INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
34100 TRIESTE (ITALY) - P.O.B. 586 - MIRAMARE - STRADA COSTIERA 11 - TELEPHONE: 2240-1
- CABLE: CENTRATOM - TELEX 460392 - 1

SMR/207 - 2

WORKSHOP ON
"SURFACE SCIENCE AND CATALYSIS"
(4 - 8 May 1987)

FOURIER TRANSFORM INFRARED SPECTROSCOPY

(Summary)

M. CHESTERS
School of Chemical Sciences
University of East Anglia
Norwich NR4 7TJ
U.K.

FOURIER TRANSFORM INFRARED SPECTROSCOPY

The first section of the lecture will be concerned with an introduction to the basic principles of molecular vibrations, characteristic group frequencies and the use of infrared spectroscopy for identifying molecular species. I go on to discuss experimental aspects and to compare dispersive instruments with Fourier Transform instruments. Finally the application of transmission infrared spectroscopy to high surface area 'catalyst-like' materials will be contrasted with the application of reflection-absorption infrared spectroscopy (RAIRS) to single crystal metal samples.

The second section of the lecture will concentrate on some specific examples. Spectra of ethane, ethene and ethyne on a Cu(111) surface will be analysed to illustrate the application of the metal surface selection rule.

Adsorption of ethylene on platinum surfaces will be used to illustrate the interplay between studies of single crystal surfaces and work on catalysts.

Adsorption and decomposition of methanol on Cu(111) will be used to illustrate possibilities for monitoring surface reactions.

Finally the prospects for improvements in the RAIRS technique will be discussed.

Outline:

1. Molecular Vibrational Spectroscopy[1,2]
   - simple harmonic oscillator
   - normal modes of vibration
   - characteristic group frequencies

2. Infrared Spectroscopy[1,2]
   - excitation mechanism
   - selection rules
   - instruments - dispersive
   - routine sensitivity.

3. Principles of FTIR[3]
   - Michelson interferometer
   - interferogram
   - typical mid-i.r. instrument
   - advantages vs dispersive instruments
     - a) multiplex
     - b) throughput
     - c) wavenumber accuracy

4. Application of Transmission Infrared Spectroscopy to High Surface Area, 'Catalyst-Like' Samples[4,5]
   - nature of supported metal samples
   - sample size
   - i.r. absorption by oxide support
   - importance of FTIR.

5. Reflection-Absorption Infrared Spectroscopy (RAIRS) [6,7,8]
   - history
   - metal surface selection rule > sample size and sensitivity
   - FT-RAIRS
   - comparison with EELS

6. Examples
   - ethane, ethene and ethyne on Cu(111)
   - methanol and methoxy on Cu(111)
   - kinetic studies

7. Prospects for the Future
   - improved sensitivity
   - improved spectral range

References

1. Gordon M. Barrow, 'Molecular Spectroscopy' McGraw-Hill 1962.
2. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds (3rd. ed). Wiley-Interscience 1978. (especially early part on symmetry and selection rules.)
3. Peter R. Griffiths and James A. De Haseth 'Fourier Transform Infrared Spectroscopy', Vol. 83 of 'Classical Analysis', Eds. P.J. Elving, J.D. Winefordner and I.M. Kolthoff, Wiley-Interscience 1986.
4. L.H. Little, Infrared, 'Soectra of Adsorbed Species', Academic Press, 1966.
5. A.V. Kiselev and V.I. Lygin, 'Infrared Spectra of Surface Compounds', Wiley, 1975.
6. R.G. Greenler, J. Chem. Phys. 44, (1966), 310, and J. Vac. Sci. Technol. 12, '1975), 1410.
7. P. Hollins and J. Pritchard, Prog. Surface Science, 19, (1985), 275.
8. M.A. Chesters, J. Electron Spectrosc. and Related Phenom. 38, (1986), 123.

M. Chesters.