

Supplementary Information for

Oxidation state and metal interactions influence aerosol oxidative potential in acellular DTT and OH assays

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Table S1. Purities of the chemicals used in the study.

Chemical	Purity
Sodium selenite pentahydrate	≥ 99.0%
Antimony(III) chloride	99.95%
Antimony(V) chloride	≥ 99.99%
Lead(II) nitrate	99.999%
Tin(II) chloride	≥ 99.99%
Iron(II) sulfate heptahydrate	99.99%
Iron(III) chloride hexahydrate	97%
Copper(I) chloride	≥ 99.995%
Copper(II) sulfate pentahydrate	99.999%
Barium chloride	99.999%
Zinc sulfate heptahydrate	≥ 99.95%
Mercury(II) chloride	99.5%
Manganese(II) chloride tetrahydrate	≥ 98%
L-Ascorbic acid	≥ 99%
L-Glutathione reduced	≥ 98%
Uric acid sodium salt	11.0-13.0% Na, anhydrous basis (ICP)
DL-dithiothreitol	≥ 99.5%
5,5'-dithiobis(2-nitrobenzoic acid)	> 98.0%
Tris Base	≥ 99.9%
Ethylenediaminetetraacetic acid disodium salt dihydrate	≥ 99%
Sodium phosphate dibasic	≥ 99.5%
Potassium phosphate monobasic	≥ 99.5%
Disodium terephthalate	> 99.0%
2-hydroxyterephthalic acid	> 98.0%
10% trichloroacetic acid	9.5–10.5% w/v

Table S2. MINTEQ-predicted Fe(II) and Fe(III) speciation in the OH and DTT assays with precipitation suppressed.

Added Fe	Assay	Dominant modeled aqueous species
Fe(II)	OH	FeHPO ₄ , ~77%
Fe(II)	DTT	FeHPO ₄ , ~84%
Fe(III)	OH	Fe(OH) ₂ Asc ⁻ , ~99%
Fe(III)	DTT	Fe(OH) ₂ ⁺ , ~89%

Table S3. Chemical species and initial concentrations used as inputs for MINTEQ calculations of Fe speciation in the OH and DTT assays.

Assay	Fe(II)		Fe(III)	
	Component	Initial concentration (M)	Component	Initial concentration (M)
OH	Na ⁺	3.57E-02	Na ⁺	3.57E-02
	K ⁺	2.20E-03	K ⁺	2.20E-03
	Asc ²⁻	2.00E-04	Asc ²⁻	2.00E-04
	G ³⁻	1.00E-04	G ³⁻	1.00E-04
	U ²⁻	1.00E-04	U ²⁻	1.00E-04
	TA ²⁻	1.00E-02	TA ²⁻	1.00E-02
	PO ₄ ³⁻	1.00E-02	PO ₄ ³⁻	1.00E-02
	Fe(II)	1.00E-06	Fe(III)	1.00E-06
	SO ₄ ²⁻	1.00E-06	Cl ⁻	3.00E-06
DTT	Na ⁺	1.56E-01	Na ⁺	1.56E-01
	K ⁺	2.20E-02	K ⁺	2.20E-02
	PO ₄ ³⁻	1.00E-01	PO ₄ ³⁻	1.00E-01
	DTT	1.00E-04	DTT	1.00E-04
	Fe(II)	1.00E-06	Fe(III)	1.00E-06
	SO ₄ ²⁻	1.00E-06	Cl ⁻	3.00E-06

Table S4. Formation constants, corresponding temperatures and literature sources for reactions added to the MINTEQ thermodynamic database.

