Journal of Electron Spectroscopy and Related Phenomena, 30 (1983) 27
Elsevier Scientific Publishing Company, Amsterdam — Printed in The Netherlands

THEORETICAL VIBRATIONAL FREQUENCIES FOR NH_x AND CH_x REACTIVE INTERMEDIATES ON NICKEL(100) AND NICKEL(111) SURFACES

John J. Low VI and William A. Goddard III

Arthur Amos Noyes Laboratory of Chemical Physics,
California Institute of Technology, Pasadena, California 91125

ABSTRACT

Theoretical studies have been performed on CH_x and NH_x species chemisorbed on threefold and fourfold sites of nickel clusters. From this work we have obtained geometries and vibrational frequencies that can be compared with experimental data concerning these species chemisorbed on Ni(100) and Ni(111) surfaces. These results can be used to help assign the observed losses in EELS spectra for CH on the Ni(111) surface.

0368-2048/83/0000—0000/$03.00