ELECTRONIC SUPPLEMENTARY INFORMATION

Formation constants of copper(I) complexes with cysteine, penicillamine and glutathione: implications for copper speciation in the human eye

Lan-Chi Königsberger*, Erich Königsberger, Glenn Hefter and Peter M. May

Chemical and Metallurgical Engineering and Chemistry, School of Engineering and Information Technology, Murdoch University, Murdoch WA6150, Australia.

E-mail:
L.Koenigsberger@murdoch.edu.au
E.Koenigsberger@murdoch.edu.au
G.Hefter@murdoch.edu.au
P.May@murdoch.edu.au

Fax number:
+61 8 9310 1711

ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1 Titration information for the determination of the protonation constants of the thioamino acids CSH, PSH and GSH[a].

System	N_t	N_{dp}	p[H] range
CSH	19	939	1.6 to 11.8
PSH	12	902	1.8 to 11.9
GSH	18	1053	1.8 to 11.9

[a] N_t: Number of titrations; N_{dp}: Number of data points.

Table S2 Titration information for the determination of the formation constants of the binary complexes of Cu(I) with CSH, PSH and GSH[a].

Ligand	N_t	N_{dp}	p[H] range
CSH	42	2011	5.2 to 11.4 [b]
PSH	15	993	1.7 to 11.5
GSH	15	617	1.5 to 2.3 and 6.9 to 12.0 [c]

[a] N_t: Number of titrations; N_{dp}: Number of data points. [b] Precipitation occurred at p[H] < 5.2. [c] Precipitation occurred in the range 2.3 < p[H] < 6.9.

Table S3 Titration information for the ternary Cu(I)–CSH–PSH and Cu(I)–CSH–GSH systems[28].

Ligands	N_t	N_{dp}	p[H] range
CSH–PSH	19	952	1.5 to 11.9
CSH–GSH	18	891	1.4 to 11.6

Table S4 Measured formation constants of the ternary Cu(I)–CSH–PSH and Cu(I)–CSH–GSH systems at 25 °C in I = 1.00 M (Na)Cl[28].

Cu(I) with	OBJT	lgβ_{1110}(σ)	lgβ_{1111}(σ)	lgβ_{1114}(σ)	lgβ_{2111}(σ)	lgβ_{2123}(σ)
CSH–PSH	3.60E–8	15.71(1)	25.89(1)		37.54(2)	
CSH–GSH	3.42E–8			44.502(8)	38.29(2)	58.92(2)

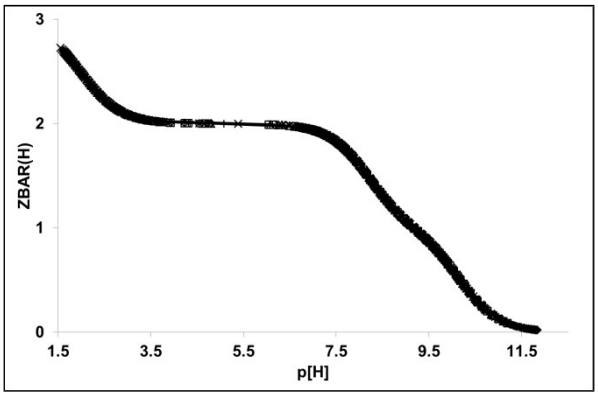

Fig. S1 Proton formation function for CSH at 25 °C and I = 1.00 M (Na)Cl. Open symbols, experimental data; solid line, calculated curve.

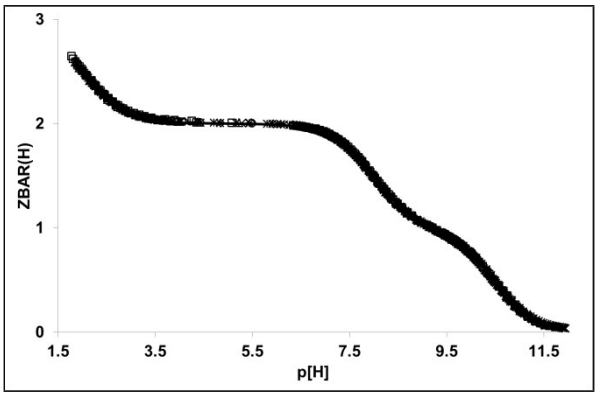

Fig. S2 Proton formation function for PSH at 25 °C and I = 1.00 M (Na)Cl. Open symbols, experimental data; solid line, calculated curve.

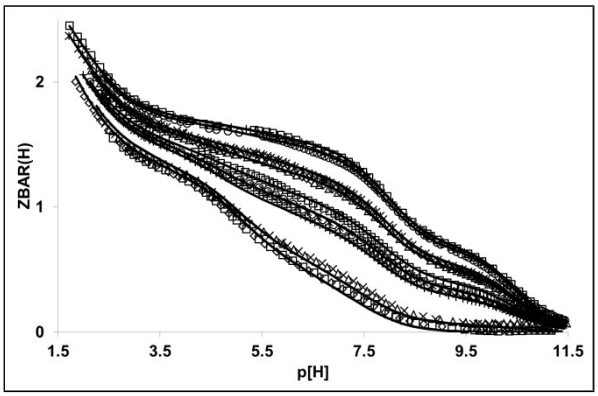

Fig. S3 Proton formation functions for Cu(I)–PSH at 25 °C and I = 1.00 M (Na)Cl with $[Cu(I)]_T$ = (4 to 5) mM. Open symbols, experimental data at Cu(I):PSH = 1:1, 2:3, 1:2 and 1:3; solid lines, calculated curves.

