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Metal Catalyzed H-D Exchange Methods Using D_2O as a Deuterium Source: A Comparative Study in Different Sealed Devices

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In order to advance neutron research, we have investigated some easy-to-implement deuteration systems through H-D exchange reactions. Sub-gram to gram scale H-D exchange reactions of 1-butyl-3-methylimidazolium chloride ([C_4mim][Cl]) and acrylate polymer raw materials, such as methyl methacrylate and butyl acrylate, were investigated. The deuteration of C_4mim cation was successfully carried out in Parr Reactor system and a stainless steel sealed reactor, while that of the acryl moieties of acrylate polymer raw materials was effectively demonstrated in a D_2O/2-PrOH solvent system (the alkyl moieties remained unaffected).

KEYWORDS: Deuterium labeling, Ionic liquid, Taiatsu-stainless steel reactor

1. Introduction

Deuterium (^{2}H) is a stable isotope of hydrogen (^{1}H) and exists only in trace amounts (0.015%) in nature. Deuterium labeled compounds have been widely used as tracers for ^{1}H Nuclear Magnetic Resonance (NMR) spectroscopy, reaction mechanisms, and neutron studies, due to the different physicochemical properties in comparison with ^{1}H such as atomic mass and nuclear spin [1, 2]. Since the FDA recently approved deutetrabenazine (Austedo®) as a deuterated (heavy) prescription medicine, the interest of deuterium-labeled compounds in the development of new drugs by pharmaceutical companies has been growing [3].

Deuterated materials have been used in neutron studies to control the neutron scattering contrast of organic molecules and/or reduce the neutron incoherent scattering background of hydrogen. Deuteration methods using Parr Reactor systems, which are generally used in the synthesis of deuterated materials for use in neutron studies, have been established, and various kinds of deuterated compounds were synthesized in the