07/07/2007

The Cordination Cemistry of the Mercury(II) Ion in Liquid and Aqueous Ammonia Solution, and the Crystal Structure of Tetraamminemercury(II) Perchlorate

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Electronic Supporting Information

Table S1. Hydrogen bonds with H···A hydrogen bonds shorter than radius of A + 2.000 Å, and a D-H···A bond angle larger than 110 °.

D-H	*d*(D-H)	*d*(H···A)	∠ D-H···A	*d*(D···A)	A
N1-H1A	0.890				
N1-H1B	0.890	2.045	169.80	2.925	O11B_b
N1-H1B	0.890	2.294	158.98	3.141	O12_a
N1-H1B	0.890	2.980	165.55	3.848	Cl1_a
N1-H1C	0.890	2.579	136.04	3.278	O11_a
N1-H1C	0.890	2.592	137.22	3.301	O12B_b
N2-H2A	0.890	2.086	158.21	2.931	O12B_b
N2-H2A	0.890	2.277	157.20	3.117	O11_a
N2-H2B	0.890	2.146	146.63	2.931	O12B_b
N2-H2B	0.890	2.341	145.70	3.117	O11_a
N2-H2C	0.890	2.313	174.03	3.200	O12_a
N2-H2C	0.890	2.924	152.93	3.739	Cl1_a
N3-H3A	0.890	2.469	136.03	3.170	O22
N3-H3B	0.890	2.441	148.87	3.236	O11_a
N3-H3B	0.890	2.530	117.32	3.043	O23
N3-H3C	0.890	2.183	162.52	3.043	O23

Cif file for the structure $[Hg(NH_3)_4](ClO_4)_2$

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 '-x, -y, -z'
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
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Legends to Figures

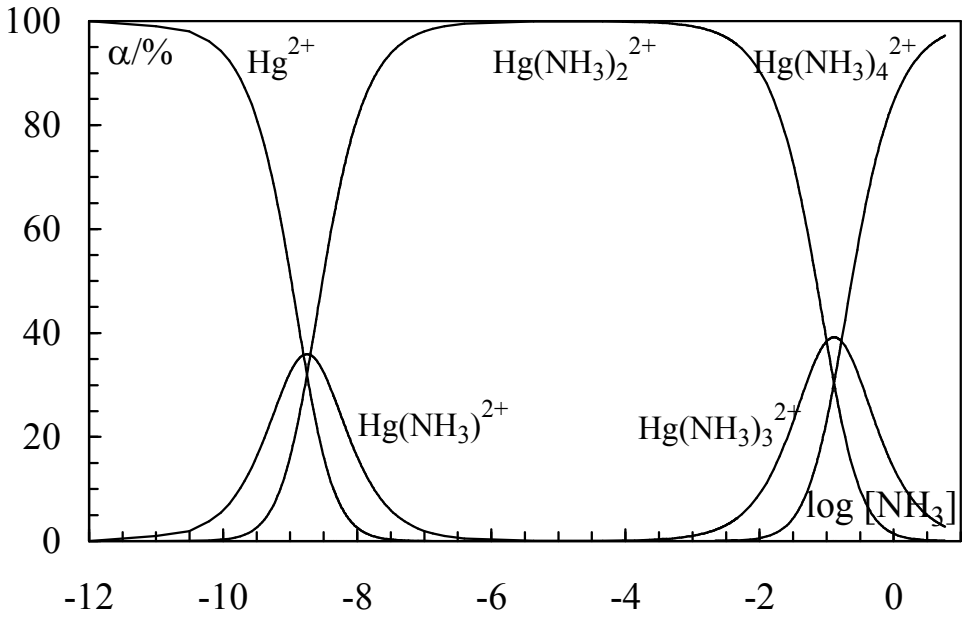
Figure S1. The distribution functions of the mercury(II)-ammonia complexes in water using the stability constants given by Bjerrum, ref. 14.

Figure S2. Normalised XANES spectra of the analysed mercury(II) complexes: $[Hg(NH_3)_4]^{2+}$ in NH_3(aq), (offset 1.75); $[Hg(NH_3)_4]^{2+}$ in NH_3(l), (offset 1.25); $[Hg(NH_3)_4](ClO_4)_2$ (s)(offset 0.5) and $[Hg(NH_3)_2](ClO_4)_2$ (s)(no offset).

Figure S3. Fourier transforms of the EXAFS data: experimental (solid line) and model (dashed) of: $[Hg(NH_3)_4]^{2+}$ in NH_3(aq), (offset 2.75); $[Hg(NH_3)_4]^{2+}$ in NH_3(l), (offset 2); $[Hg(NH_3)_4](ClO_4)_2$ (s)(offset 1.5), and $[Hg(NH_3)_2](ClO_4)_2$ (s)(no offset).

Figure S4. UV-VIS spectra (l = 0.1 mm) of the aqueous ammonia solutions of mercury(II) perchlorate with $\boldsymbol{R}$ = (a) 0, (b) 2, (c) 4 and (d) 8, $C_{Hg^{2+}}$ = 0.15 (a) and 0.064 (b) mol·dm^{-3}.

