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

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September 1981

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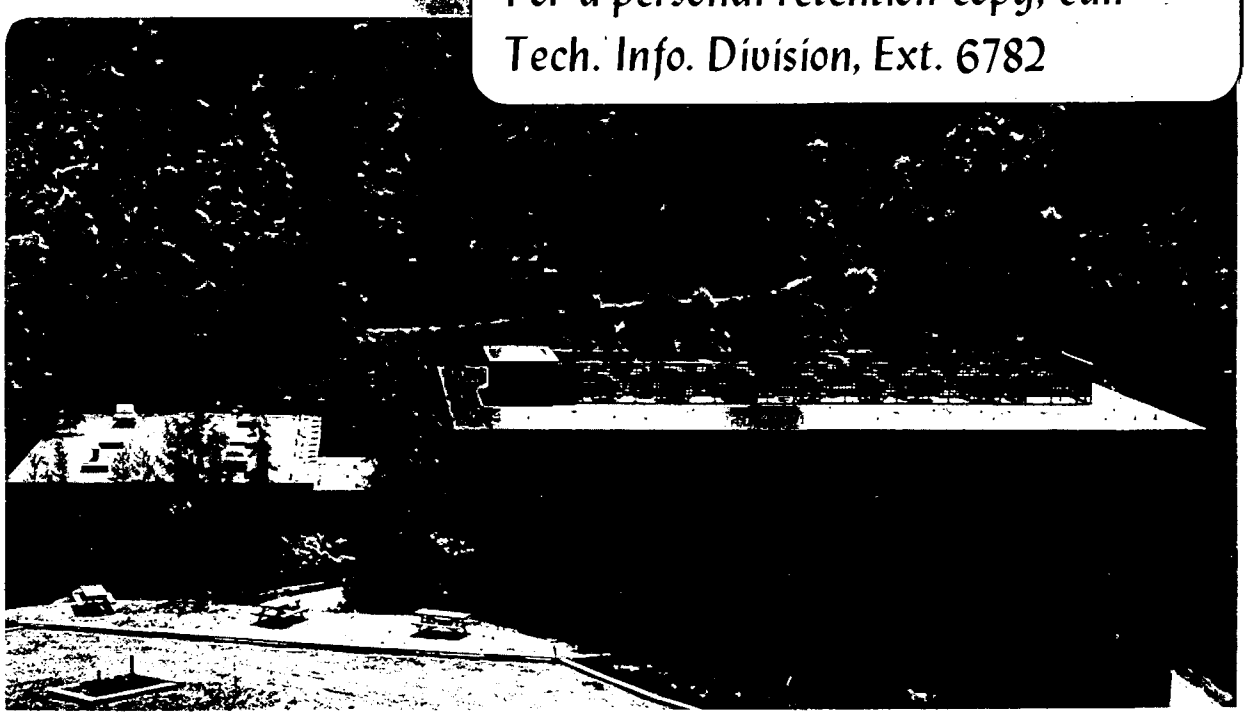

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LBL 13300

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

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Ethylene ($H_2C{=}CH_2$) 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 ($\rightarrow C{-}CH_3$), 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 ($H{-}C \equiv C{-}H$) by coadsorption of H_2.

The (2x2) ethylidyne species on Rh(111) can be converted under gentle heating or addition of H_2 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 ($H_2C{=}CH{-}CH_3$) 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 ($\rightarrow C{-}CH_2{-}CH_3$) has been obtained whose $\rightarrow C{-}C$ base is identical to that of ethylidyne. The extra methyl groups ($-CH_3$) 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 ($H{-}C \equiv C{-}CH_3$) 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.

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5. M.A. Van Hove and G.A. Somorjai, submitted to Surface Science.

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 $(2\sqrt{3}x2\sqrt{3})R30°$ lattice on Rh(111).

