

REACTION CHEMISTRY OF EPOXIDES WITH FLUORINATED CARBOXYLIC ACIDS

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During measurements designed to develop a chiral tag rotational spectroscopy methodology for establishing the absolute configuration of a known persistent fluorinated carboxylic acid pollutant (FRD-903), an interesting reaction chemistry was observed. In several cases, highly fluorinated carboxylic acids participate in ring opening of epoxides under ambient conditions. Reactions of three 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. Reactions were performed by adding 4:1 molar equivalents of PO to carboxylic acid, and each reaction was 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 the products, both the ring-opening at the least- and most-substituted carbon on the epoxide ring, are racemized. While these results are not useful for obtaining the absolute configuration, these results further our understanding of the chemistry involved in these reactions. Covalently modifying fluorinated carboxylic acids can be achieved, and establishing absolute configuration could be possible with a more controlled reaction to prevent racemization of the chiral center on the epoxide.