Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

How the Spontaneous Insertion of Amphiphilic Imidazolium-Based Cations Change Biological Membranes: A Molecular Simulation Study

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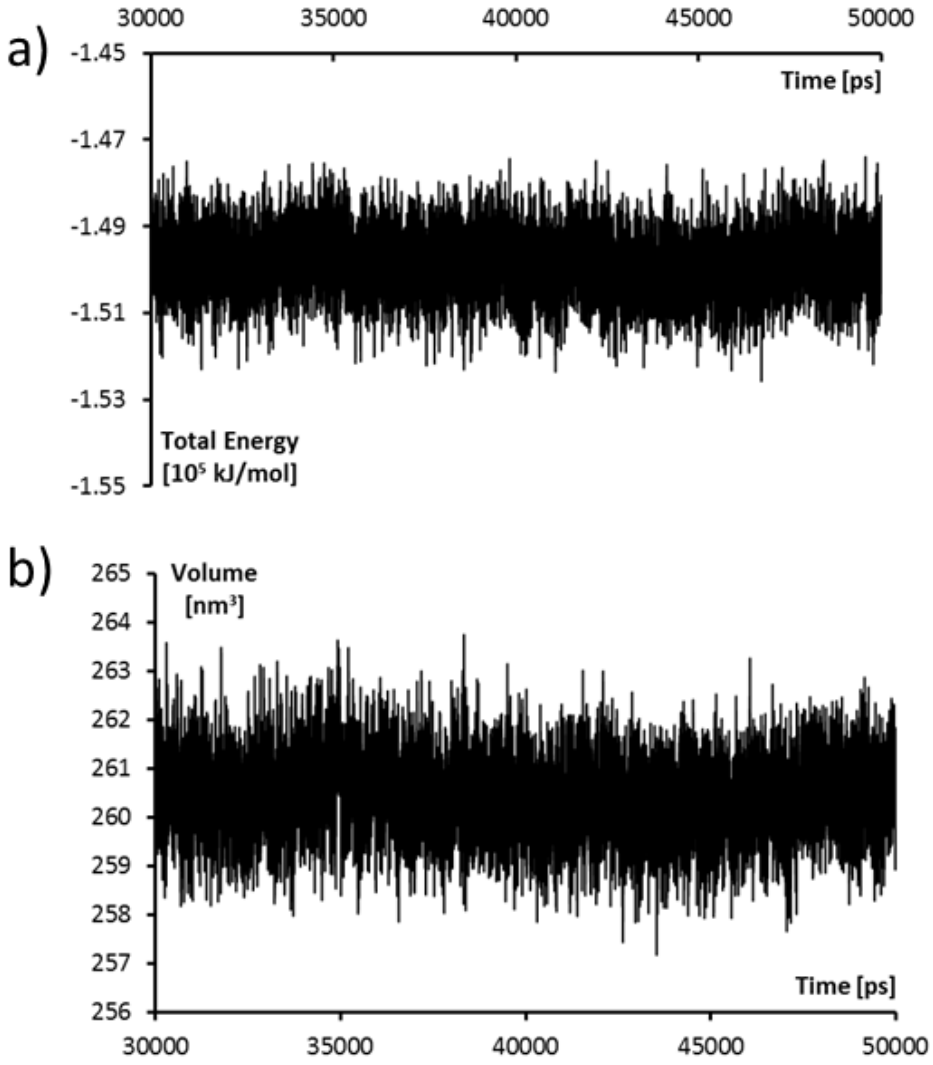

Figure S1: Total energy (a) and volume (b) of solvated membrane system over the last 20 ns of equilibration simulation. Results were subsequently used to initiate free energy calculations.

