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In-situ Raman-spectra of oxygen-containing adspecies on

Article Author:

Zhang, H. B.; Liu, Y

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# **ABSTRACTS OF PAPERS**

## **Part 1**

**207th ACS National Meeting**

**0-8412-2774-8**

**American Chemical Society**

**San Diego, CA.**  
**March 13-17, 1994**

29 ACS Divisions, 2 Secretariats, 4 Committees have scheduled 5717 papers to be presented at the 207TH ACS National Meeting.

The completed final program with exact presentation times for all papers is in the February 7, 1994 issue of CHEMICAL & ENGINEERING NEWS.

ACS Divisions and Committees are identified by CODE as shown in the Table of Contents. CODE letters and paper number should be used when citing or reprinting abstracts. For example: Lytch, R.G., FERT, O2, 195th ACS National Meeting, Toronto, Canada, June 5-10, 1988. Abstracts may be reprinted freely. Divisional Preprints are copyrighted by the American Chemical Society and require permission from the ACS Divisions to reprint. Preprint information is listed in the front section of this book. A section also list ACS and Divisional journals, and Symposia from recent ACS National Meetings which are available in the ACS SYMPOSIUM SERIES and the ADVANCES IN CHEMISTRY SERIES.

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Abstracts of Meeting Papers  
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5. AN INFRARED SPECTROSCOPY AND TEMPERATURE PROGRAMMED DESORPTION STUDY OF ADSORBED THIOPHENE ON ALUMINA SUPPORTED Mo AND Rh CATALYSTS  
M. E. Bussell, W. W. C. Quigley, P. M. Sofarelli and H. D. Yamamoto, Dept. of Chemistry, Western Washington University, Bellingham, WA 98225.

The surface chemistry of adsorbed thiophene on sulfided Mo/Al<sub>2</sub>O<sub>3</sub> and Rh/Al<sub>2</sub>O<sub>3</sub> catalysts has been investigated under ultrahigh vacuum conditions using infrared (IR) spectroscopy and temperature programmed desorption (TPD). At ~120 K, thiophene adsorbs molecularly on the sulfided catalyst surfaces as identified by IR spectroscopy. Upon heating, both thiophene desorption and decomposition are observed and these processes have been characterized in detail for the Mo and Rh catalysts. In conjunction with the thiophene studies, carbon monoxide adsorption has been used both to identify and to quantify adsorption sites on the catalyst surfaces. Others have shown that a direct correlation exists between the CO chemisorption capacity of alumina supported sulfide catalysts and their thiophene HDS activity, and this relationship will be discussed in the context of the adsorption properties of the two species.

6. A MOLECULAR LEVEL MECHANISM OF n-BUTANE OXIDATION TO MALEIC ANHYDRIDE OVER VANADYL PYROPHOSPHATE. A.A. Agaskar, L. DeCaul, and R.K. Grasselli, Mobil R&D Corporation, Central Research Laboratory, P.O. Box 1025, Princeton, NJ 08540.

A molecular level mechanism is proposed for the highly selective transformation of n-butane to maleic anhydride on the surface of vanadyl pyrophosphate. The mechanism suggests that the dimeric active sites transform among four possible inter-convertible states which differ from each other in the number of available oxygen atoms and the formal oxidation states of the individual vanadium atoms. The relative ratios of active sites in each of the four states are dictated by the reaction conditions, the redox properties of the reacting gases, and the structure of the vanadyl pyrophosphate active surface. A crucial feature of the mechanism is a "pseudo-ozonide" surface species formed by the interaction of a chemisorbed dioxygen molecule and an adjacent metal oxo group, which serves to activate butane. The proposed mechanism is entirely consistent with literature reports describing the behavior of (VO)<sub>2</sub>P<sub>2</sub>O<sub>7</sub> in flow, pulse, and TAP reactors.

7. IN-SITU RAMAN SPECTRA OF OXYGEN-CONTAINING ADSPECIES ON Th-La-O<sub>x</sub>/BaCO<sub>3</sub> CATALYSTS FOR METHANE OXIDATIVE COUPLING. H.-B. Zhang, Y.-D. Liu, G.-D. Lin, Y.-Y. Liao, and K.-R. Tsai, Department of Chemistry & State Key Laboratory for Physical Chemistry of the Solid Surface, Xiamen University, Xiamen 361005, China

Raman spectra of oxygen-containing adspecies on highly active Th-La-O<sub>x</sub>/BaCO<sub>3</sub> catalysts for oxidative coupling of methane have been taken *in situ* under cofeed reaction conditions of CH<sub>4</sub>/O<sub>2</sub> = 4/1 v/v, GHSV = 2.0x10<sup>4</sup> h<sup>-1</sup>, atmospheric pressure and 740°C. Observed Raman peaks at 1056 cm<sup>-1</sup> (vs), 1120cm<sup>-1</sup> (w) and 1148cm<sup>-1</sup>(w) are ascribable, respectively, to CO<sub>3</sub><sup>2-</sup> and two O<sub>2</sub><sup>-</sup> adspecies in different microenvironments. In the same flowing feed stream but at 500°C, the latter two peaks increased in intensity noticeably; moreover, a new peak around 940cm<sup>-1</sup> (w) appeared (which might be ν<sub>1</sub> of surface stabilized O<sub>3</sub><sup>2-</sup>, as to be explained in text). Besides these peaks, two weak and blur peaks at 812cm<sup>-1</sup> and 824cm<sup>-1</sup>(w), insensitive to temperature change from 740° to 500°C, can not be unambiguously ascribed to O<sub>2</sub><sup>2-</sup>. The results strongly support our previous proposal that O<sub>2</sub><sup>-</sup> is an active and OCM-selective oxygen-adspecies.

8. A SCHEME FOR METAL OXIDE PROMOTION OF CO AND CO<sub>2</sub> HYDROGENATION OVER RH BASED ON THE CORRELATION OF RATE ENHANCEMENT AND OXIDATION STATE. A.B. Boffa<sup>1</sup>, A.T. Bell<sup>2</sup>, and G.A. Somorjai<sup>1</sup>, Departments of Chemistry<sup>1</sup> and Chemical Engineering<sup>2</sup>, University of California, Berkeley, California 94720.

The effect of sub-monolayer oxide deposits on the rate of methane formation of CO and CO<sub>2</sub> hydrogenation over a Rh foil has been determined and compared with XPS measurements of the oxide after reaction. The oxides investigated were AlOx, TiOx, VOx, FeOx, ZrOx, NbOx, TaOx, and WOx. With the exception of AlOx, each of the oxides was found to enhance the rate of CO methanation relative to that