Supplementary Information

Binding and removal of octahedral, tetrahedral, square planar and linear anions in water by means of activated carbon functionalized with a pyrimidine-based anion receptor

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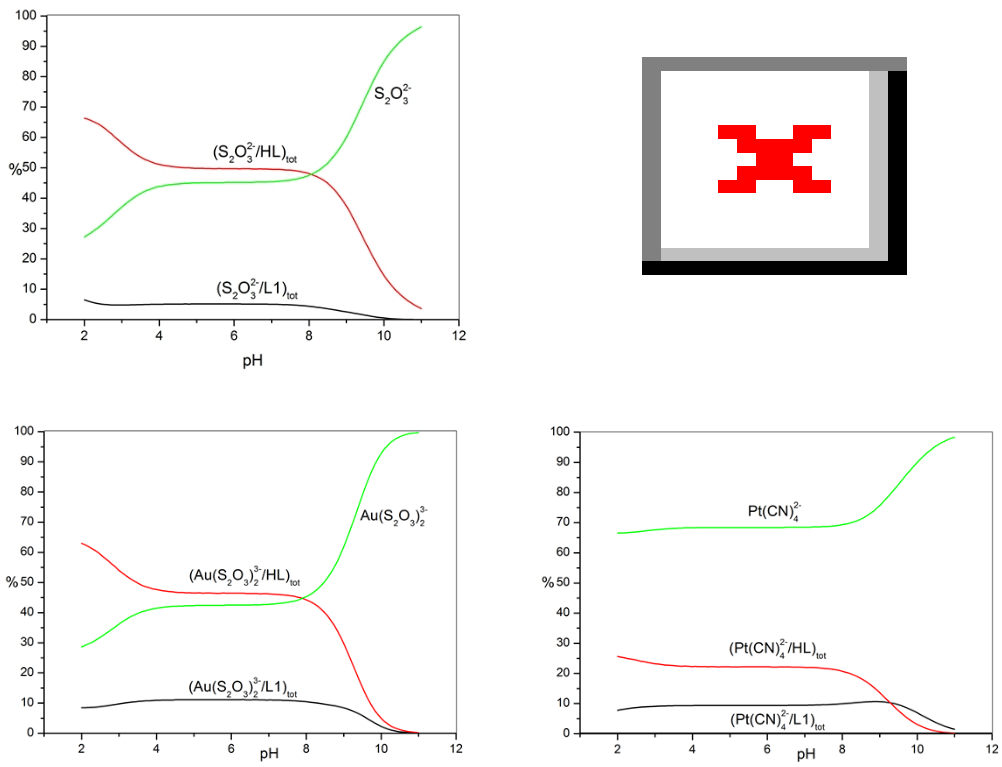

Figure S1. Selectivity diagrams calculated for the systems HL/L1/$S_2O_3^{2-}$, HL/L1/$Co(CN)_6^{3-}$, HL/L1/$Au(S_2O_3)_2^{3-}$ and HL/L1/$Pt(CN)_4^{2-}$, showing the percentage of anion bound to each ligand as a function of pH. All reagents 1×10^{-3} M.