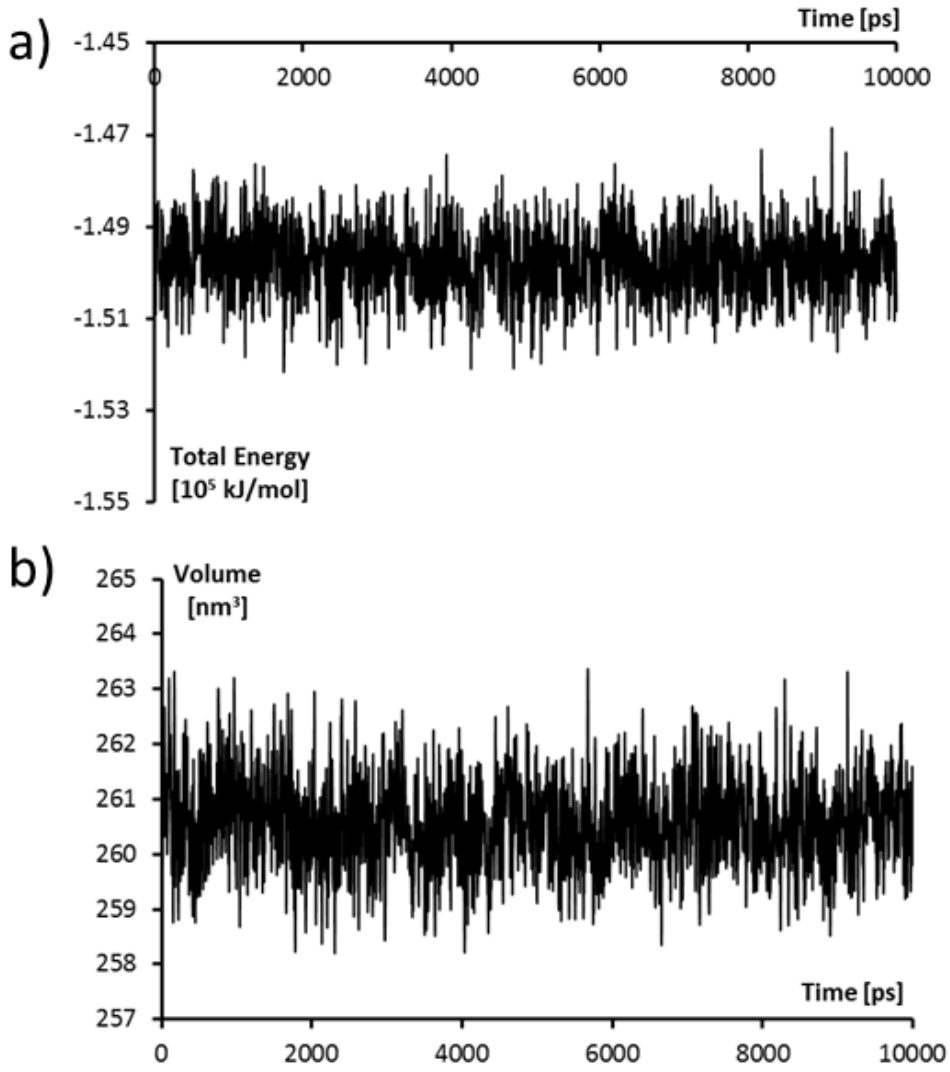

Figure S2: A representative plot of the total energy (a) and volume (b) as a function of simulation time. This was recorded during an MD run, which was used to derive free energy changes that were induced by pulling $OMIM^+$ from water into the membrane.

