

Mercury capture on a supported chlorocuprate(II) ionic liquid adsorbent studied using *operando* synchrotron X-ray absorption spectroscopy

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Electronic Supplemental Data

EXAFS of mercury standards, MCA fluorescence data capture times, XANES and IPD data from Hg captured by the supported ionic liquid

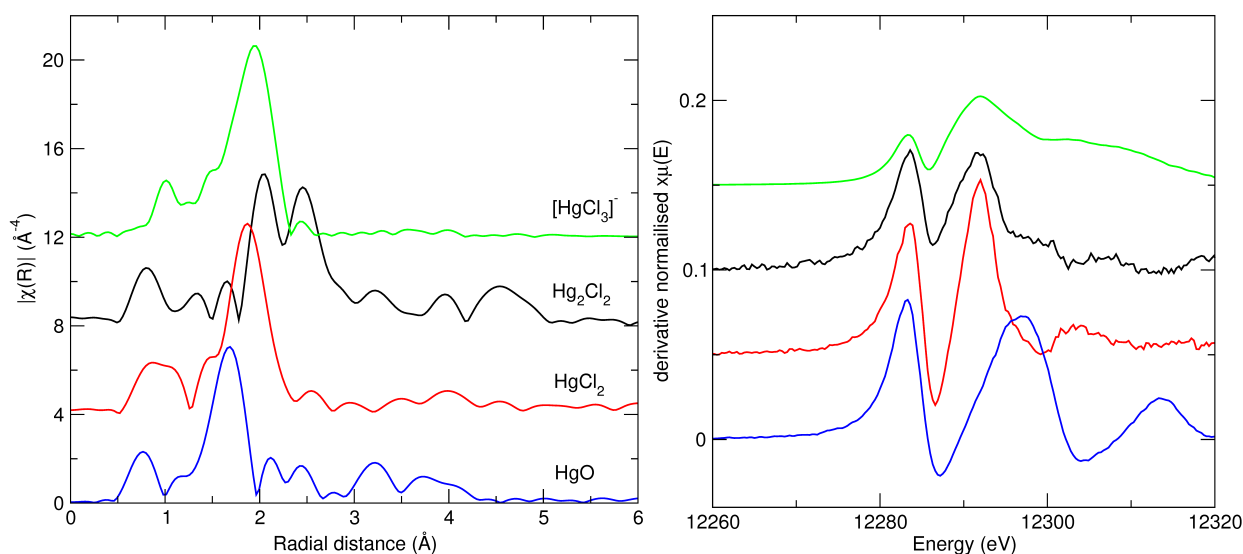


Figure S1: k^3 -weighted mercury EXAFS *pseudo*-radial distribution functions (*left*) and IPD shown from the first derivative of the EXAFS L_3 -edge jump (*right*) for the standards Hg_2Cl_2 , HgCl_2 , HgO , and $[\text{HgCl}_3]^-$ from $[\text{omim}]\text{Cl}/\text{HgCl}_2$ $X=0.50$. Data collected on beamline I20.

Table S1: IPD values for the mercury standards and chloromercurate(II) ionic liquids.

Standard	IPD /eV
Hg(0)	0
HgO	12.9
HgCl ₂	8.5
Hg ₂ Cl ₂	8.3
[omim]Cl/HgCl ₂ ($\chi_{\text{HgCl}_2} = 0.33$)	4.8
[omim]Cl/HgCl ₂ ($\chi_{\text{HgCl}_2} = 0.50$)	8.8

Table S2: Times of XAS fluorescence data collection at each position in the bed. Averaged times from each cycle of data collection are used for reference in the manuscript.

Position	Cycle 1		Cycle 2		Cycle 3	
	Time /h	Data set #	Time /h	Data set#	Time /h	Data set#
1	02:26	198716	05:27	198776	08:28	198836
2	02:43	198722	05:45	198782	08:46	198842
3	03:01	198728	06:02	198788	09:04	198848
4	03:19	198734	06:20	198794	09:22	198854
5	03:37	198740	06:38	198800	09:39	198860
Average	03:01		06:02		09:03	
Stdev	00:28		00:27		00:28	

Position	Cycle 4		Cycle 5		Cycle 6	
	Time /h	Data set #	Time /h	Data set #	Time /h	Data set #
1	11:29	198896	14:30	198956	17:31	199017
2	11:47	198902	14:48	198962	17:49	199023
3	12:05	198908	15:06	198968	18:07	199029
4	12:23	198914	15:24	198974	18:25	199035
5	12:41	198920	15:41	198980	18:42	199041
Average	12:05		15:06		18:07	
Stdev	00:28		00:28		00:28	

