_4^+ (0.72), C_5F_3^+ (100), ClF_2^+ (1.1), ClF^+ (0.7), and Cl^+ (0.2). Metastable ions were observed in the following region: 184.5, 170.0, 165.6 and 56.0. The peak at m/e 240 showed a very weak metastable peak at $m^* = 144.0$ from the process: $240 \longrightarrow 186 + \text{ClF}^\circ$.