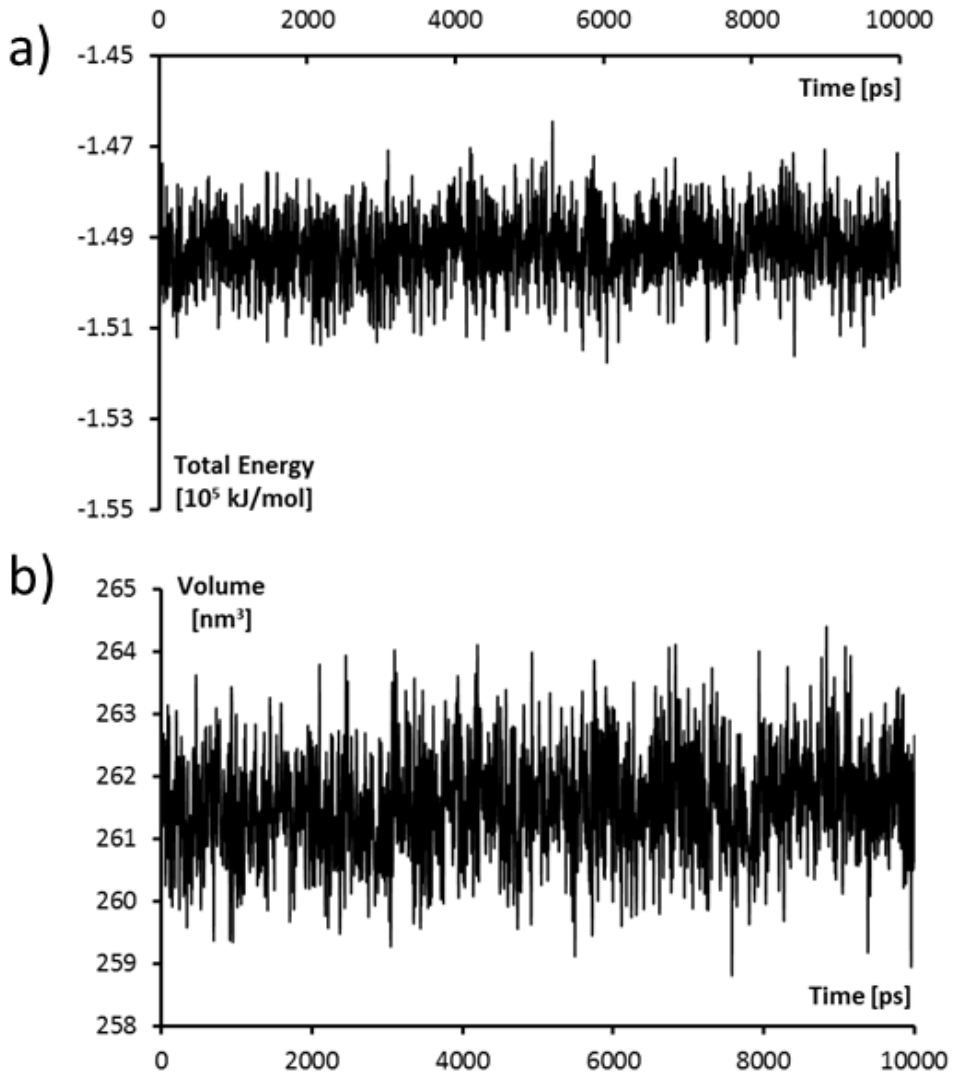

Figure S3: A representative plot of the total energy (a) and volume (b) as a function of simulation time. This was recorded during an MD run, which was used to derive free energy changes that were induced by pulling $OMIM^+$ from the membrane into water, while a second cation remained inside the membrane. At the start of these simulations, the two cations were placed inside the membrane *closer* than their energetically optimum distance.

