Electronic supplementary information (ESI) for PCCP

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

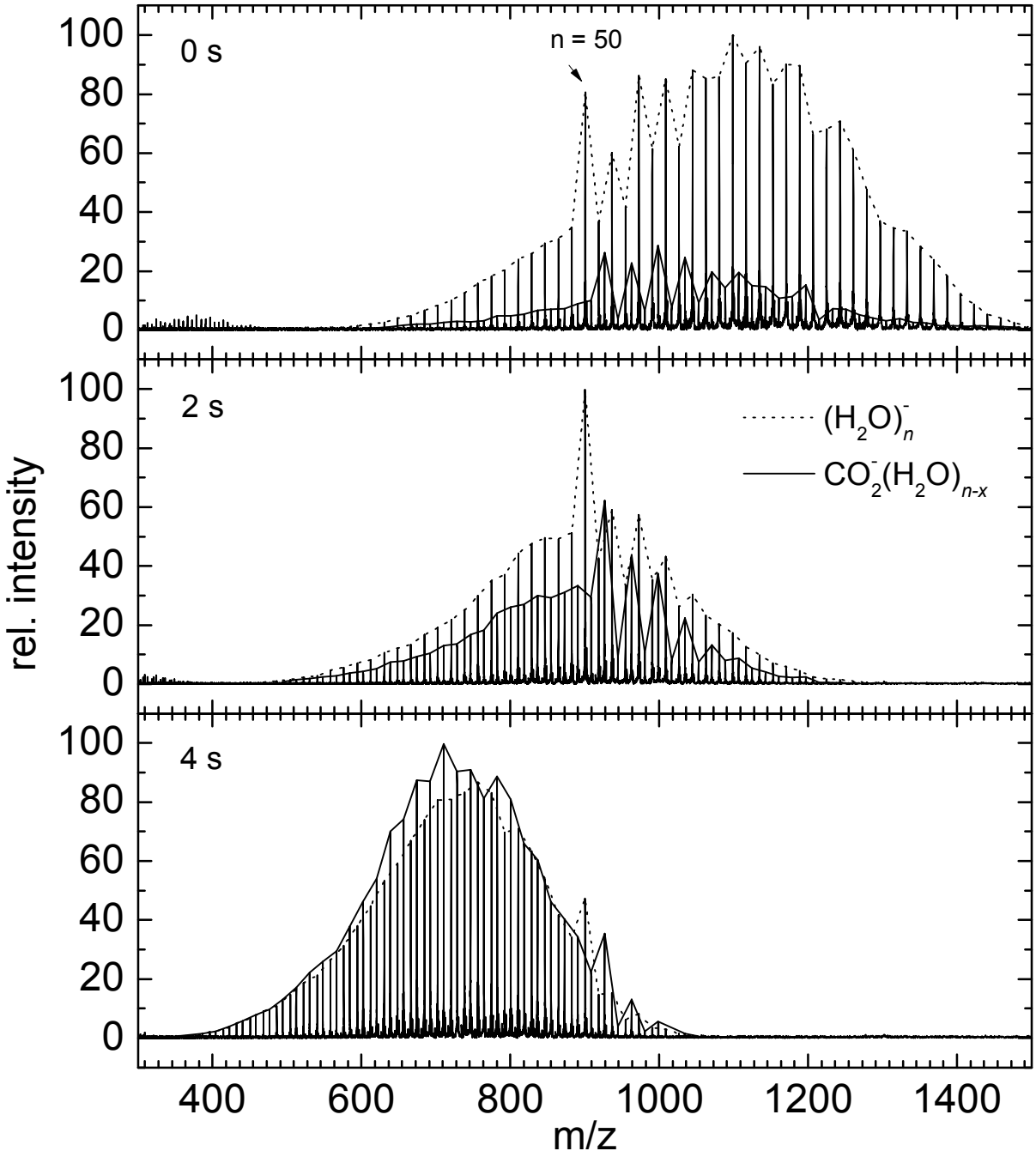

Figure S1: Mass spectra taken at different reaction delays for the reaction of hydrated electrons with CO_2.