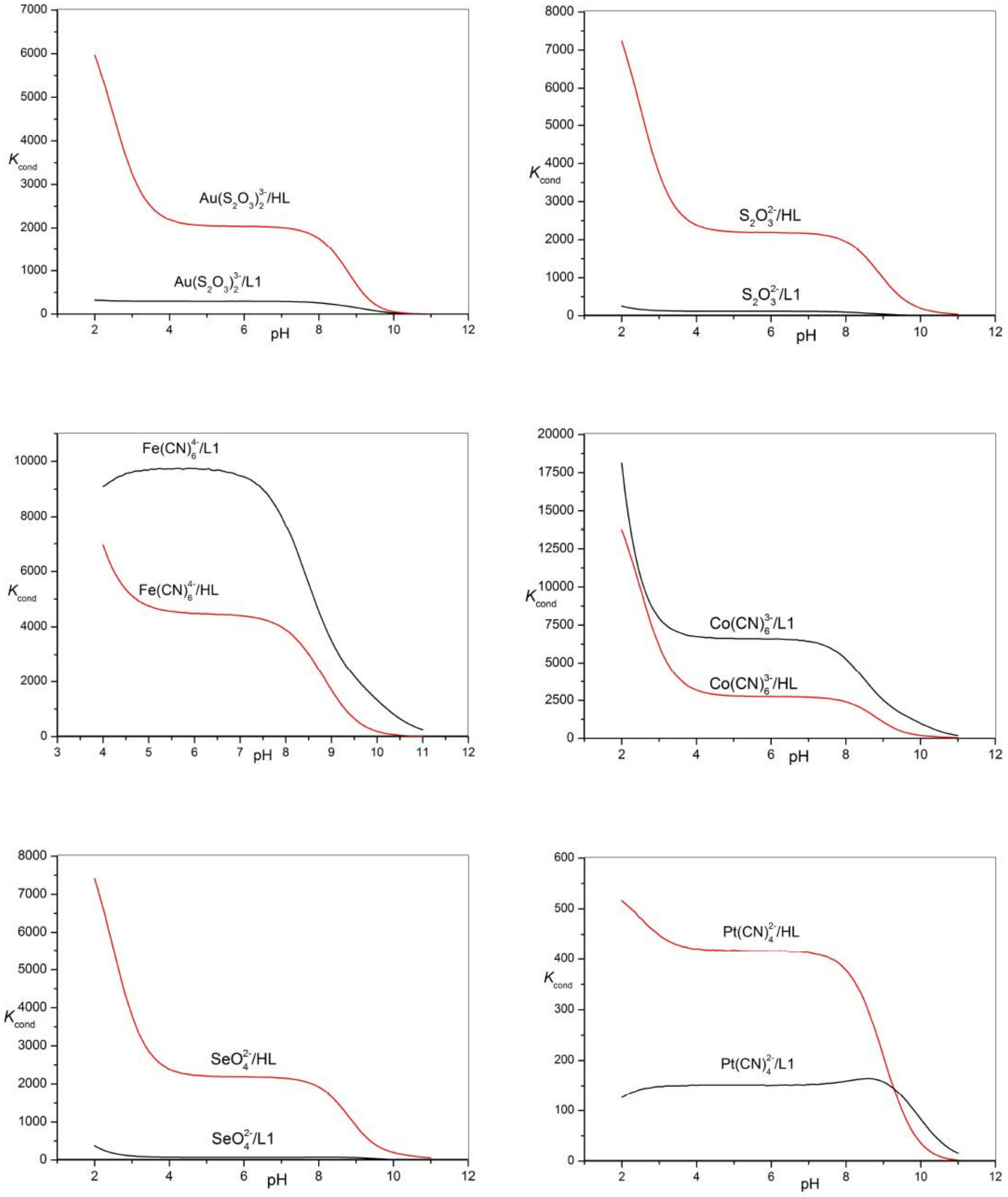

Figure S2. Conditional stability constants calculated as a function of pH for the systems HL/L1/$Au(S_2O_3)_2^{3-}$, HL/L1/$S_2O_3^{2-}$, HL/L1/$Fe(CN)_6^{4-}$, HL/L1/$Co(CN)_6^{3-}$, systems HL/L1/SeO_4^{2-} and and HL/L1/$Pt(CN)_4^{2-}$.

