

Catalytic Reduction of Carbonyl Functional Groups in 2-Propanol by Molybdocene
Hydrides

by

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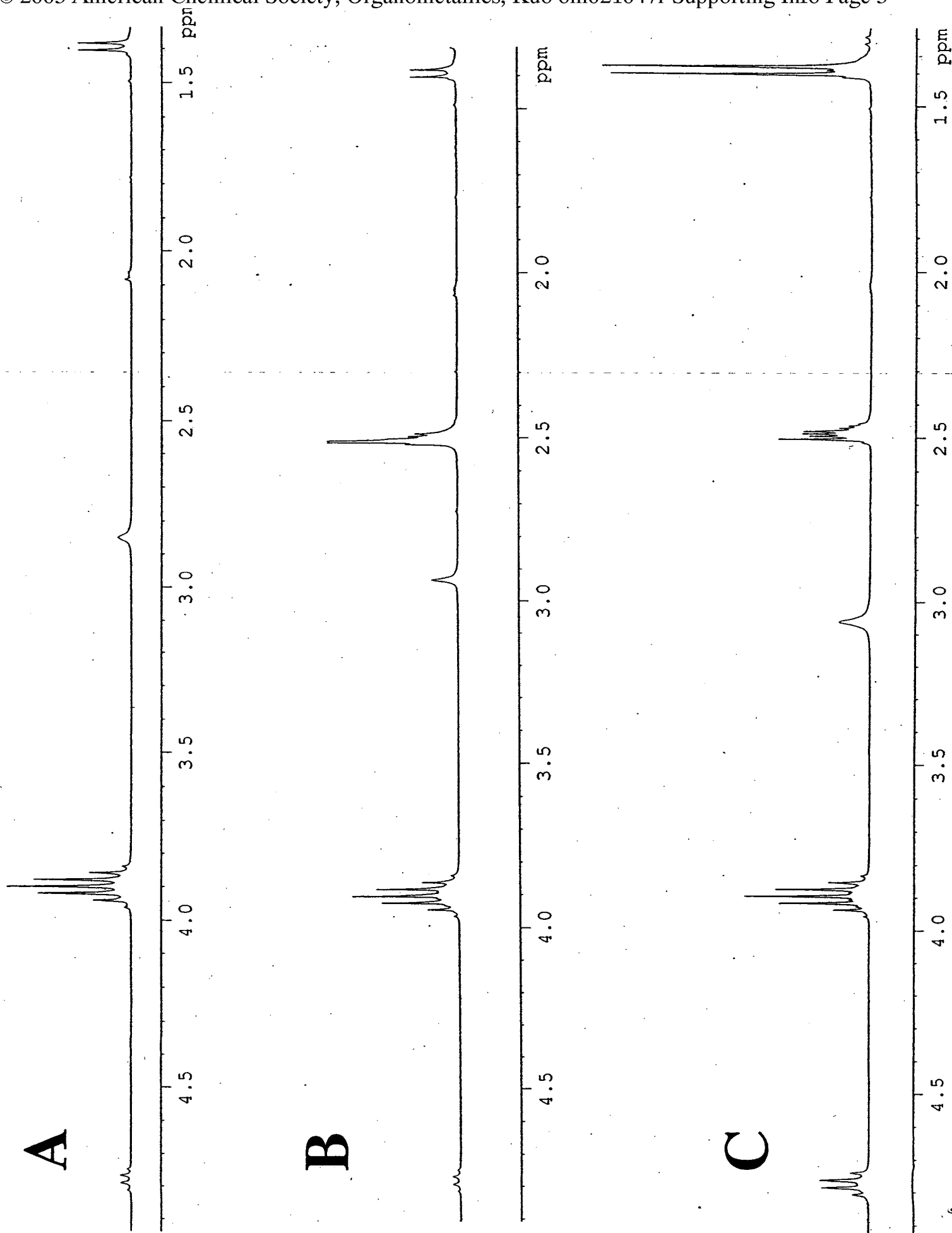
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SUPPORTING INFORMATION

