# Electronic Supplementary Information – Environmental Science: Nano

***for "Colloidal stability of hematite nanoparticles in the presence of a common quaternary ammonium compound at environmentally-relevant concentrations"*** *by Deborah M.* Aruguete, Andy Zhuang, Cameron Canonaco, Trevor Sheckler, Corryn Schmidt and Rituraj Borgohain[c]

## I. Mass spectrometry

**Table S1. Operating conditions for Agilent 7900 ICP-MS**

| | |
|---|---|
| Plasma gas flow | 15 L/min |
| Auxiliary gas flow | 0.9 L / min |
| Nebulizer gas flow* | 0.75 – 1.03 L / min |
| ICP RF power | 1600 W |
| Mode of operation | He Collision Cell on |
| He gas flow | 4.3 mL/min |
| Spray chamber temperature | 2° C |
| Sample uptake | 0.32 mL/min |
| Ion optic voltages* | Vary |
| Integration time | 0.1 s |
| Replicates / sample | 3 |
| Nebulizer type | Agilent MicroMist Glass U-series |
| Spray chamber type | Agilent 7900 UHMI Spray Chamber (Scott-style quartz) |
| Sample cone | Agilent 7900 Ni Sampler Cone with Cu base |
| Skimmer cone | Agilent 7900/8900 Ni Skimmer Cone |

*Tuned daily using Agilent Tuning Solution for ICP-MS containing 1 μg/L each of Li, Y, Ce, Tl and Co in a matrix of 2% $HNO_3$ (stock solution #5188-6564).

Parameters for this instrument are adjusted to maximize the $^{59}Co$, $^{89}Y$ and $^{205}Tl$ signals (in tuning solution standard). Parameters were also adjusted to reduce the formation of doubly-charged species and oxides by minimizing the ratios of $^{140}Ce^{++}/^{140}Ce$ (70/140 ratio) and $^{156}CeO/Ce$ (≤0.03). To reduce the amount of polyatomic species formed, a collision cell was utilized. He flow was tuned to keep $^{40}Ar^{38}Ar$ at a minimum.

All stable isotopes of iron were monitored, namely $^{54}Fe$, $^{56}Fe$, $^{57}Fe$ and $^{58}Fe$. The reported measurements were based on $^{57}Fe$ due to polyatomic interferences with N and Cl (both present in the surrounding matrix), along with our monitoring of the discrepancy between the signal with and without the He collision cell. Other than the expected polyatomic species with Ar, O and H, $^{57}Fe$ has mass interferences with polyatomics containing Ca and F. Given that the high purity of our reagents makes Ca and F unlikely contaminants, we believed $^{57}Fe$ was the best choice.

The following table contains the common mass interferences for iron. Those expected to be particularly significant are indicated in red.

**Table S2. Common mass interferences for iron***

| Isotope | Natural abundance | Common interferences |
|---|---|---|
| $^{54}Fe$ | 5.85% | $^{37}Cl^{16}OH$, $^{40}Ar^{14}N$, $^{36}Ar^{18}O$, $^{38}Ar^{16}O$, $^{36}Ar^{17}OH$, $^{36}S^{18}O$, $^{35}Cl^{18}O$, $^{37}Cl^{17}O$ |
| $^{56}Fe$ | 91.8% | $^{40}Ar^{16}O$, $^{40}Ca^{16}O$, $^{40}Ar^{15}NH$, $^{38}Ar^{18}O$, $^{38}Ar^{17}OH$, $^{37}Cl^{18}OH$ |
| $^{57}Fe$ | 2.12% | $^{40}ArOH$, $^{40}CaOH$, $^{40}Ar^{17}O$, $^{38}Ar^{18}OH$, $^{38}Ar^{19}F$ |
| $^{58}Fe$ | 0.28% | N/A (Signal too low) |

*Reference: May, T.W. and Wiedmeyer, R.H. "A Table of Polyatomic Interferences in ICP-MS" *Atomic Spectroscopy* Vol 19(5) 1998 150-155.

## II. Semiquantitative analysis of NP content in suspension

Absorption spectroscopy was utilized as an immediate, rapid means to characterize the remaining NP content in suspensions. As optical absorbance of NP suspensions is affected by concentration, particle size/aggregation, and other size-influenced physicochemical parameters, it was only utilized as a semiquantitative measurement. Due to the semiquantitative nature of this data, no detailed statistical analysis was performed.

