



Simulation and experiment for heavy element gas phase chromatography

Dominik Dietzel^{1,2}, Alexander Yakushev², Christoph E. Düllmann^{1,2,3}, Jadambaa Khuyagbaatar², Jörg Krier², Egon Jäger²

¹ *Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany*

² *GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*

³ *Helmholtz-Institut Mainz, 55099 Mainz, Germany*

In preparation of gas phase chemical experiments with element 115, we studied the chemical behavior of single short-lived ^{211}Bi atoms in rare gases (helium and argon) and in oxygen atmosphere. For that purpose, we performed off-line isothermal gas chromatography experiments at room temperature. The short-lived volatile ^{219}Rn precursor, provided from an ^{227}Ac -source, was transported into the miniCOMPACT setup (mini Cryo-Online Multi detector for Physics and Chemistry of Transactinides), using different carrier gases. The internal chromatograms were modeled by Monte Carlo simulations, which account for the precursor effect of beta-decaying ^{211}Pb that decays to the detected alpha-decaying ^{211}Bi and compared them to experimental results to determine a lower limit of the adsorption enthalpy of bismuth on silicon dioxide. Furthermore, we present a new advance of the Monte Carlo code that has been adapted to study the chemical properties of superheavy elements and their lighter homologs in greater detail. The inclusion of an activation energy barrier that enables the simulation of physisorption and chemisorption, substitutes the simple mobile adsorption surface process. By applying this code to the analysis of gas chromatography experiments, valuable insights into the behavior of SHE and lighter homologs can be obtained. Our results demonstrate the potential of the new Monte Carlo simulations to advance our understanding of these systems and suggest promising directions for future research.