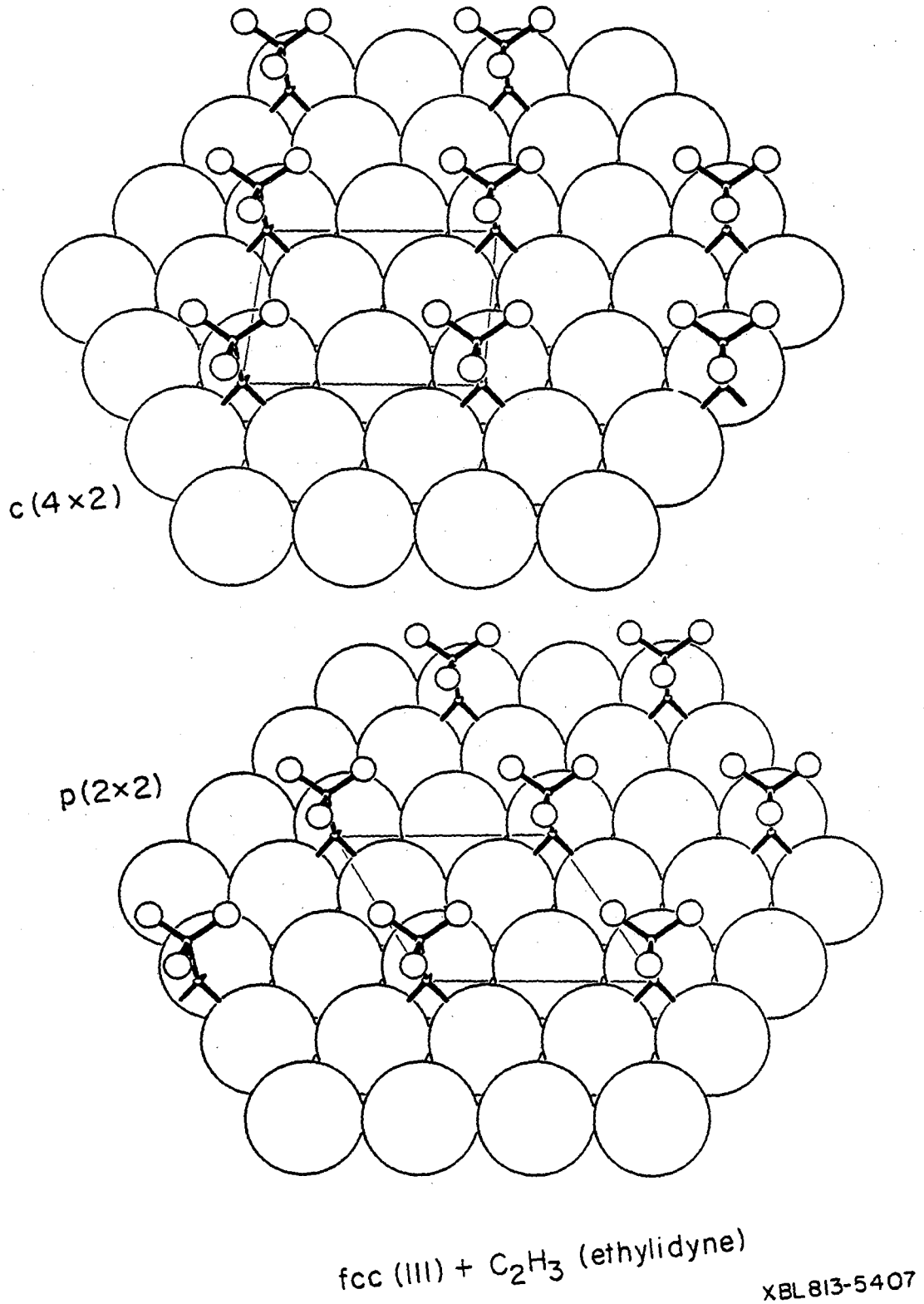
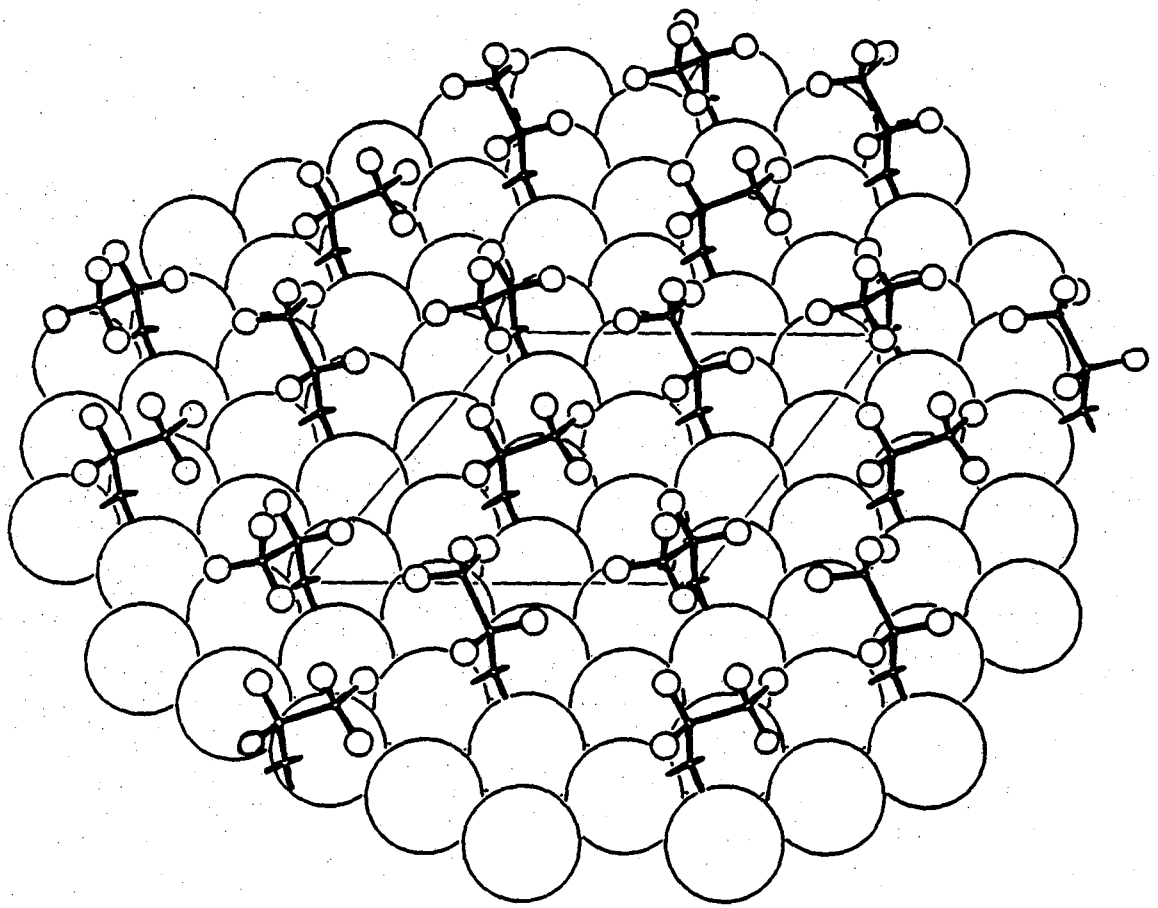


Fig.1



fcc(111) + $(2\sqrt{3} \times 2\sqrt{3})R30°$ C_3H_5 (propylidyne)

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Fig.2

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