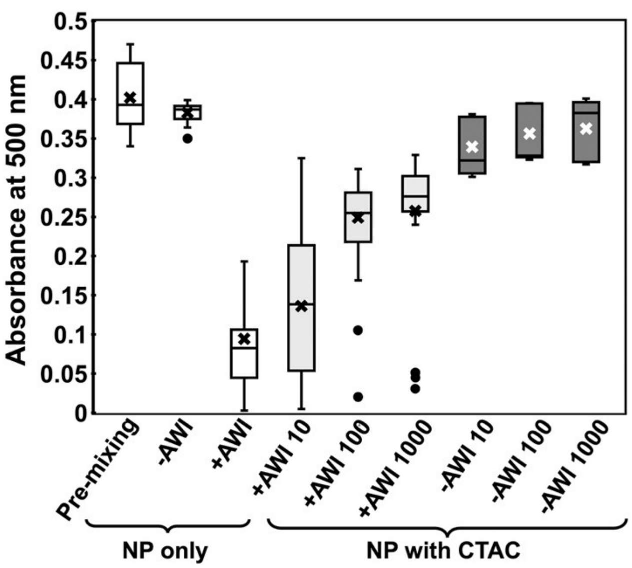



**Figure S1.** Box-and-whiskers plot of absorbance values at 500 nm ($A_{500}$) for aliquots of NP suspensions collected after 22 h of mixing. White boxes are data from NP-only trials, light gray boxes are data from +AWI trials with CTAC, and the dark gray boxes are data from -AWI trials with CTAC. The concentrations of CTAC were 10, 100, and 1000 μg / L. Mean $A_{500}$ values are denoted with the symbol "X". The dots mark outlier measurements, namely data points >1.5 interquartile ranges above the third quartile or below the first quartile.

**Table S3. Absorbance values of NP suspensions at 500 nm.**

| Treatment | Mean $A_{500}$ | Std dev $A_{500}$ | Median $A_{500}$ | Replicates (*n*) |
|---|---|---|---|---|
| **Sonicated, pre-mixing*** | 0.419 | 0.043 | 0.429 | 10 |
| **-AWI (NP only)** | 0.367 | 0.053 | 0.387 | 26 |
| **+AWI (NP only)** | 0.094 | 0.120 | 0.083 | 30 |
| **+AWI 10 µg CTAC / L** | 0.137 | 0.088 | 0.139 | 30 |
| **+AWI 100 µg CTAC / L** | 0.249 | 0.084 | 0.255 | 29 |
| **+AWI 1000 µg CTAC / L** | 0.258 | 0.082 | 0.276 | 27 |
| **-AWI 10 µg CTAC / L** | 0.340 | 0.037 | 0.322 | 9 |
| **-AWI 100 µg CTAC / L** | 0.356 | 0.036 | 0.328 | 9 |
| **+AWI 1000 µg CTAC / L** | 0.362 | 0.038 | 0.383 | 12 |

*After sonication, $A_{500}$ decreased from the original value of 0.5 (prior to sonication).

## III. *p*-values resulting from pairwise comparisons (Mann-Whitney)

For all dataset groups, p-values were <0.0005 for Kruskal – Wallis tests. Note that for DLS or zeta potential data, the -AWI 10, -AWI 100, and -AWI 1000 treatments were not included as these treatments' sample sizes were too low.

**Pink numbers** indicate $p < 0.05$, but not reaching the Bonferroni-corrected threshold of $p \leq 0.001$ (or 0.003 for DLS and zeta potential data).

**Yellow-highlighted boxes** are for $p \leq 0.001$ ($p \leq 0.002$ for surface tension data, $p \leq 0.003$ for DLS and zeta potential data), indicating that the Bonferroni-corrected significance threshold was met or exceeded.

**Table S4. Mann-Whitney Test *p*-values for [Fe] data**

| | Initial | -AWI | +AWI | +AWI 10 | +AWI 100 | +AWI 1000 | -AWI 10 | -AWI 100 | -AWI 1000 |
|---|---|---|---|---|---|---|---|---|---|
| **Initial** | | 0.403 | <0.0005 | <0.0005 | <0.0005 | <0.0005 | 0.553 | 0.495 | 0.179 |
| **-AWI** | | | <0.0005 | <0.0005 | <0.0005 | <0.0005 | 0.249 | 0.416 | 0.450 |
| **+AWI** | | | | 0.057 | <0.0005 | <0.0005 | <0.0005 | <0.0005 | <0.0005 |
| **+AWI 10** | | | | | **0.004** | <0.0005 | <0.0005 | <0.0005 | <0.0005 |
| **+AWI 100** | | | | | | <0.0005 | <0.0005 | <0.0005 | <0.0005 |
| **+AWI 1000** | | | | | | | <0.0005 | <0.0005 | <0.0005 |
| **-AWI 10** | | | | | | | | 0.473 | **0.019** |
| **-AWI 100** | | | | | | | | | **0.027** |
| **-AWI 1000** | | | | | | | | | |