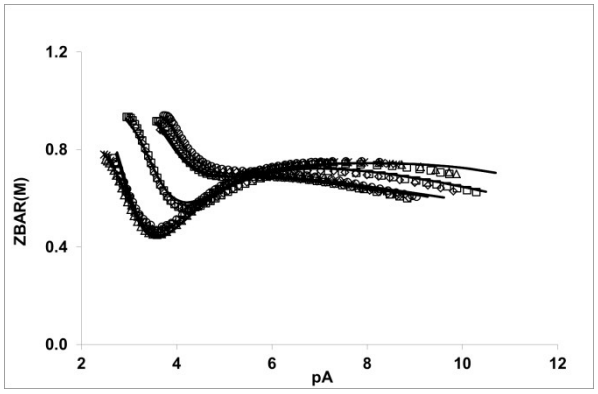

Fig. S4 Metal formation functions for Cu(I)–CSH at 25 °C and I = 1.00 M (Na)Cl with $[Cu(I)]_T$ = (4 to 5) mM. Open symbols, experimental data at Cu(I):CSH = 1:1, 2:3, and 1:3; solid lines, calculated curves.

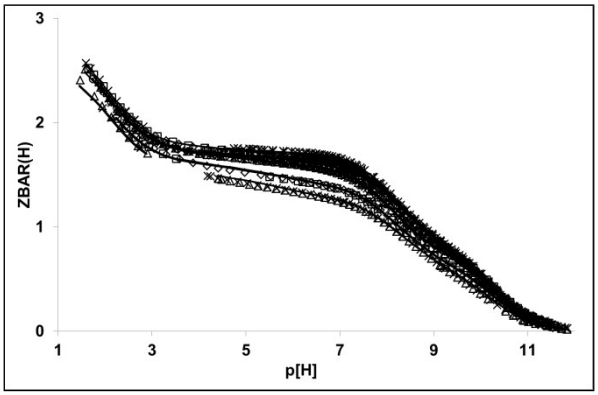

Fig. S5 Proton formation functions for Cu(I)–CSH–PSH at 25 °C and I = 1.00 M (Na)Cl with $[Cu(I)]_T$ = (4 to 10) mM. Open symbols, experimental data at Cu(I):CSH:PSH = 1:1:1, 1:1:2, 1:1:3, 1:2:2, and 1:3:1; solid lines, calculated curves.

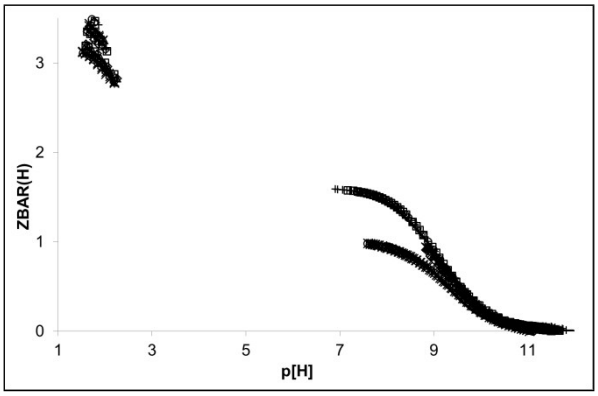

Fig. S6 Proton formation functions for Cu(I)–GSH at 25 °C and I = 1.00 M (Na)Cl with $[Cu(I)]_T$ = (4 to 7) mM. Open symbols, experimental data at Cu(I):GSH = 1:1, 2:3, 1:2 and 1:3; solid lines, calculated curves.

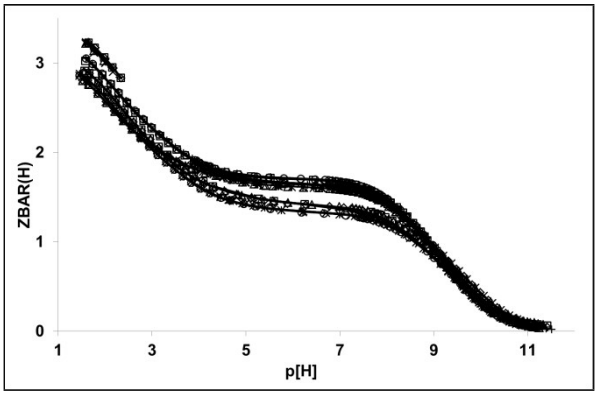

Fig. S7 Proton formation functions for Cu(I)–CSH–GSH at 25 °C and I = 1.00 M (Na)Cl with $[Cu(I)]_T$ = (4 to 10) mM. Open symbols, experimental data at Cu(I):CSH:GSH = 1:1:1, 1:1:2, 1:1:3, 1:2:2, and 1:3:1; solid lines, calculated curves.