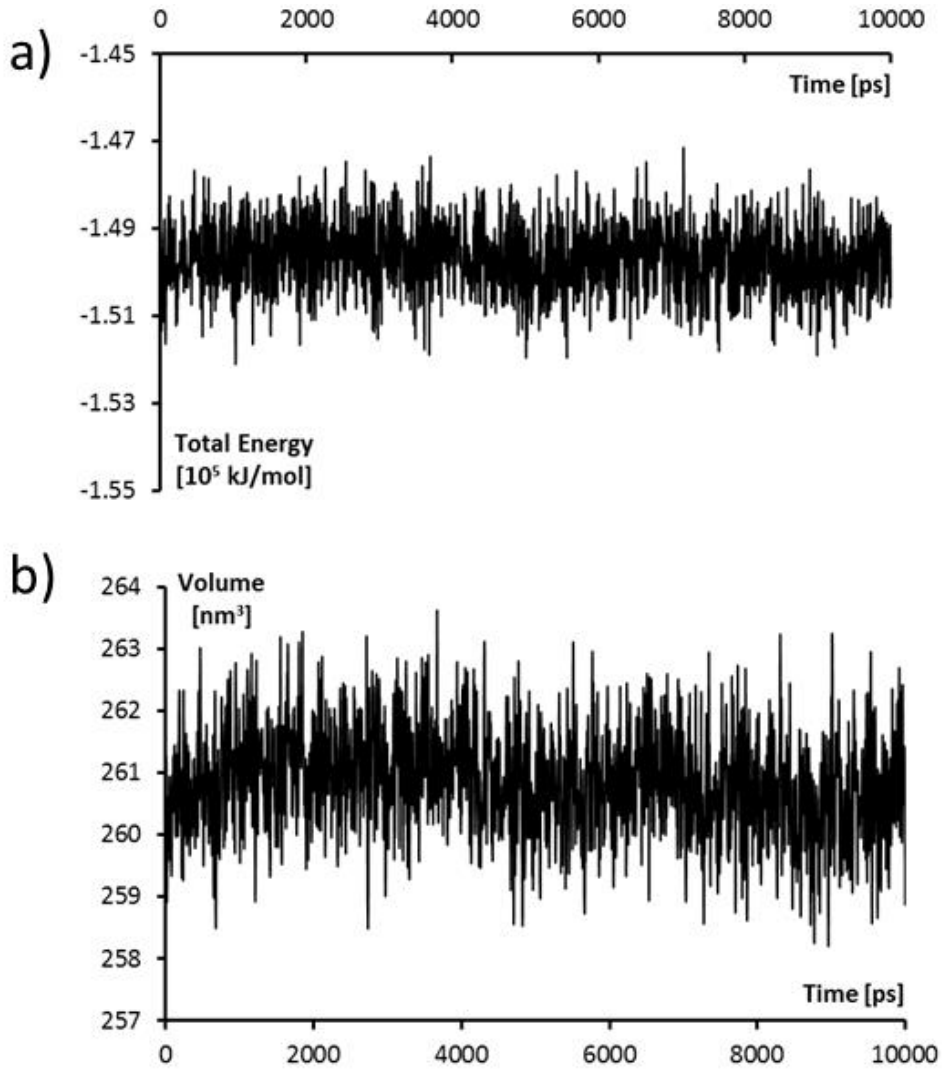

Figure S4: A representative plot of the total energy (a) and volume (b) as a function of simulation time. This was recorded during an MD run, which was used to derive free energy changes that were induced by pulling $OMIM^+$ from the membrane into water, while a second cation remained inside the membrane. At the start of these simulations, the two cations were placed inside the membrane *at* their energetically optimum distance.