**Table S5. Mann-Whitney Test *p*-values for DLS data (Z-average sizes)**

| | Initial | -AWI | +AWI | +AWI 10 | +AWI 100 | +AWI 1000 |
|---|---|---|---|---|---|---|
| **Initial** | | 0.023 | <0.0005 | <0.0005 | 0.075 | 0.312 |
| **-AWI** | | | 0.001 | 0.001 | 1.000 | 0.374 |
| **+AWI** | | | | 0.421 | <0.0005 | <0.0005 |
| **+AWI 10** | | | | | <0.0005 | <0.0005 |
| **+AWI 100** | | | | | | 0.078 |
| **+AWI 1000** | | | | | | |

**Table S6. Mann-Whitney Test *p*-values for Zeta Potential**

| | Initial | AWI - | AWI+ | AWI+ 10 | AWI+ 100 | AWI+1000 |
|---|---|---|---|---|---|---|
| **Initial** | | 0.927 | 0.210 | 0.074 | 0.144 | 0.023 |
| **AWI-** | | | 0.121 | 0.027 | 0.031 | 0.006 |
| **AWI+** | | | | 1.000 | 0.523 | 0.510 |
| **AWI+ 10** | | | | | 0.943 | 0.298 |
| **AWI+ 100** | | | | | | 0.175 |
| **AWI+1000** | | | | | | |

**Table S7. Mann-Whitney Test *p*-values for polydispersity indices**

| | Initial | AWI - | AWI+ | AWI+ 10 | AWI+ 100 | AWI+1000 |
|---|---|---|---|---|---|---|
| **Initial** | | 0.210 | <0.0005 | <0.0005 | 0.022 | 0.006 |
| **AWI-** | | | 0.001 | 0.001 | 0.002 | 0.002 |
| **AWI+** | | | | 0.272 | <0.0005 | <0.0005 |
| **.AWI+ 10** | | | | | <0.0005 | <0.0005 |
| **AWI+ 100** | | | | | | 0.707 |
| **AWI+1000** | | | | | | |

**Table S8. Mann-Whitney Test *p*-values for surface tension**

| | Water only | 10 µg CTAC/L | 100 µg CTAC/L | 1000 µg CTAC/L |
|---|---|---|---|---|
| **Water only** | | 0.001 | <0.0005 | <0.0005 |
| **10 µg CTAC/L** | | | <0.0005 | <0.0005 |
| **100 µg CTAC/L** | | | | <0.0005 |
| **1000 µg CTAC/L** | | | | |

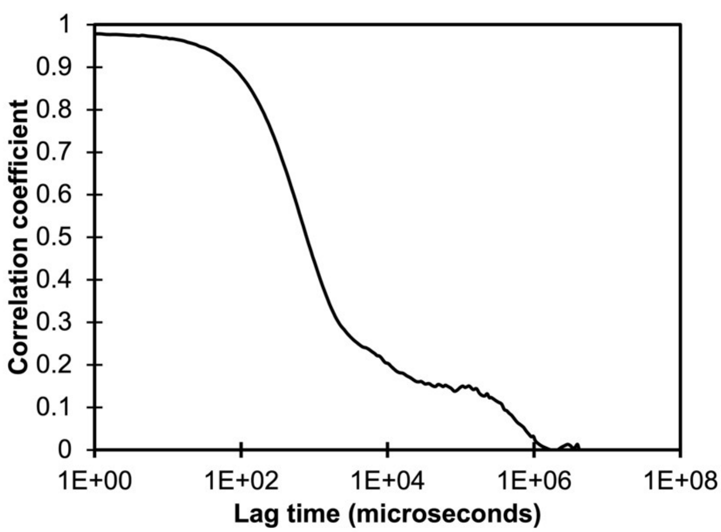
**Table S9. Mann-Whitney Test *p*-values for contact angles**

| | Water only | 10 µg CTAC/L | 100 µg CTAC/L | 1000 µg CTAC/L |
|---|---|---|---|---|
| **Water only** | | 0.625 | 0.175 | 0.082 |
| **10 µg CTAC/L** | | | 0.138 | 0.505 |
| **100 µg CTAC/L** | | | | 0.023 |
| **1000 µg CTAC/L** | | | | |

Note that all other M-W comparisons with and between $10^4$, $10^5$ and $10^6$ µg CTAC/L found significant differences ($p < 0.0005$).

# IV. Comments on DLS measurements of the +AWI (no CTAC)

Number fluctuation refers to variations in the number of particles within the scattering volume during a DLS measurement and can generally be caused by the presence of large particles or aggregates. Here is a correlogram for one of the DLS measurements. The discontinuities in the curve are typical for samples with number fluctuations.




All DLS measurements were performed as soon as possible after the mixing portion of our experiments. Whereas a way to “solve” the number fluctuations issue is to let the sample settle or filter it, we wanted to be consistent in our sampling, rather than processing the +AWI only trials differently from all the other treatments. Regardless of the number fluctuations, this data invariably indicates that the +AWI treatment results in samples and NP aggregation very different from most of the other treatments.