Table S1. Overall equilibrium constants for the formation of anion complexes with HL determined by means of potentiometric measurements in 0.1M Me_4NCl aqueous solution at 298.1 K.

	log β
Equilibria	
$2H^+ + L^- + Fe(CN)_6^{4-} = [H_2L(Fe(CN)_6)]^{3-}$	23.55(6)[a]
$3H^+ + L^- + Fe(CN)_6^{4-} = [H_3L(Fe(CN)_6)]^{2-}$	33.04(5)
$4H^+ + L^- + Fe(CN)_6^{4-} = [H_4L(Fe(CN)_6)]^-$	36.56(7)
$5H^+ + L^- + Fe(CN)_6^{4-} = [H_5L(Fe(CN)_6)]$	39.40(6)
$2H^+ + L^- + Au(S_2O_3)_2^{3-} = [H_2L(Au(S_2O_3)_2)]^{2-}$	22.97(6)
$3H^+ + L^- + Au(S_2O_3)_2^{3-} = [H_3L(Au(S_2O_3)_2)]^-$	32.70(4)
$4H^+ + L^- + Au(S_2O_3)_2^{3-} = [H_4L(Au(S_2O_3)_2)]$	35.37(5)

[a] Values in parentheses are standard deviations on the last significant figures.

Table S2. Overall equilibrium constants for the formation of anion complexes with tren (L1) determined by means of potentiometric measurements in 0.1M Me_4NCl aqueous solution at 298.1 K.

	log β
Equilibria	
$2H^+ + L1 + S_2O_3^{2-} = [H_2L1(S_2O_3)]$	21.23(6)[a]
$3H^+ + L1 + S_2O_3^{2-} = [H_3L1(S_2O_3)]^+$	30.09(5)
$4H^+ + L1 + S_2O_3^{2-} = [H_4L1(S_2O_3)]^{2+}$	32.28(5)
$2H^+ + L1 + SeO_4^{2-} = [H_2L1(SeO_4)]$	21.20(4)
$3H^+ + L1 + SeO_4^{2-} = [H_3L1(SeO_4)]^+$	29.94(4)
$4H^+ + L1 + SeO_4^{2-} = [H_4L1(SeO_4)]^{2+}$	32.59(4)
$H^+ + L1 + Pt(CN)_4^{2-} = [HL1(Pt(CN)_4)]^-$	12.20(6)
$2H^+ + L1 + Pt(CN)_4^{2-} = [H_2L1(Pt(CN)_4)]$	21.88(5)
$3H^+ + L1 + Pt(CN)_4^{2-} = [H_3L1(Pt(CN)_4)]^+$	30.19(5)
$H^+ + L1 + Co(CN)_6^{3-} = [HL1(Co(CN)_6)]^{2-}$	13.28(7)
$2H^+ + L1 + Co(CN)_6^{3-} = [H_2L1(Co(CN)_6)]^-$	22.92(5)
$3H^+ + L1 + Co(CN)_6^{3-} = [H_3L1(Co(CN)_6)]$	31.83(5)
$4H^+ + L1 + Co(CN)_6^{3-} = [H_4L1(Co(CN)_6)]^+$	34.19(5)
$H^+ + L1 + Fe(CN)_6^{4-} = [HL1(Fe(CN)_6)]^{3-}$	13.41(5)
$2H^+ + L1 + Fe(CN)_6^{4-} = [H_2L1(Fe(CN)_6)]^{2-}$	23.04(6)
$3H^+ + L1 + Fe(CN)_6^{4-} = [H_3L1(Fe(CN)_6)]^-$	32.00(7)
$4H^+ + L1 + Fe(CN)_6^{4-} = [H_4L1(Fe(CN)_6)]$	34.78(5)
$2H^+ + L1 + Au(S_2O_3)_2^{3-} = [H_2L1(Au(S_2O_3)_2)]^-$	21.85(4)
$3H^+ + L1 + Au(S_2O_3)_2^{3-} = [H_3L1(Au(S_2O_3)_2)]$	30.48(6)
$4H^+ + L1 + Au(S_2O_3)_2^{3-} = [H_4L1(Au(S_2O_3)_2)]^+$	31.97(5)

[a] Values in parentheses are standard deviations on the last significant figures.