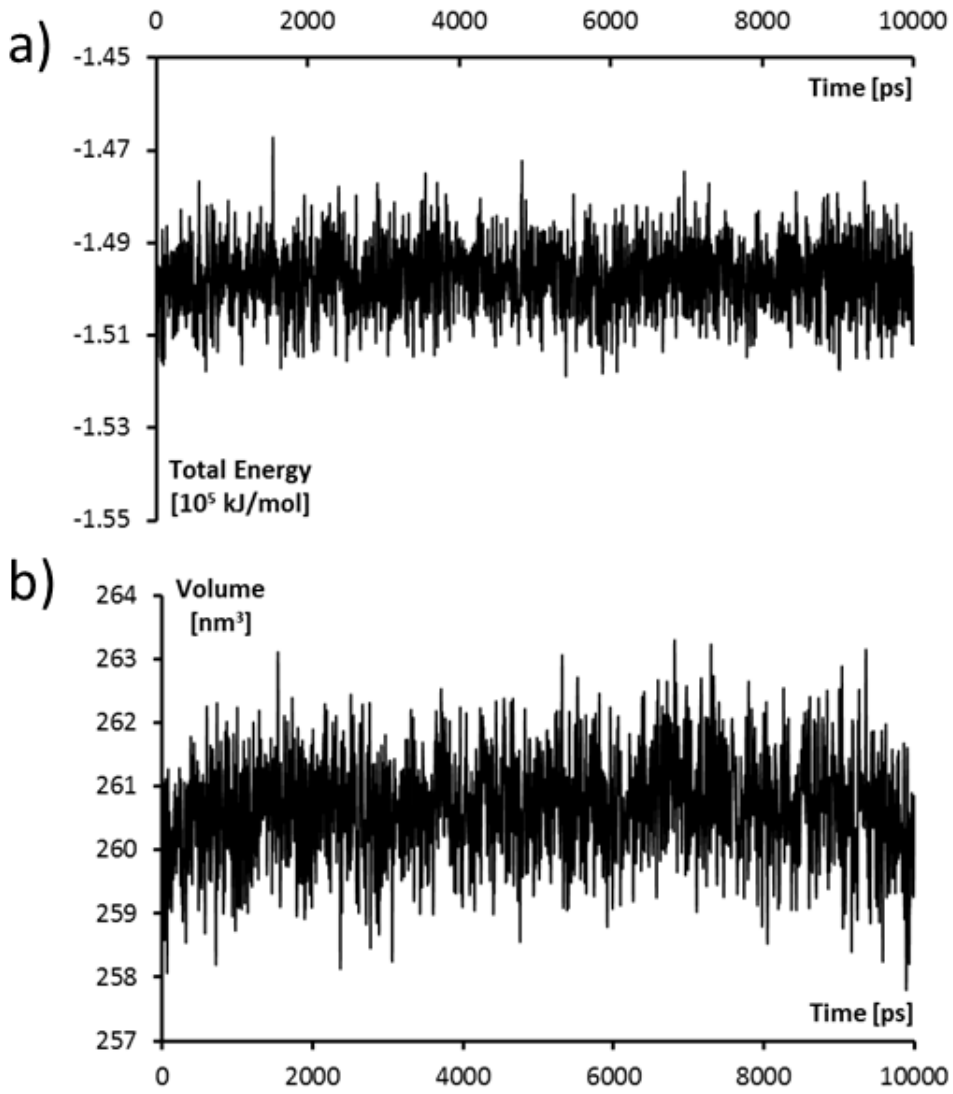

Figure S5: A representative plot of the total energy (a) and volume (b) as a function of simulation time. This was recorded during an MD run, which was used to derive free energy changes that were induced by pulling $OMIM^+$ from the membrane into water, while a second cation remained inside the membrane. At the start of these simulations, the two cations were placed inside the membrane *farther* than their energetically optimum distance.