Fig. S1.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60
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20
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α/%
Hg2+
Hg(NH3)2 2+
Hg(NH3)4 2+
Hg(NH3)2+
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-8
-6
-4
-2
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Fig. S2.

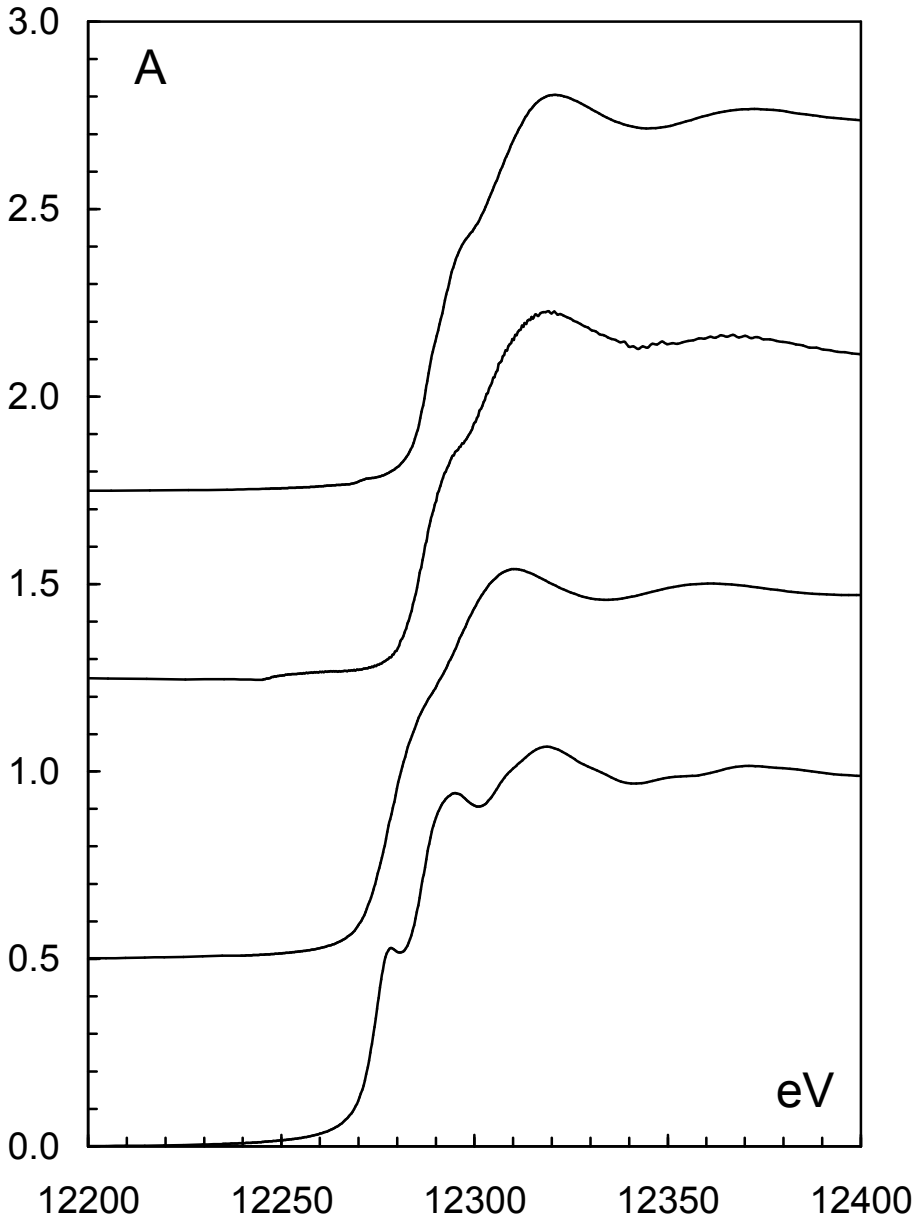


Fig. S3.

