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INVITED LECTURE - Vacuum thermochromatography - prospective method for heaviest element studies

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The title technique for separating species with dissimilar adsorbability uses deeply evacuated columns with imposed negative longitudinal temperature gradient. Then the molecular flow, though convectionless, produces deposits peaking in individual temperature ranges. This fundamental mechanism - random walks from wall to wall - calls for rigorous Monte Carlo (MC) simulations, which require a minimum of assumptions, are very versatile in accounting for numerous parameters and conditions of real experiments, but are slow. Diffusional approximation of random walks with solution to the appropriate differential equation gives excellent agreement with MC. The calculations are faster for some basic conditions, but the versatility is much poorer. Meanwhile, the structure of the solution suggests a way to a semi theoretical explicit formula for the peak. The one presented here is negligibly inaccurate, reasonably versatile, and unmatched in the speed of the necessary calculations. It greatly enables evaluation of the experiments with a few radioactive atoms or labeled molecules, which is the case in today chemical studies of the superheavy elements. This is demonstrated by simulating experimental data of this kind for certain desorption energy and then, backward, evaluating the confidence intervals for the “experimental” value of the energy. The Bayesian approach is used; several caveats on hasty conclusions at poor statistics are emphasized. Some considerations about the real experiments are presented.

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