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Formation of HIV-1 capsids based on an extended Becker-Döring Model by stochastic self-assembly

The HIV-1 virions include various components such as MA(matrix protein), CA (capsid proteins), NC (nucleocapsid proteins) and RNA (ribonucleic acid) during the period of maturation. The CA monomers play important role to form capsids. Before formation of capsid, CA monomers become the CA hexamers. About 1000-1500 CA monomers are needed to build a typical cone-shaped capsid [5]. The self-assembly of HIV-1 will be modeled here using an extended Becker-Döring model, and the mean first assembly time to form CA hexamers will be determined.

The Becker-Döring model is one of the most popular models to describe aggregation and detachment in the self assembly of molecules.

$$C_r + C_s \underset{k^-_{r+s}}{\overset{k^+_r}{\rightleftharpoons}} C_{r+s}$$

Here, C_r are the concentrations of a cluster of size r, where r can be referred to as aggregation number and, $r = 1, 2, 3...$. The r^{th} forward reaction rate constant is k^+_r, and k^-_{r+s} is the $(r+s)^{st}$ backward reaction rate constant. One of the limitations of the Becker-Döring model is that only monomers can attach or detach to a given cluster. The Becker-Döring model is extended here to include attachment and detachment of molecules of size two or more in a cluster(s=2,3,... in above equation), one at a time, with the help of a chemical master equation and stochastic approaches. The mean first assembly times of molecules of different sizes based on the extended Becker Döring Model will be determined stochastically.