Memo 4

DIVERSIFIED CHEMICAL PRODUCTS
Research and Product Development Division
Blacksburg VA

TO: U. R. Engineer
FROM: Phil D. Chemist
DATE: 2007 Sep 13
SUBJECT: Kinetic Model for Reaction 1

A detailed study of possible kinetic models for Reactions IA and IB has been underway for some time now at the Research Center. Evidence from experiments such as the one carried out just recently at your request has suggested that the overall reactions:

$$2R1 + R2 \rightarrow A$$

$$R1 + R2 \rightarrow C + H_2$$

are not elementary. A number of possible reaction mechanisms were proposed by the organic chemists here in Blacksburg. Kinetic models were developed and tested using experimental data similar to that which we collected for you.

The following mechanism was determined to best describe the data:

$$R1 + R2 \rightarrow I1 \text{ (Pt catalyzed)} \quad (1)$$

$$R1 + I1 \rightarrow A \quad (2)$$

$$I1 \rightarrow C + H_2 \quad (3)$$

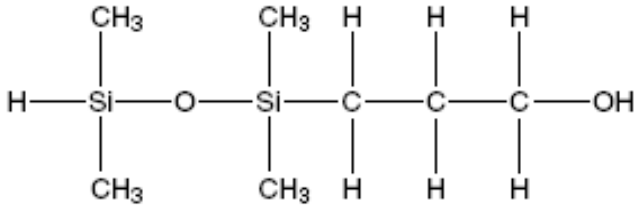
$$C + I1 \leftrightarrow I2 \text{ (reversible)} \quad (4)$$

$$Pt \rightarrow Pt^* \quad (5)$$

These reactions are elementary and follow the "expected" mechanisms with the exception of the catalyzed reaction (1). C further reacts to form an unwanted byproduct I2 in a reversible reaction (4). The catalyst deactivates during the course of the reaction (5). The molecular structures of I1 and I2 are shown in Figure 1.

Kinetic rate constants were determined from the data. With the help of Art Jockey's Technical Services Group, a computer simulation program was developed to simulate the reaction network numerically. This program will allow you to analyze various operating strategies and design the first reactor.

Molecule I1



Molecule I2

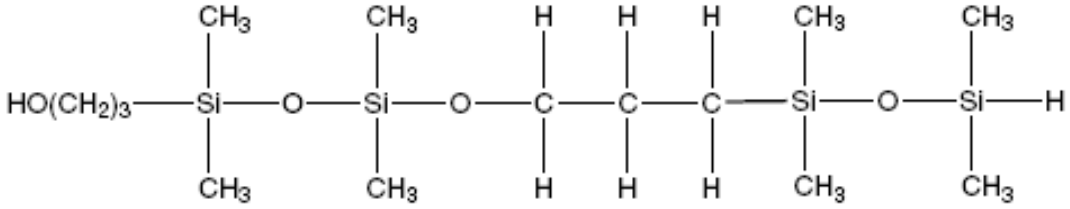


Figure 1: Molecular Structure for I1 and I2