400  16-Molecular Structure Determination by Methods other than Diffraction

Fig. 1. X-ray absorption spectrum near the Ta-LIII edge of KTa3 at 32 K.

Fig. 2. Radial structure function around Ta atom at 32 K.


PS-9.01.07 RELATIONSHIP BETWEEN CATALYTIC ACTIVITY FOR WATER-GAS SHIFT AND STRUCTURE OF Co-Mo-Al Oxide CATALYST

Li Xiaoming, Lu Xinwan, Li Yuxiang, Quan Jingrong, Feng Tuhua. Zhejiang Research Institute of Chemistry. Wuhan. 430074, China.

The dehydration of two commercial Co-Mo-Al oxide KWS catalysts has been studied by XRD, TPD, IR, SEM-XPS etc. The results showed that the catalysts' surface properties and regenerative and mechanical strength of catalysts have significant effects on the activity except the rate of CO2 generation and CO content in operating temperature.

The Co-Mo-Al-Oxide catalyst was prepared by impregnation of Al2O3 with a Mo (MoO3) mixed solution.

A typical Y-Al2O3 XRD pattern was obtained with Co-Mo-Al oxide catalyst A in the cobalt state. The element was well dispersed on the support. Catalyst B showed three XRD patterns consistent with Mo6Al2O13 and Mo6Al2O12.

The crystal structures of the catalysts were studied using a powder diffractometer (J. P. B. 500, Cu, 1984, 85, 86).

The spinel-like Al2O3 structure formation was observed by increasing the calcination temperature and it is correlated with the procedure of catalyst preparation.

The specific surface area of the catalyst A (9.50 m2/g) decrease to about 5.00 mg/g as the catalyst converted to sulfided state. It was about 7.00 mg/g after the catalyst used for a year, and the catalyst mechanical strength decreased to 1/3 after regeneration-comparing with new one.

The Co-Mo and Mo catalysts were not last after used for four years. The catalysts were not last after used for four years.

The catalyst activity is mainly due to the formation of sulfates, increasing of Na2O and MgAl2O4. The active center Co-Mo-S is destroyed over-boiling in the regeneration sulfidation and operation process enhance formation of inactive MgAl2O4 and crystal phase MgO. The higher ratio of Na2O and MgO, higher concentration of Sulfate enhance also the sulfates formation.

Fig. 1. ICP results of catalyst A and B.

PS-9.01.08 CRYSTAL STRUCTURE AND HALOGEN NQR OF DIAMMONIUMHALOGEN BISERIDES

Helmut Paulus and Alan Weiss, Institut für Physikalische Chemie, Technische Hochschule Darmstadt, Petersenstr. 20, D-6100 Darmstadt, Germany.

The crystal structures of the isomorphous compounds 1,3-di ammonium propyl dibromide and - iodide are reported. Monoclinic, P21/n, 2-4. Lattice constants in pm: (1) a=1343.6(6), b=457.9(1), c=1347.1(1), β=103.4(1); (2) a=1293.6(5), b=427.6(1), c=1299.6(5), β=110.10(1). The diammonium propyl cations are centrosymmetric and there are two crystallographic independent anions and two independent cations in the unit cell. The positive (NaCNH21) and negative halogen anions are proportionately distributed in the lattice. Weak hydrogen bonds N-H...X, X=Br, I are observed. The discrepancy in the 19Br and 127I NQR spectra, respectively, [1] from which 1H NQR was banned, is removed by investigation of the spectra. Additionally to the already known 19Br line at 22.95MHz a second line at 12.07MHz was found at room temperature. Structures and NQR spectra are compared and discussed.