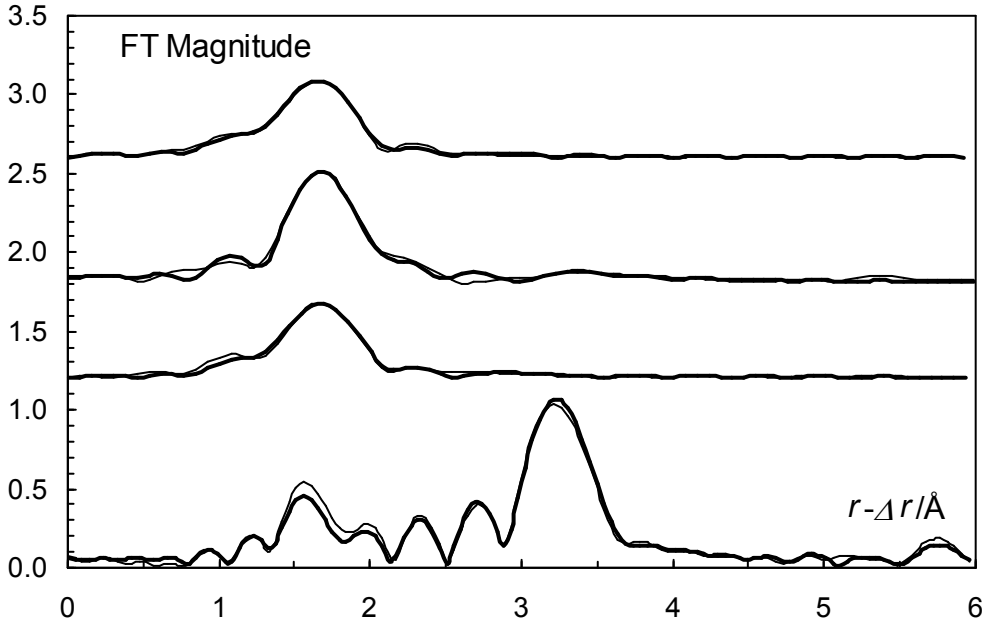
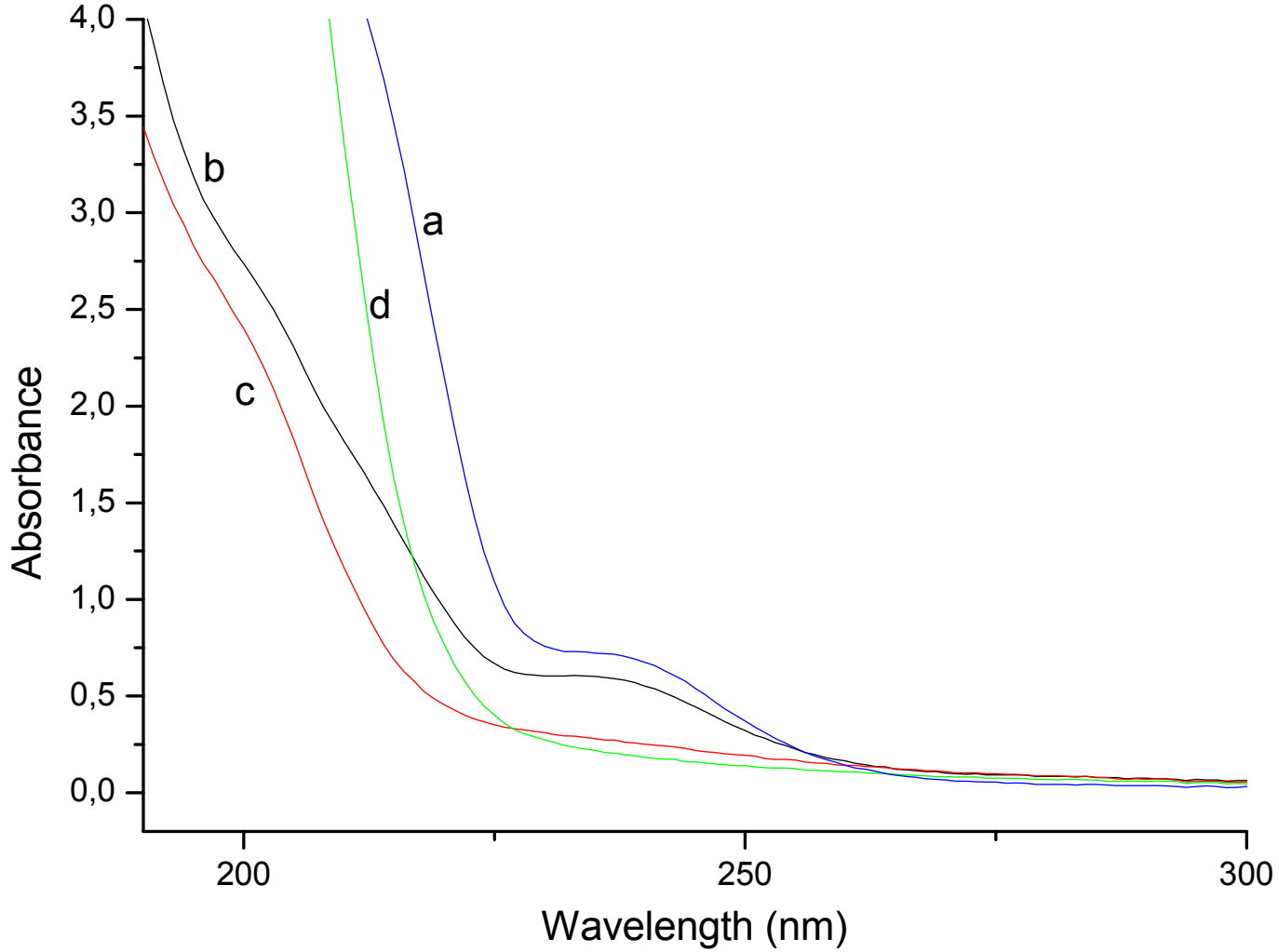


Fig. S4.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b
c
d