Armstrong and Hoshi, http://www.jgp.org/cgi/content/full/jgp.201411223/DC1

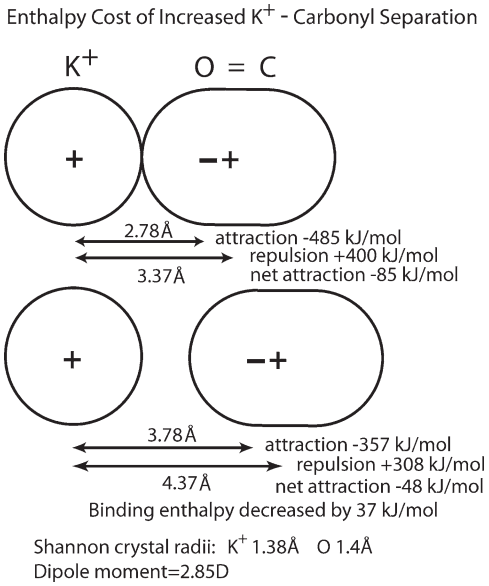

Figure S1. An approximate calculation of the interaction of a carbonyl dipole with a K^+ ion. The diagram shows the K^+ and the carbonyl dipole in close contact. The separation of charges in the carbonyl is appropriate for a dipole moment of 2.85 Debye (acetone). When K^+ and carbonyl are separated by 1 Å, the binding enthalpy decreases by 27.2 kJ/mol. At 21°C, this would decrease the binding affinity for K^+ by a factor of roughly 50,000.

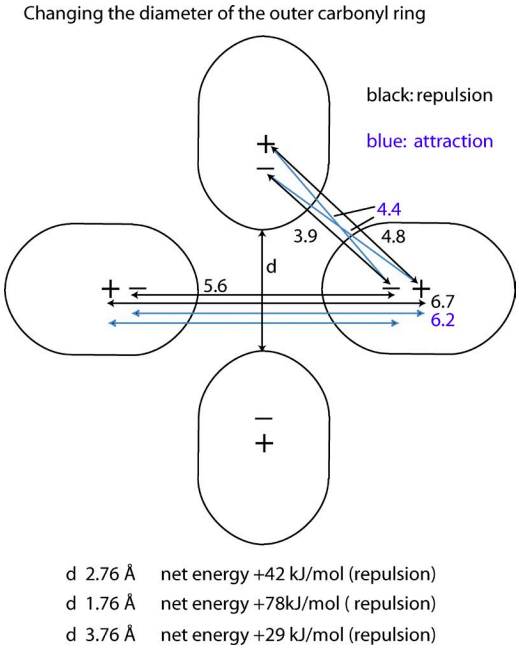

Figure S2. Comparing the energy change upon constricting an empty carbonyl ring from d = 2.76 Å (a good fit for a dehydrated K^+ ion) to 1.76 Å or dilating it to 3.76 Å. The diagram shows the distances between dipole charges (dipole moment 2.85D) of the rightmost carbonyl and the adjacent one above and the one opposite. Analogous distances for the other carbonyls are not illustrated. Carbonyl repulsion makes dilation much more probable than constriction, by 49 kJ/mol, or a factor of $\sim 3 \times 10^8$. Upon dilation a partially hydrated cation could enter the site.

THE JOURNAL OF GENERAL PHYSIOLOGY