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Ruthenium(II)-Catalyzed Transfer Deuteration of Acetophenone and Derivatives

Felix R. Perez and Saeed Attar, Department of Chemistry, California State University, Fresno, CA 93740.

Abstract

Deuterated compounds play an important role in research because they give scientists the ability to study specific aspects of a reaction. In this study, using $\text{RuCl}_2(\text{PPh}_3)_3$ (**1**) as a catalyst, various deuterated 1-phenylethanol derivatives were prepared by transfer deuteration of acetophenone and derivatives, R-PhC(=O)CH_3 where $\text{R} = \text{H}$, 3-Cl, 3- CH_3 , and 2- OCH_3 . Isopropanol- d_8 was used as the deuterium donor and acetophenone as the acceptor. The percent conversion to the deuterated product was calculated using gas chromatography and compared with that obtained in the corresponding transfer hydrogenation reaction. The products formed were analyzed using mass spectrometry. The deuterium kinetic isotope effect slowed these reactions but did not affect the percent conversion. Mass spectrometry results also indicate that (a) sodium isopropoxide does not donate protons according to one mechanistic scenario, (b) other deuterated products are formed due to abstraction of alpha protons of acetophenone ($\text{R} = \text{H}$), and (c) benzophenone does not participate in this reaction due to steric reasons.