

Stereochemical reduction by NaBH₄ of ketone-β-cyclodextrin complexes

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A β-cyclodextrin (β-Cyd) inclusion complex containing some cyclic ketones (4-t-butylcyclohexanone, 2-methylcyclohexanone, 4-methylcyclohexanone, 3,3,5-trimethylcyclohexanone) as a guest was prepared by kneading method with aliquot addition of ethanol. The product was characterized by Fourier Transform Infrared (FTIR) spectrometer and UV spectrometer which proves the formation of inclusion complex where alkyl part is encapsulated with the hydrophobic part of β-cyclodextrin. Such inclusion compound was used for reduction of these ketones using NaBH₄ as reducing agent in ethanol. The reaction was monitored using thin layer chromatography (TLC) and FTIR. Exclusive formation of trans-4-t-butylcyclohexanol (Fig) was observed this case. In case of reduction of other substituted

cyclohexanones, propensity to form more of equatorial alcohol was observed. This is due to the complexation of β-cyclodextrin and 4-t-butylcyclohexanone by H bonding. Another advantage of 4-t-butylcyclohexanone is that the ketone is conformationally locked. Hence, once H bonding takes place from the equatorial side, the molecule cannot flip. It behaves like a rigid system. The chemical yields of various alcohols were high (~95-99%). The rates of reductions of the ketones were also appreciably high. All reduced products were characterized by standard instrumental techniques like FTIR and ¹HNMR (Figure 1).

Reference

1. K. P. Sambasevam, S. Mohamad, N. M. Sarih, N. A. Ismail, Int. J. Mol. Sci. 14 (2013) 3671-3682.

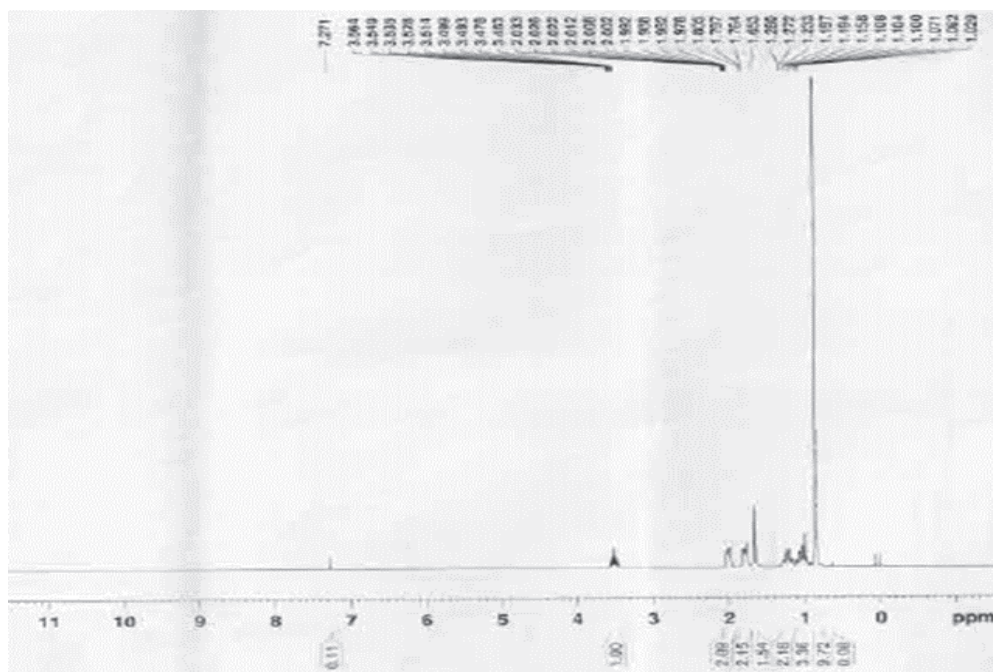


Figure 1: ¹HNMR spectrum of reduction product of 4-t-butylcyclohexanone