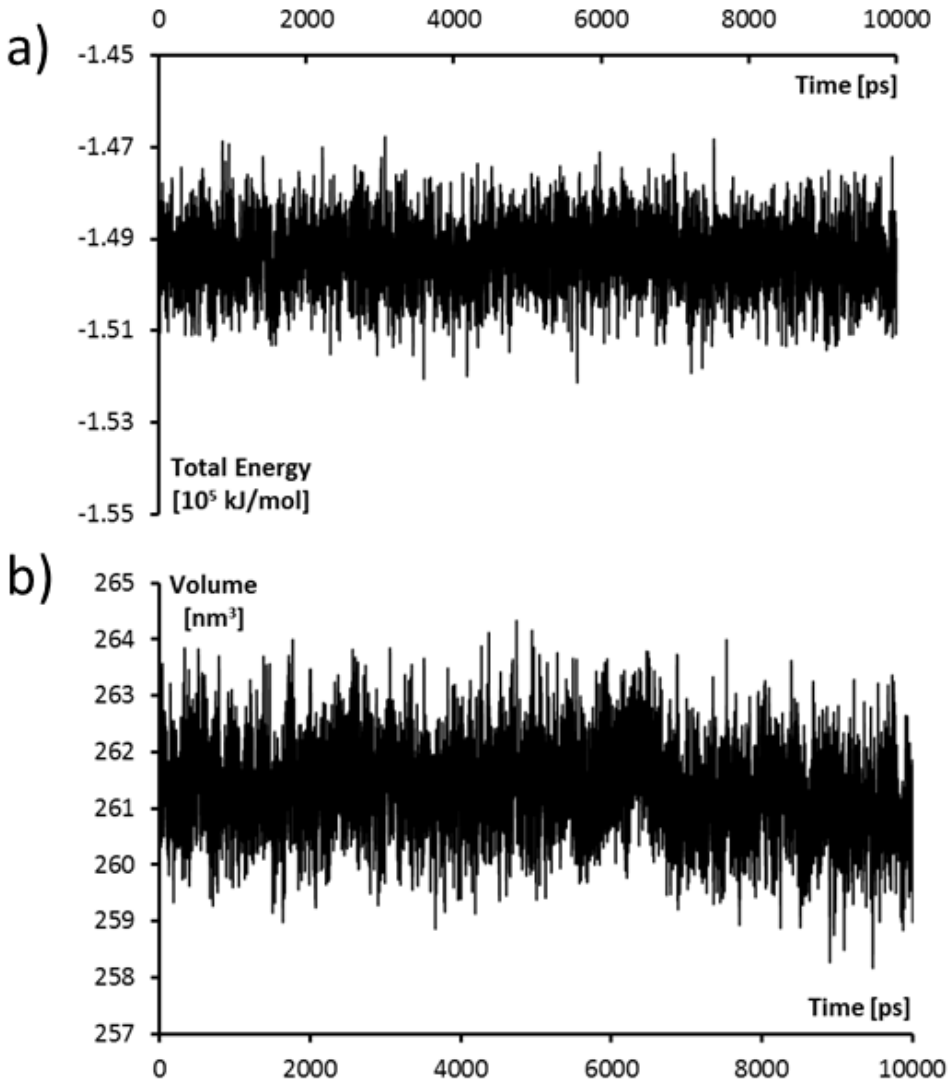

Figure S6: A representative plot of the total energy (a) and volume (b) as a function of simulation time. This was recorded during an MD run, which was used to derive free energy changes that were induced by pulling $OMIM^+$ across the membrane relative to a second cation, while both cations remained inside the membrane.

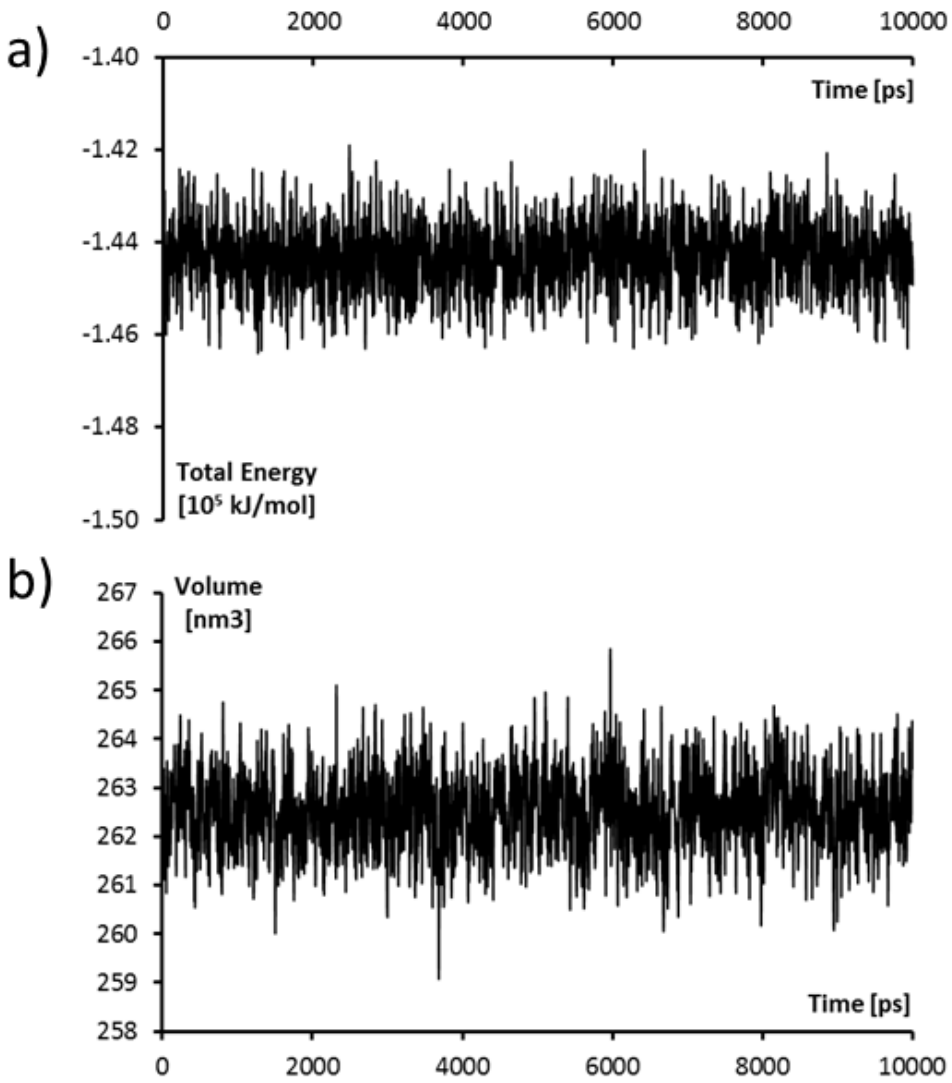

Figure S7: A representative plot of the total energy (a) and volume (b) as a function of simulation time. This was recorded during an MD run, which was used to derive free energy changes that were induced by pulling ammonia through the membrane.