REACTION CHEMISTRY OF EPOXIDES WITH FLUORINATED CARBOXYLIC ACIDS

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In the course of measurements to develop a chiral tag rotational spectroscopy methodology for establishing the absolute configuration of fluorinated carboxylic acids, an interesting reaction chemistry was found. In most cases, fluorinated carboxylic acids undergo ring opening of epoxides under ambient conditions. Reactions of four fluorinated carboxylic acids, difluoroacetic acid, trifluoroacetic acid, and pentafluoropropionic acid, with propylene oxide (PO) were explored. The reactions were performed externally to the spectrometer and internally in the gas phase by flowing PO over the fluorinated acid samples. External reactions were performed by adding volumetric amounts of PO with each carboxylic acid in a 4:1 molar ratio. The reactions were highly exothermic. The reaction mixtures were analyzed by rotational spectroscopy using a chirped-pulsed Fourier transform rotational spectrometer. These measurements showed that the reaction products are created through epoxide ring-opening at both epoxide ring carbons. This reaction chemistry, in principle, offers a way to perform chiral analysis through covalent tagging, but this application would require retention of configuration in the reaction. The reaction products were subsequently chiral tagged to determine the extent of configuration retention. These experiments show that partial retention of configuration is achieved. The scope of reaction was further explored using trifluoropropylene oxide and styrene oxide. Using trifluoropropylene oxide no reaction or reaction products were observed. Styrene oxide produced epoxide ring-opening products both at most- and least-substituted carbon. In contrast to propylene oxide, only one conformer was observed for the reaction product of the fluorinated acids and styrene oxide.