Plenary and Session Lectures

B1

Experimental Access to the Electronic Structure of Organo-f-element Complexes

R. D. FISCHER

Institut für Anorganische und Angewandte Chemie, Universität Hamburg, F.R.G.

(To be published later as a full paper)

B2

Optical and Magnetic Properties of Uranium and Neptunium Borohydrides and Tetrakismethylborohydrides

K. RAJNAK, E. GAMP, R. BANKS, R. SHINOMOTO and N. M. EDELSTEIN*

Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, Calif, 94720, U.S.A.

(To be published later as a full paper)

B3

Spectroscopy and Nonradiative Phenomena of Rare Earths in Glasses: Future Applications

RENATA REISFELD[†]

Department of Inorganic and Analytical Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

The radiative transition probabilities of rare earth ions in glasses can be calculated from the measured intensity parameters and calculated transition matrix elements using the Judd-Ofelt theory. The Judd-Ofelt parameters in oxide, fluoride and chalcogenide glasses were obtained for a variety of rare earth ions. These intensity parameters depend on the chemical bonding between the rare earths and the glass matrix and the viscosity of the medium. The nonradiative transition probabilities are calculated using a phenomenological theory, experimentally measured fluorescence lifetimes and quantum efficiencies. The nonradiative transition probabilities

show an exponential dependence of the phonon energy of the network forming material. Experimental results according to this theory show that Er³⁺ has the highest quantum efficiency in fluoride glasses. Technological implementation of the above theory will be discussed for glass lasers, sources for fiber waveguides and luminescent solar concentrators.

B4

Photoelectron Spectroscopy of f-Element Complexes

IGNAZIO L. FRAGALÀ

Dipartimento di Chimica, Università di Catania, V.le A. Doria 6, 95125 Catania, Italy

Although the chemical bonding of actinide complexes is far from being well understood and, hence, there is a high demand of details of their electronic structure, only few theoretical and/or experimental approaches are capable to probe deep insight into such aspects.

Today almost all informations on the bonding have been generally drawn from reactivity data [1]!

In fact, sophisticated MO calculations are hardly practicable with 5f-element complexes because of the very large basis set required while responses of most usual spectroscopic techniques are very hard to be rationalized and/or provide informations only on crystal field aspects.

By contrast, gas-phase UV photoelectron spectroscopy is a well established spectroscopic technique which provides:

- 1) the energy ordering of 'valence' MOs,
- 2) the possible contribution of metal AOs to various MOs by using compared He-I vs. He-II relative intensity variations (this specially applies to spectra of 5f-element complexes).
- 3) and, finally, an adequate reference to test results of theoretical calculations at any level.

This discussion will be mainly limited to investigations carried out at the Chemistry Department of University of Catania on several classes of complexes of f-elements.

Organometallic Complexes

The wider group of complexes which attracted attention were cyclopentadienyl complexes of Th(IV),

[†]Enrique Berman Professor of Solar Energy.