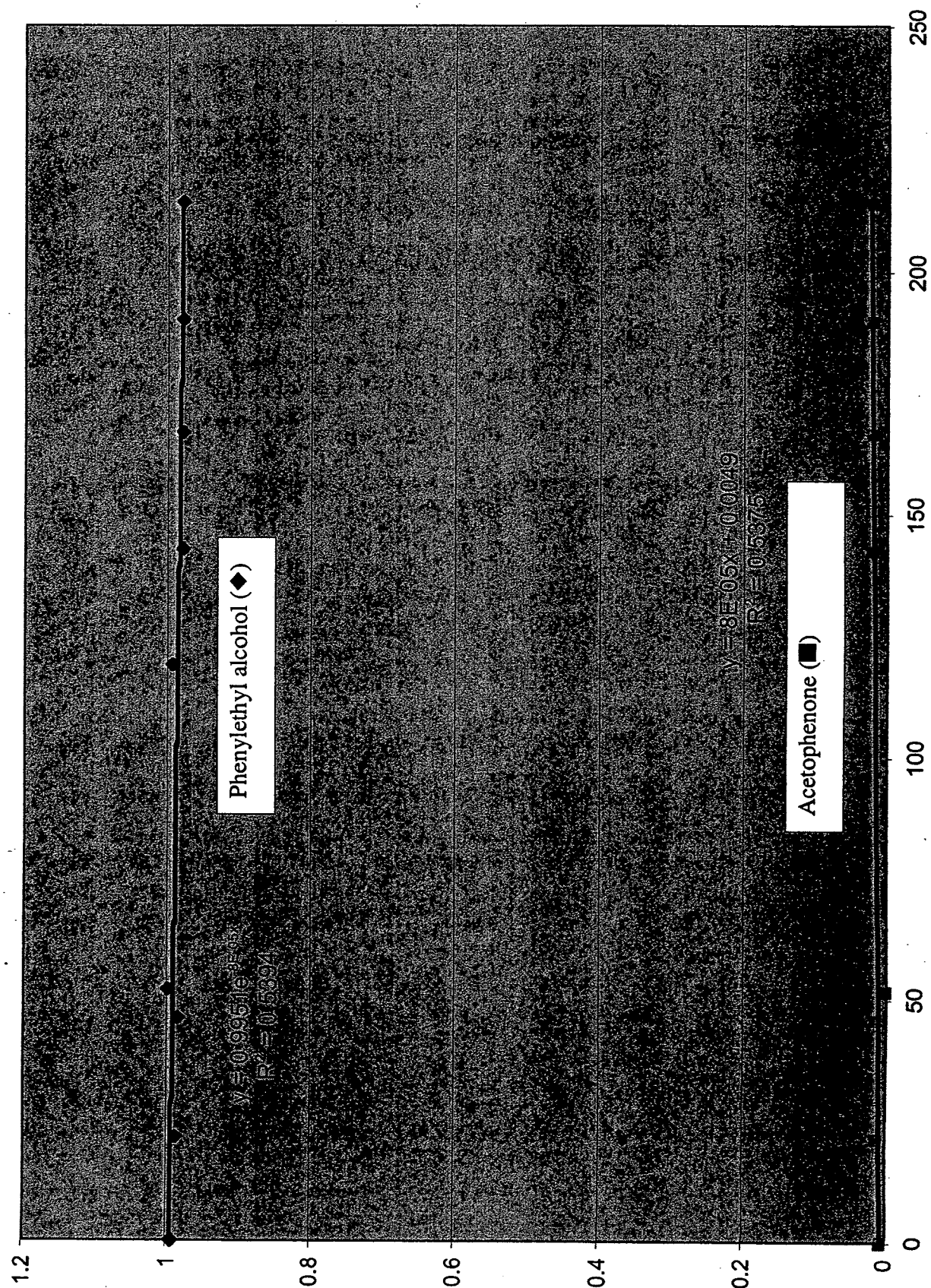
1. Supporting ^1H NMR spectrum
 2. Plot of reverse reaction for the oxidation of phenylethyl alcohol to acetophenone.
 3. Plot of dimer to monomer conversion for compound I.
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This supporting information includes plots for the reverse reaction-the oxidation of phenyl ethyl alcohol, which show the backwards reaction was negligible as well as the dimer-to-monomer conversion in isopropanol- d_8 .

Included in this supplementary material are the ^1H NMR spectra of the hydrogenation of acetophenone with **I** in 2-propanol (A) after evaporation of the solvent. Authentication of the product alcohol (1.4 ppm and 4.9 ppm) was confirmed by addition of the acetophenone (2.5 ppm) (B) followed by 1-phenylethyl alcohol (C). Spectra were taken in CDCl_3 where the broad peak at 2.8-3.1 ppm is water, and the septet at 3.9 ppm is the residual 2-propanol solvent that was not evaporated.



Backwards Reaction of Phenylethyl Alcohol Oxidation by [Cp2Mo(OH)]2 Dimer



Breakdown of Dimer in 2-propanol- d_8 at 65°C. Diamonds represent the dimeric form of molybdocene, and the squares represent the monomeric form. Rate constant for this conversion from dimer to monomer is $8.95 \times 10^{-2} \text{ sec}^{-1}$