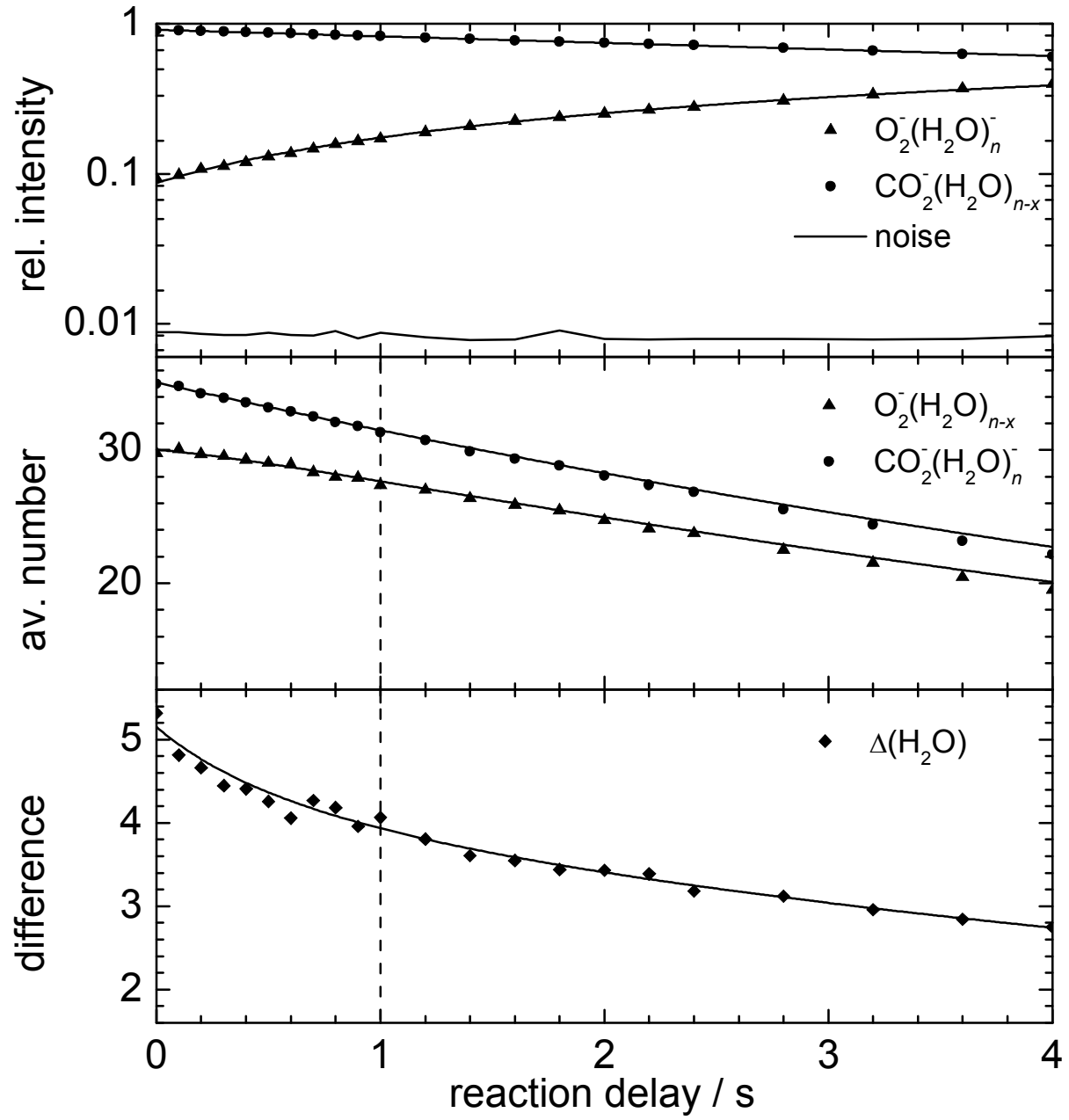

Figure S2: Optimized fit parameters slope k_f, intercept $N_{0,CO2}$, the number of evaporating water molecules ΔN_{vap} and the least-square error of the fit, with the intercepts for the hydrated electrons $N_{0,el}$ scanned from 1 to 10. Although most fit parameters are quite flexible, the desired result ΔN_{vap} and the least-square error stay constant.