Assay	Species	Formation reaction using fully deprotonated ligand	log β	Temperature (°C)	References
OH	$HAsc^-$	$H^+ + Asc^{2-} \rightleftharpoons HAsc^-$	11.72	25	Charrier and Anastasio 2011 ¹
	H_2Asc	$2H^+ + Asc^{2-} \rightleftharpoons H_2Asc$	15.89	25	
	$FeAsc$	$Fe^{2+} + Asc^{2-} \rightleftharpoons FeAsc$	0.66	25	
	$FeHAsc^+$	$H^+ + Fe^{2+} + Asc^{2-} \rightleftharpoons FeHAsc^+$	12.38	25	
	$FeAsc^+$	$Fe^{3+} + Asc^{2-} \rightleftharpoons FeAsc^+$	9.5	37	Ritacca et al. 2022 ²
	$Fe(OH)Asc$	$Fe^{3+} + Asc^{2-} + H_2O - H^+ \rightleftharpoons Fe(OH)Asc$	7.8	37	
	$Fe(OH)_2Asc^-$	$Fe^{3+} + Asc^{2-} + 2H_2O - 2H^+ \rightleftharpoons Fe(OH)_2Asc^-$	5.0	37	
	$FeAsc_2^-$	$Fe^{3+} + 2Asc^{2-} \rightleftharpoons FeAsc_2^-$	18.8	37	
	HG^{2-}	$H^+ + G^{3-} \rightleftharpoons HG^{2-}$	9.123	37	Bugarín and Filella 1999 ³
	H_2G^-	$2H^+ + G^{3-} \rightleftharpoons H_2G^-$	17.42	37	
	H_3G	$3H^+ + G^{3-} \rightleftharpoons H_3G$	20.78	37	
	H_4G^+	$4H^+ + G^{3-} \rightleftharpoons H_4G^+$	22.93	37	
	HU^-	$H^+ + U^{2-} \rightleftharpoons HU^-$	10.4	37	Lotan et al. 2025 ⁴
	H_2U	$2H^+ + U^{2-} \rightleftharpoons H_2U$	15.75	37	
	HTA^-	$H^+ + TA^{2-} \rightleftharpoons HTA^-$	4.82	25	Guseva et al. 2025 ⁵
	H_2TA	$2H^+ + TA^{2-} \rightleftharpoons H_2TA$	8.33	25	
DTT	$HDTT^-$	$H^+ + DTT^{2-} \rightleftharpoons HDTT^-$	9.811	37	Gnonlonfoun et al. 1991 ⁶
	H_2DTT	$2H^+ + DTT^{2-} \rightleftharpoons H_2DTT$	18.672	37	

Table S5. Individual experimental measurements of OH formation by tested elements and metal mixtures.

Element/mixture	Individual measurements (nM min ⁻¹)
1 μ M Ba(II)	0.020, -0.22, 0.21
1 μ M Zn(II)	0.31, 0.19, 0.26, 0.32
1 μ M Hg(II)	-0.49, 0.24, 0.41, 0.28, 0.30, 0.21, 0.15
1 μ M Sn(II)	-1.2, -0.70, -0.56, -0.85
1 μ M Pb(II)	-2.7, -1.8, -1.8, -1.6
1 μ M Cu(I)	6.2, 6.2, 5.6
1 μ M Cu(II)	9.1, 7.8, 9.6, 7.2, 7.5, 7.1, 7.2, 8.2, 7.8, 7.5, 7.2
1 μ M Fe(II)	8.6, 8.0, 7.3
1 μ M Fe(III)	2.3, 2.6, 2.3
1 μ M Sb(III)	-0.51, -0.41
1 μ M Sb(V)	0.14, 0.18, 0.18
1 μ M Mn(II)	0.26, 0.030, 0.30, 0.12, 0.18
1 μ M Se(IV)	1.2, 1.2, 1.1, 0.58
1 μ M Cu(II) + 1 μ M Pb(II)	-2.1, -1.1, -1.1, -1.1, -1.2, -1.3, -1.4
1 μ M Cu(II) + 0.2 μ M Pb(II)	1.1, 1.0
1 μ M Cu(II) + 0.05 μ M Pb(II)	6.1, 5.8, 6.3, 4.7, 5.5, 4.8, 5.5, 5.1
1 μ M Fe(II) + 1 μ M Pb(II)	6.9
1 μ M Fe(III) + 1 μ M Pb(II)	1.6

All values are blank-corrected. The mean OH formation rate of blanks (Milli-Q water) was 2.19 ± 0.69 nM min⁻¹.

Table S6. Individual experimental measurements of DTT consumption by tested elements and metal mixtures.

Element/mixture	Individual measurements (μ M min ⁻¹)
1 μ M Ba(II)	0.013, -0.037, -0.00084, -0.0052
1 μ M Zn(II)	0.019, 0.031, 0.080, 0.060, 0.050
1 μ M Hg(II)	0.011, 0.0068, -0.015, -0.033, -0.062, -0.0080
1 μ M Sn(II)	-0.0070, -0.018, 0.049, -0.015
1 μ M Pb(II)	-0.016, -0.011, -0.011
1 μ M Cu(I)	0.58, 0.53, 0.51, 0.53, 0.54
1 μ M Cu(II)	0.73, 0.71, 0.80, 0.67, 0.72, 0.61, 0.72, 0.84
1 μ M Fe(II)	0.0080, 0.057, 0.049, 0.0080, 0.027
1 μ M Fe(III)	0.017, 0.031, 0.0020, 0.021
1 μ M Sb(III)	-0.075, -0.082, -0.074
1 μ M Sb(V)	-0.045, -0.051, -0.081
1 μ M Mn(II)	0.14, 0.15, 0.15
1 μ M Se(IV)	-0.0029, 0.0087, 0.032
1 μ M Cu(II) + 1 μ M Pb(II)	0.66, 0.61, 0.59, 0.62
1 μ M Cu(II) + 0.05 μ M Pb(II)	0.70, 0.63, 0.69, 0.71

All values are blank-corrected. The mean DTT consumption rate of blanks (Milli-Q water) was 0.095 ± 0.05 μ M min⁻¹.

References

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