Thermochemistry from Ion-Molecule Reactions of Hydrated Ions in the Gas Phase: A New Variant of Nanocalorimetry Reveals Product Energy Partitioning

Robert F. Höckendorf, O. Petru Balaj, Christian van der Linde, and Martin K. Beyer*

Institut für Physikalische Chemie, Christian-Albrechts-Universität zu Kiel, Olshausenstraße 40, 24098 Kiel, Germany

email: beyer@phc.uni-kiel.de
Figure S1: Mass spectra taken at different reaction delays for the reaction of hydrated electrons with CO$_2$. 
Figure S2: Optimized fit parameters slope $k_f$, intercept $N_{0,CO_2}$, the number of evaporating water molecules $\Delta N_{vap}$ and the least-square error of the fit, with the intercepts for the hydrated electrons $N_{0,el}$ scanned from 1 to 10. Although most fit parameters are quite flexible, the desired result $\Delta N_{vap}$ and the least-square error stay constant.
Figure S3: Least-square error in a 2D scan of the fit parameters $\Delta N_{vap}$ and $N_{0,el}$ for the reaction of hydrated electrons towards CO$_2$, with all other parameters optimized by the genetic algorithm. The minimum error is always found for $\Delta N_{vap} = 1.0$, illustrating the stability of the fit.