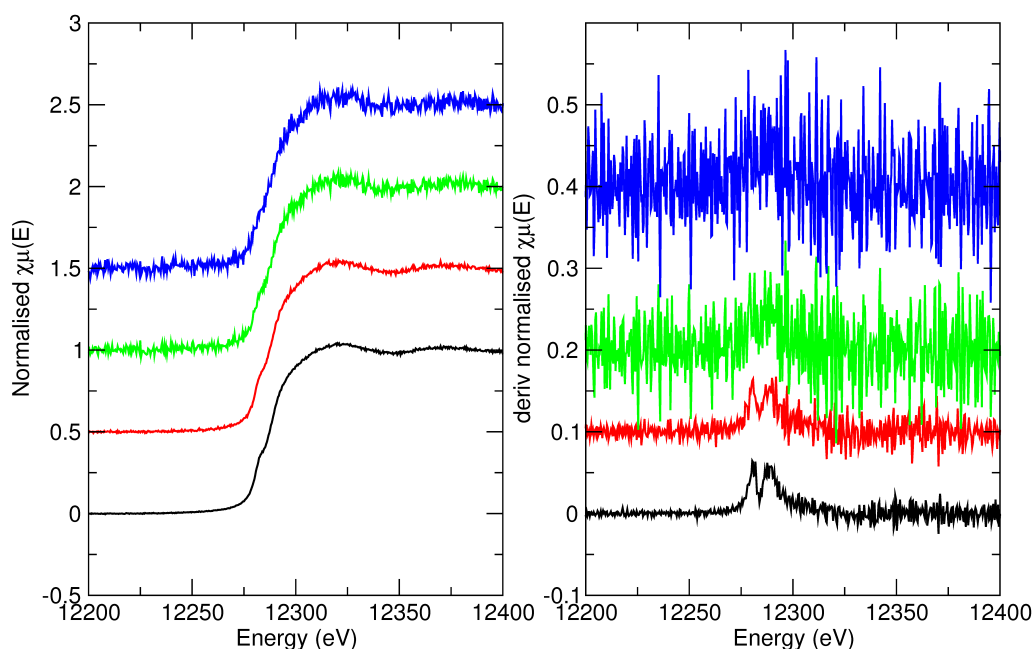


Figure S2: Hg L₃-edge XANES and first derivative data for adsorbed mercury on the supported ionic liquid bed taken after 3 h from the start of the experiment at positions 1 (black), 2 (red), 3 (green) and 4 (blue) along the bed. No mercury L₃-edge jump could be detected at position 5.

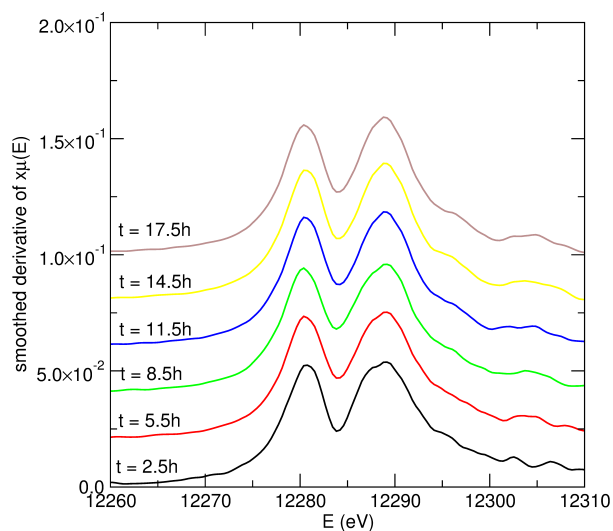


Figure S3: Change in the inflection point difference spectra for the Hg L₃ XANES data from position 1 (front edge of the adsorbant bed) through the experiment. Data collected on beamline B18.

Table S3: Change in the inflection point difference in the Hg L₃ XANES data from position 1 (front edge of the adsorbant bed) through the experiment. Throughout the experiment, the IPD value is 8.45 eV (stdev 0.19), in the range of both Hg(II)-Cl and Hg(I)-Cl compounds.

Hg(0) exposure time/ hour	Inflection point difference (IPD)/ eV
2.5	8.2
5.5	8.3
8.5	8.7
11.5	8.4
14.5	8.6
17.5	8.5