Abstract Submitted for the MAR09 Meeting of The American Physical Society

Temperature Dependent Adsorption Dynamics of Binary Mixtures of Halomethanes on Graphite and α -quartz Surfaces¹ JONATHAN NEHRING, North Park University, G. LEUTY, MESFIN TSIGE, Southern Illinois University at Carbondale — Using atomistic molecular dynamics simulations, we have investigated the structure and dynamics of binary mixtures of halomethanes $(CF_4, CF_3Cl, \text{ and } CF_3Br)$ as a function of temperature on two structurally and chemically different surfaces. The initial distribution of the binary mixtures is either they are uniformly mixed or a layer or layers of one component is placed on top of a layer or layers of the other component. As a function of temperature (below and above the melting temperature of CF_4) and the two surface types, we observed a marked change on the concentration, dynamics, orientation, and structure of each of the components in the first layer of the binary mixtures next to the surfaces.

¹Work supported by the Donors of the American Chemical Society Petroleum Research Fund.

> Jonathan Nehring North Park University

Date submitted: 24 Nov 2008

Electronic form version 1.4