Electrostatic Theory of the Acidity of the Solution in the Lumina of Viruses and Virus-Like Particles

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1. Abstract

Recently, Maassen et al. measured an appreciable pH difference between the bulk solution and the solution in the lumen of virus-like particles, self-assembled in an aqueous buffer solution containing the coat proteins of a simple plant virus and polyanions (Maassen, S. J.; et al. Small 2018, 14, 1802081). They attribute this to the Donnan effect, caused by an imbalance between the number of negative charges on the encapsulated polyelectrolyte molecules and the number of positive charges on the RNA binding domains of the coat proteins that make up the virus shell or capsid. By applying Poisson–Boltzmann theory, we confirm this conclusion and show that simple Donnan theory is accurate even for the smallest of viruses and virus-like particles. This, in part, is due to the additional screening caused by the presence of a large number of immobile charges in the cavity of the shell. The presence of a net charge on the outer surface of the capsid we find in practice to not have a large effect on the pH shift. Hence, Donnan theory can indeed be applied to connect the local pH and the amount of encapsulated material. The large shifts up to a full pH unit that we predict must have consequences for applications of virus capsids as nanocontainers in bionanotechnology and artificial cell organelles.
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