XAFS Evidence for the Formation of Pb(II) Inner-sphere Adsorption Complexes and Precipitates at the Calcite-Water Interface

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Supporting Information:

3 Pages

1 Table, 2 Figures

	μM initial Pb				
	1	**5**	**10**	**20**	**60**
Pb-phases SI					
Cerussite	-0.16	0.54	0.84	1.14	1.62
Hydrocerussite	-0.74	1.35	2.26	3.16	4.59
Batch Uptake					
$^*\Gamma$ (moles Pb per m^2)	1.0×10^{-6}	5.1×10^{-6}	1.1×10^{-5}	2.9×10^{-5}	9.8×10^{-5}
Pb on calcite (ppm)	2170	10491	22814	59757	202484
Pb atoms per Ca site	0.13	0.61	1.33	3.47	11.77

Table S1. Saturation indices for Pb-bearing phases and results from batch uptake experiments for relevant sorption samples.
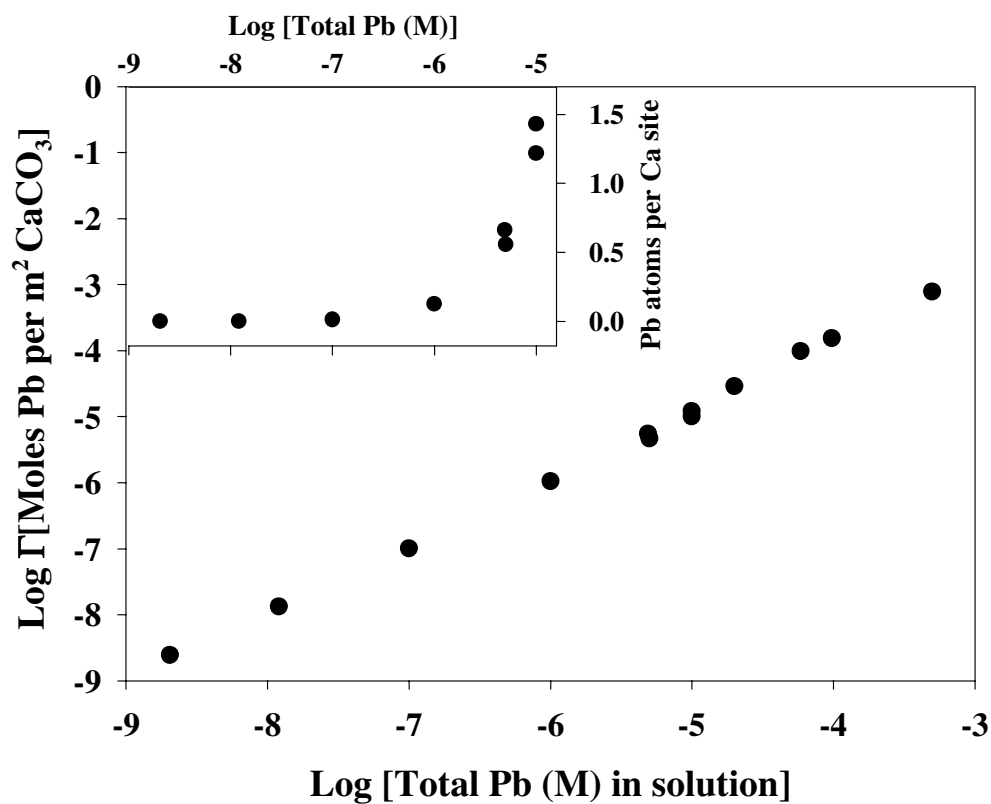
$^*\Gamma$ = Pb sorption density

Figure S1. a) The effect of initial Pb concentration on sorption density Γ. Inset: b) Theoretical site occupancy as a function of initial Pb concentration for the concentration range 10^{-9} to 10^{-5} M Pb showing the onset of oversaturation.
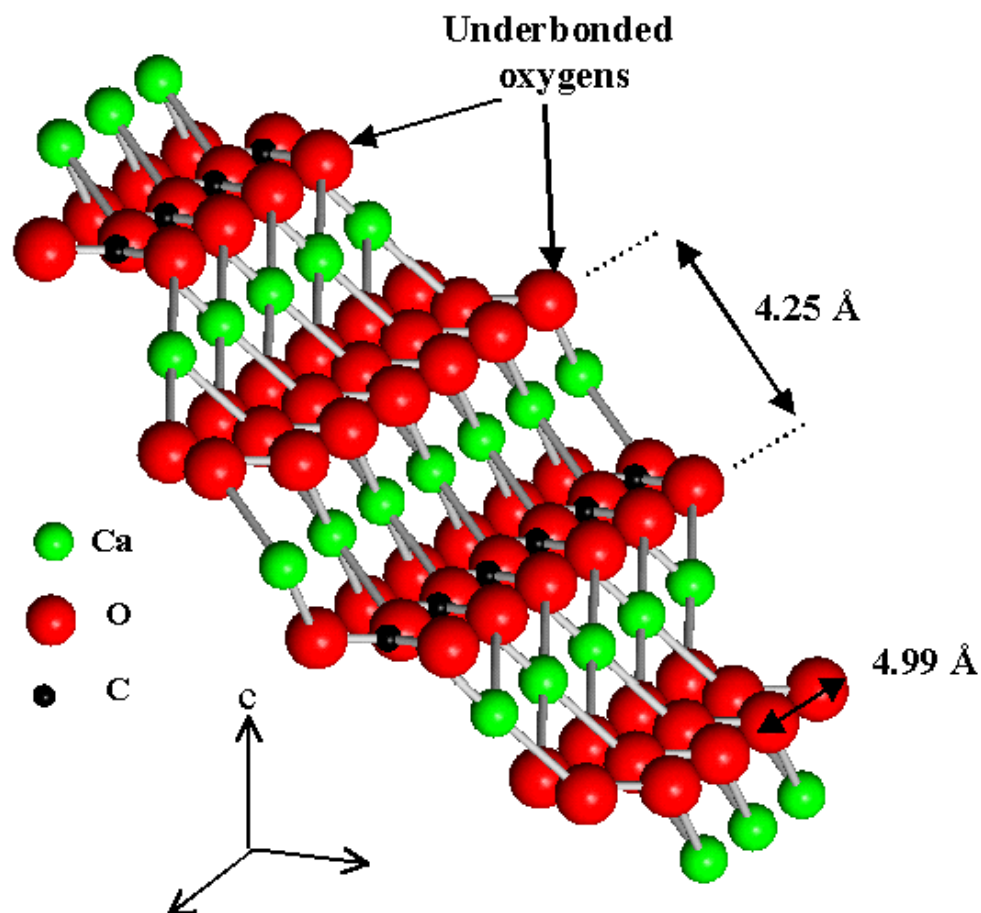
Figure S2. Location and O-O distances of underbonded oxygens on a calcite $(10\bar{1}4)$ terrace. These atoms have one unsatisfied bond compared to those at step kink sites, which have two, and therefore more degrees of freedom. O-O separations are too long, and flexibility insufficient to expect binding of the Pb adsorption complex to two of these oxygen atoms.