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# **ABSTRACTS OF PAPERS**

**Part 2**

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241. COLLISIONS OF LOW TRANSLATIONAL ENERGY IONS WITH SOLID, LIQUID AND GASEOUS FLUORINATED TARGETS: A CASE STUDY OF  $W(CO)_6^+$ , R.G. Cooks, T. Pradeep, T. Ast and J. Patrick, Department of Chemistry, Purdue University, West Lafayette, IN 47907

The traditional method of ion activation in mass spectrometry involves collisions with gaseous targets; alternative techniques, in which gases are substituted by solid or liquid surfaces, have seen development and expansion in the recent years. The results will be presented of a comparative investigation, in which the behavior of  $W(CO)_6^+$  derived ions has been examined in low translational energy (10 - 100 eV) collisions with solid, liquid and gaseous targets.  $W(CO)_6^+$  is a "thermometer" ion: by studying its fragmentation, the internal energy content of the fragmenting ion can be assessed. Fluorinated targets have been shown to be especially effective in translational to internal energy conversion; in this study, we have utilized and compared the properties of fluorinated alkanethiol monolayers on gold (solid), perfluorinated polyethers (liquid) and perfluorocarbons (gases). In addition to collision induced dissociation, reactive collisions have been observed at all surfaces, resulting in the formation of  $WF_n^-$  ( $n = 1-5$ ) products. These multiple W-F bonds are formed in single collision sequences and the mechanism involved is discussed.

242. AB INITIO STUDIES OF SUBSTITUTED HYDROXYPHENYL TEREPHTHALATES: MODEL SYSTEMS FOR LIQUID CRYSTALLINE POLYESTERS. Jing-Yue Yeh, Debbie B. Saebø and Svein Saebø, Department of Chemistry, Mississippi State, MS 39762

Four liquid crystalline polymers: 3-methyl-4-hydroxyphenyl terephthalate, 3-phenyl-4-hydroxyphenyl terephthalate, 3-phenylethyl-4-hydroxyphenyl terephthalate, and 3-chloro-4-hydroxyphenyl terephthalate are under investigation using several different experimental and theoretical techniques. As part of these studies a series of *ab initio* calculations have been performed on model systems representing the repeat units of each of the four polyesters. The conformations relative to the ester linkage are expected to be particularly important for the geometrical shape of the polymers, and thus for their physical properties. A series of calculations on the unsubstituted molecule 4-hydroxyphenyl terephthalate at different levels of theory as well as calculations of conformational energy differences and barriers to internal rotation for the repeat units for the four polyesters mentioned above. In the minimum energy conformation, the benzene ring of the hydroquinone moiety is twisted about 65 degrees relative to the planar terephthalic acid fragment of the molecule. The barrier to internal rotation around the ester bond is estimated to be approximately 2 kcal/mole.

243. BRIDGE THEORY AND PHYSICAL CHEMISTRY IN MOLECULAR DESIGN OF CATALYST. D. W. Liao, Z. N. Huang, H. L. Wan and K. R. Tsai, Department of Chemistry, Xiamen University, Xiamen, Fujian 361005, CHINA

Catalysis is a kind of chemical reaction in nature. However, the explanation of catalysis will involve not only both chemical and physical images but also mathematical image. A new explanation of catalysis was described according to the bridge theory proposed by us. A catalytic reaction can be defined as  $[\text{reagent matrix}] \times [\text{bridge matrix}] = [\text{product matrix}]$ . The mathematical model, involving such concepts as matrix, group, collective, mapping and so on, was also suggested. Based on the periodic properties of elements and compounds, the physicochemical bases of molecular design of catalysts, namely, (1) geometric adaptability, (2) electronic structure adaptability, (3) magnetic adaptability, (4) other physicochemical property adaptability and (5) catalytic active model adaptability, were suggested for computer-assistant catalyst design on molecular level. Again, the program of catalyst component design was written in C language by us with methods of pattern recognition and artificial intelligence.

244. DYNAMICAL BEHAVIOR OF ELECTRONIC STATES OF METHYLAMINE DICATION PREPARED FROM N 1S ELECTRON IONIZATION. Robert G. Hayes, Department of Chemistry, University of Notre Dame, Notre Dame, IN 46556; K. Lee, C. I. Ma and D. M. Hanson, Department of Chemistry, State University of New York, Stony Brook, NY 11794-3400

We have prepared methylamine dication in a broad spectrum of electronic states by N 1s ionization followed by Auger decay. We have observed the ionic products from groups of closely-spaced electronic