

Investigation of the reaction between Mu and Acetone in Trihexyl (Tetradecyl) Phosphonium Chloride Ionic Liquid

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The kinetics of H atom reactions in condensed phase is usually studied by pulse radiolysis. Such kinetics studies cannot be investigated in pure ionic liquid solvents because a high concentration of acid must be used to produce the H atom. Alternatively, in this study we employed transverse field- μ SR to probe H atom addition to acetone in a phosphonium ionic liquid and compared that with water. The measured activation energy and pre-exponential factor in ionic liquid is $E_a = 60.7 \pm 4.9$ kJ/mol and $\ln(A/M^{-1} s^{-1}) = 42.2 \pm 2.0$ respectively. The activation energy is greater than that for the same reaction carried out in water. The rate constants in ionic liquid and water are also significantly smaller than in heptane. *Ab initio* calculations have been used to describe the role of solvent on different potential reaction channels.