Analysis of Eutectic Formation of Amino Acids by Molecular Dynamics Simulations

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Abstract

Computer-aided molecular dynamics techniques were used to investigate the mechanism of eutectic formation in a substrate mixture. Experimental data for the melting phenomena of eutectic forming (CBZ-Asp and $AlaNH_2$) and non-forming (Asp and $AlaNH_2$) mixtures were obtained[1]. Molecular dynamics simulations[2~4] were conducted to calculate energy differences of the mixtures of CBZ-Asp & $AlaNH_2$, or Asp & $AlaNH_2$ as the temperature increased from 298 K to 333 K. For a eutectic mixture of CBZ-Asp and $AlaNH_2$, the increment of kinetic energy was much bigger than that of potential energy as the temperature increased from 298 K to 333 K. Under a temperature jump, the self-diffusion constant (D) value of the mixture CBZ-Asp and $AlaNH_2$ increased compared to that of the mixture Asp and $AlaNH_2$. The periodic boundary conditions for molecular dynamics calculations were confirmed to be effective.

References

1. C. Kim and C. S. Shin, Solvent-free Enzymatic Synthesis of Alitame Precursor Using Eutectic Substrate Mixtures, 2001, *Enzyme Microb. Tech.*, Vol. 28, pp 611-616.
2. D. C. Rapaport, *The Art of Molecular Dynamics Simulation*, 1995, Cambridge University Press, UK.
3. G. H. Grant and W. G. Richards, *Computational Chemistry*, 1995, Oxford University Press, NY.
4. Y. Tsuchiya, H. Hasegawa, and T. Iwatsubo, Prediction of the Melting Point of n-Alkanes Using the Molecular Dynamics Method, 2001, *J. Chem. Phys.*, Vol. 114, pp 2484-2488.