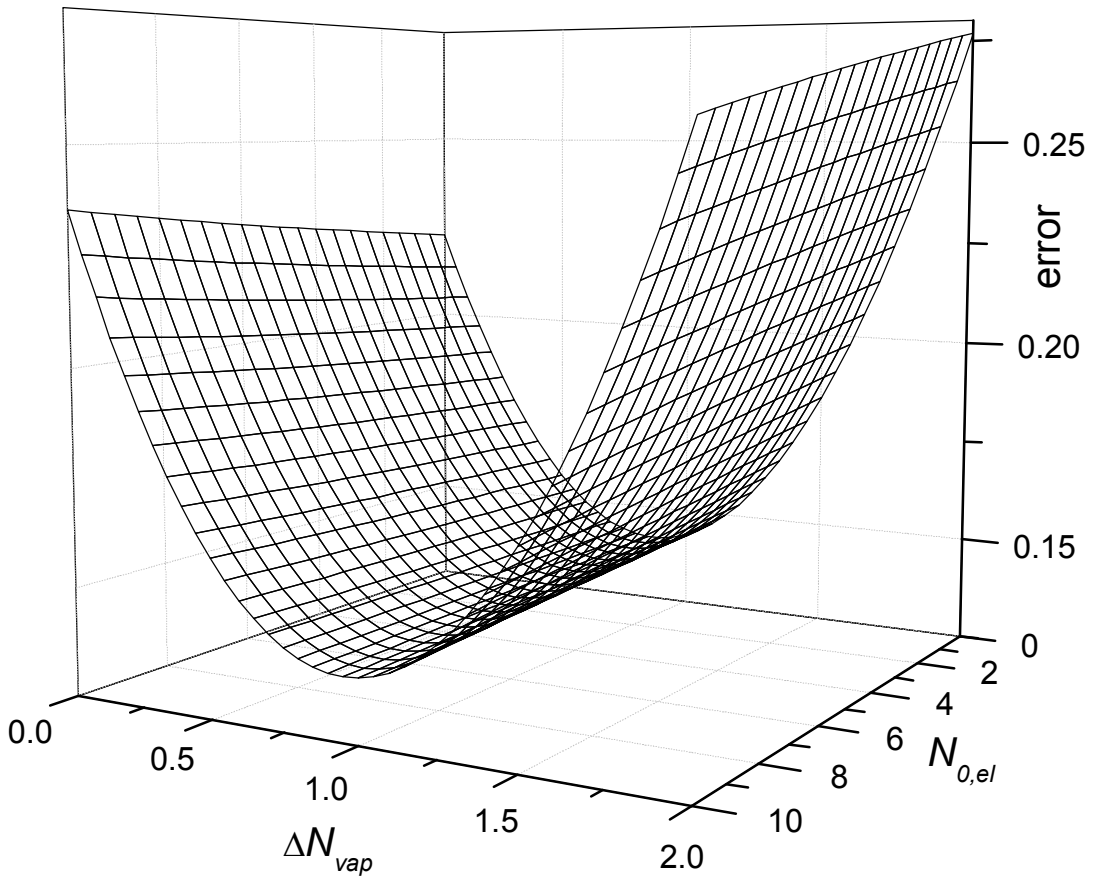

Figure S3: Least-square error in a 2D scan of the fit parameters ΔN_{vap} and $N_{0,el}$ for the reaction of hydrated electrons towards CO_2, with all other parameters optimized by the genetic algorithm. The minimum error is always found for $\Delta N_{vap} = 1.0$, illustrating the stability of the fit.