Data Files Accompanying: "Reactions of N2O5 with Salty and Surfactant-Coated Glycerol: Interfacial Conversion of Br– to Br2 Mediated by Alkylammonium Cations"

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Figure 3

These are surface tension reduction data collected using the Wilhelmy plate method. Data files show change in surface tension as a function of surfactant (THABr or CTABr) concentration in glycerol or glycerol with additional salts (0.5 M NaCl or 0.5 M NaBr). Units are mN/m vs mM. For each species, the data have been fit to a Langmuir fit (equation given below). Please see paper for full details.

Langmuir eq: $\gamma_0-\gamma(c_b)=c_\infty RT\ln(HKC_b)$

All time-of-flight (TOF) spectra discussed below are plotted as ion counts vs time (microseconds). These spectra were obtained by scattering a gas-phase species (Ar seeded in H2, N2O5 seeded in H2, or N2O5 seeded in argon) off a glass wheel rotating in a solution of glycerol containing surfactants, salts, or a mixture of the two. (The solvent for all solutions

studied here is glycerol.) Scattering and desorbing species are "chopped" into pulses, ionized by electron impact, and detected with a channeltron. Scattering species leave the glycerol surface with energy falling into one of two categories. Molecules or atoms that only lose a portion of their energy form the inelastically scattered (IS) portion of the signal. Molecules the adsorb on the liquid surface and assume the thermal energy of the surface before desorbing and traveling to the detector compose the thermal desorption (TD) component of the signal. The TD component can be fit to a Maxwell-Boltzmann distribution at the temperature of the surface. Some of the data files provided here contain a vector labeled "Sample"_MB. These are the values for the Maxwell-Boltzmann fits, and can be plotted against the same time axis as the "Sample" signal data within a given file. The Maxwell-Boltzmann equation cast in terms of time is given below. For additional fitting details, please see Michael Shaloski's dissertation, "Reactive Collisions of N_2O_5 at Salty Surfaces: Formation of Interfacial Halogen Species" completed in 2016.

MB equation: n(t)=C(1/t^4)e^-((mL^2)/(2RTt^2))

Figure 4

Time of flight (TOF) spectra for argon seeded in H2 scattering from the surface of NaBr (2.7 M), THABr (0.03 M), and THABr (0.03 M) + NaCl (0.5 M) solutions (all in glycerol). Spectra show ion counts as a function of arrival time (in microseconds) while monitoring m/z = 40.

Figure 5a

TOF spectra for N2O5 seeded in argon scattering from the surface of pure glycerol compared with scattering from a solution containing 0.03 M THABr in glycerol. m/z = 46 is used to monitor N2O5 scattering.

Figure 5b

TOF spectra monitoring Br2 signal produced from N2O5 seeded in argon scattering from the surface of 2.7 M NaBr in glycerol compared with scattering from the surface of 0.03 M THABr in glycerol. m/z = 160 is used to monitor Br2 signal.

Figure 6a

TOF spectra with IS component explicitly included and fits for N2O5 seeded in H2 signal from the surface of 2.7 M NaBr in glycerol. m/z = 46 is used to monitor N2O5.

Figure 6b

TOF spectra with IS components explicitly included and fits for N2O5 seeded in H2 signal from the surface of 0.03M THABr in glycerol. m/z = 46 is used to monitor N2O5.

Figure 6c

TOF spectra comparing Br2 signal from N2O5 seeded in H2 scattering on 0.03 M THABr and 2.7 M NaBr in glycerol.

Figure 7

In rows 1-13, 15 columns summarize 15 mass spectra of glycerol samples with excess N2O5 blown over the top at the flow rate of roughly 100 sccm. These scans are dated in row 1, and sorted in row 2 into one of three categories: Glyc (pure de-gassed glycerol only), BrGlyc (degassed glycerol containing 2.7 M NaBr), and SaltGlyc (degassed glycerol containing both 0.03 M tetrahexyl ammonium bromide (THABr) and 2.7 M NaCl). The labels in row 2 also contain a number equal to the iteration of that sorted sample. Dates and labels seen in rows 1 and 2 hold true for all rows 3-39.

Column A specifies a target peak monitored over time, with columns B through P specifying the sum amount of counts seen after blank subtraction. This sum was found by first looking into a respective day's raw data finding the respective experiment's run time and integrating the area under a curve from the moment the target peak was first seen on the mass spectrometer's time trace (a trough in the raw data's spectra) to the moment all signal disappears after removal of the sample (the break seen at the bottom of the signal's trough chronologically following). This represents the target's raw integrated signal. This raw sum was then background-subtracted by extrapolating the decay of a signal's trough and integrating area under the baseline. Subtracting this amount from the raw integrated signal yielded the true signal seen in rows 1-13, which would then be normalized in rows 14 and 15.

Values of zero denote either a negative value after background subtraction or that data was not recorded for the select experiment. Rows 17-34 normalize data obtained in rows 3-13 and sum hydrate clusters. Dates and labels are again used in rows 17 and 18. In rows 36-39, the targets Br2, mononitroglycerin (MNG), and dinitroglycerin (DNG) are summed and the fractional percentages of each product's contribution towards the overall product counts are calculated. Rows 41-46 contain basic data analysis of rows 36-39, with averages (columns B-D), standard deviations (columns G-I), and 90% confidence intervals (columns L-N) being calculated. This data is reiterated in decimal form for graphing purposes in rows 48-51.

The data is arranged in the form of "average +/- standard deviation (and 90% confidence interval)" in rows 53-59. Here, numbers are also sorted by sample, with blank glycerol compiling columns B-E, NaBr in columns G-J, and SaltMix in columns L-O.