Title
THE STRUCTURES OF SMALL HYDROCARBON MOLECULES ON Rh(111) STUDIED BY LOW ENERGY ELECTRON DIFFRACTION: ACETYLENE, ETHYLENE, METHYLACETYLENE, AND PROPYLENE

Permalink
https://escholarship.org/uc/item/6jx4c8j8

Authors
Hove, M.A. Van
Koestner, R.J.
Somorjai, G.A.

Publication Date
1981-09-01
Submitted to the Journal of Vacuum Science and Technology

THE STRUCTURES OF SMALL HYDROCARBON MOLECULES ON Rh(111) STUDIED BY LOW ENERGY ELECTRON DIFFRACTION: ACETYLENE, ETHYLENE, METHYLACETYLENE, AND PROPYLENE

M.A. Van Hove, R.J. Koestner, and G.A. Somorjai

September 1981

TWO-WEEK LOAN COPY

This is a Library Circulating Copy which may be borrowed for two weeks. For a personal retention copy, call Tech. Info. Division, Ext. 6782

Prepared for the U.S. Department of Energy under Contract W-7405-ENG-48
DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.
THE STRUCTURES OF SMALL HYDROCARBON MOLECULES ON Rh(111)

STUDIED BY LOW ENERGY ELECTRON DIFFRACTION:
ACETYLENE, ETHYLENE, METHYLACETYLENE, AND PROPYLENE

M.A. Van Hove, R. J. Koestner, and G.A. Somorjai

Materials and Molecular Research Division,
Lawrence Berkeley Laboratory, and
Department of Chemistry,
University of California, Berkeley, CA 94720

This work was supported by the Director, Office of Energy Research, Office of
Basic Energy Sciences, Materials Sciences Division of the U. S. Department of
Energy under Contract W-7405-ENG-48
Ethylene (H₂C=CH₂) deposited on Rh(111) at temperatures between 230 and 270 K produces a sharp (2x2) pattern at a 1/4 monolayer coverage. The surface species obtained in this way is ethylidyne (≡C-CH₃), bonded to 3 metal atoms and standing perpendicularly to the metal surface [1,2] cf. Fig.1. It is identical to the ethylidyne species found on Pt(111) in similar circumstances [3]. It can also be obtained [2] from acetylene (H-C≡C-H) by coadsorption of H₂.

The (2x2) ethylidyne species on Rh(111) can be converted under gentle heating or addition of H₂ to a species having a c(4x2) pattern and the same 1/4 monolayer coverage [2]. High resolution electron energy loss spectroscopy indicates that the ethylidyne species is maintained, cf. Fig.1. However, at the time of writing, dynamical LEED calculations do not agree well with experiment for this structure or any other structure.

Propylene (H₂C=CH-CH₃) deposited on Rh(111) at temperatures between 230 and 270 K produces a (2x2) pattern with weak diffuse spots in extra \((2\sqrt{3}x2\sqrt{3})R30°\) positions. The I-V curves of the (2x2) spots are nearly identical to those of (2x2) ethylidyne. Prolonged exposure to propylene produces a sharp \((2\sqrt{3}x2\sqrt{3})R30°\) pattern with concurrent changes in the I-V curves. We suggest that a propylidyne species (≡C-CH₂-CH₃) has been obtained whose ≡C-C base is identical to that of ethylidyne. The extra methyl groups (-CH₃) on neighboring molecules interact with each other because of their size and can produce the \((2\sqrt{3}x2\sqrt{3})R30°\) unit cell, cf. Fig.2. LEED calculations are in progress to check this model and determine the various structural parameters.

Both propylene and methylacetylene (H-C≡C-CH₃) can produce a c(4x2) pattern with I-V curves identical to those of the c(4x2) species obtained from ethylene and acetylene.
A new theoretical approximation is used in a first stage of this LEED analysis: the multiple scattering is ignored within the molecular overlayer, but not in other parts of the surface, including between the substrate and the overlayer.

Acknowledgement

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under contract W-7405-ENG-48.

References


Figure Captions

1. Perspective view of ethylidyne arranges in a (2x2) (bottom) and a c(4x2) (top) lattice on Rh(111).
2. Perspective view of propylidyne arranged in a (2 √3x2 √3)R30° lattice on Rh(111).
Fig. 1

fcc (III) + C₂H₃ (ethyldyne)

XBL813-5407
$\text{fcc(III)} + (2\sqrt{3} \times 2\sqrt{3}) \text{ R30°} \quad \text{C}_3\text{H}_5 \quad \text{(propylidyne)}$

XBL813-5409

Fig. 2
This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Department of Energy to the exclusion of others that may be suitable.