Prepared for submission to PhysChemChemPhys
Sept. 16, 2006

Electronic supplementary information for

Theoretical and Spectroscopic Study of the Reaction of Diethylhydroxylamine on Si(100)-2×1

Gino A. DiLabio,[*1] Stanislav A. Dogel[2], Amsalu Anagaw,[1,2] Jason L. Pitters,[1] and Robert A. Wolkow[1,2]

[1] National Institute for Nanotechnology, 11421 Saskatchewan Drive, Edmonton, Alberta, Canada T6G 2M9

[2] Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2G7.

[*] *National Institute for Nanotechnology, 11412 Saskatchewan Drive, Edmonton, Alberta, Canada T6G 2M9 . E-mail: Gino.DiLabio@nrc.ca; Tel: +1-780-641-1729.*

Figure S1. Experimental HREEL spectrum for dissociatively adsorbed DEHA on Si(100)-2×1. Calculated IR (red) and Raman (blue) spectra for the $(C_2H_5)_2N$ + OH dissociation of DEHA (Fig. 1, **E**).

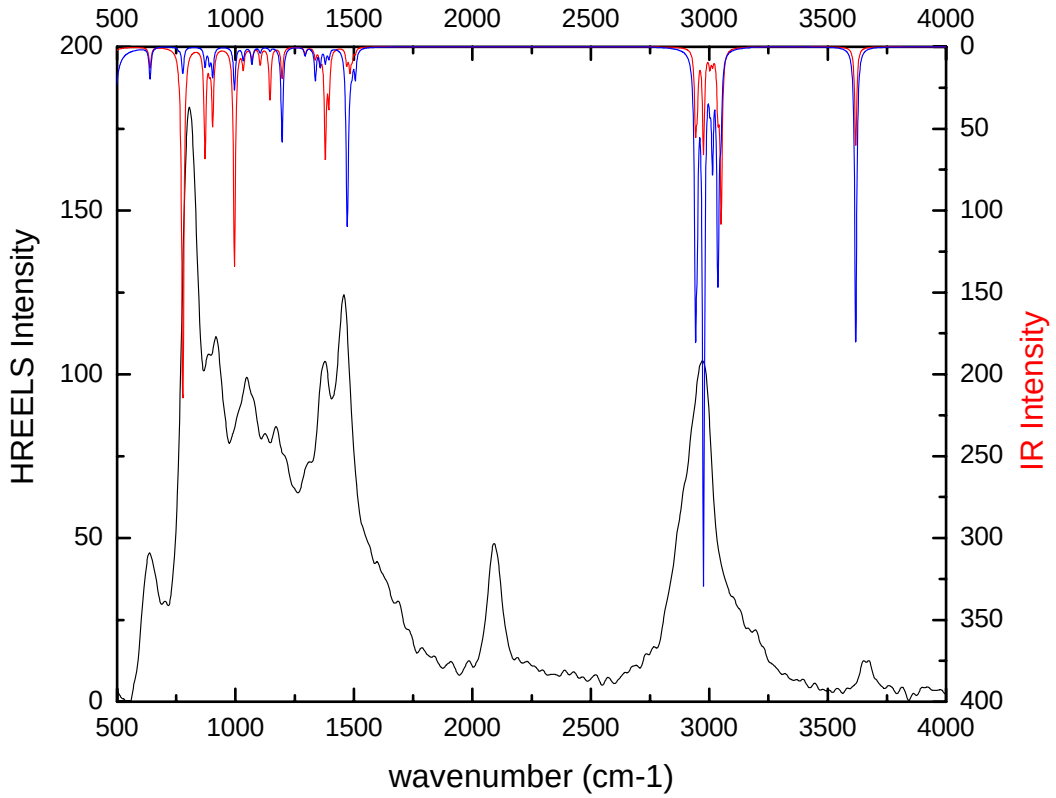
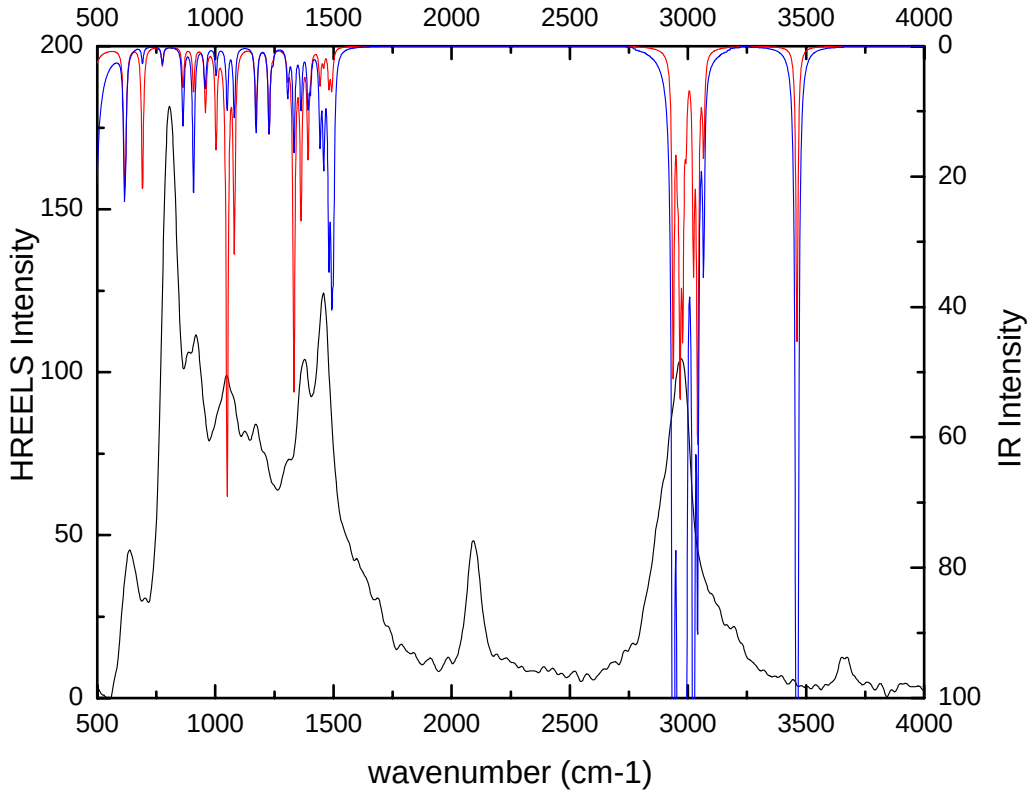


Figure S2. Experimental HREEL spectrum for dissociatively adsorbed DEHA on Si(100)-2×1. Calculated IR (red) and Raman (blue) spectra for the $(C_2H_5)NOH + C_2H_5$ dissociation of DEHA (Fig. 1, **F**).



The calculated low-energy O-H stretch at 3462 cm^{-1} is due to the fact that the O-H BDE is quite low.[33] The absence of the unusual frequency is the HREEL spectra also contributed to us discounting **F** as the dissociation product,