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Gas-phase reactions of singly and multiply-charged fullerene cations, C_{60}^{x+} ($x = 1$–3), with iron pentacarbonyl: kinetic control by Coulombic barriers[1]

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Abstract

Selected-ion flow tube measurements of rate coefficients and product distributions are reported for the reactions of $C_{60}^{\cdot+}$, C_{60}^{2+} and $C_{60}^{\cdot 3+}$ with iron pentacarbonyl in helium buffer gas at 0.35 ± 0.01 torr and 294 ± 3 K. A fast bimolecular reaction is observed with $C_{60}^{\cdot+}$ leading to a stable derivatized C_{60} cation, $C_{60}Fe(CO)_4^{\cdot+}$, but the chemistry switches for the higher charge states to charge separation by dissociative-electron transfer leading to the elimination of one and two molecules of CO with C_{60}^{2+} and $C_{60}^{\cdot 3+}$, respectively. The specificity of these CO eliminations is rationalized in terms of favourable entropy changes and kinetic control by energy barriers arising from Coulombic repulsion between product ions. © 1997 Elsevier Science B.V.

Keywords: Fullerene ions; Iron pentacarbonyl; Charge separation; Coulombic barriers

1. Introduction

The remarkable stability and ready availability of multiply-charged fullerene cations affords an opportunity to explore the chemistry of these cations as a function of charge state. We have shown previously in our laboratory that new chemical pathways often become accessible in the gas phase at room temperature (in helium buffer

[1] Dedicated to Keith Jennings on the occasion of his 65th birthday, in part for his outstanding contributions in the field of mass spectrometry and gas-phase ion chemistry.

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