

Elemental and Molecular Segregation in Oil Paintings due to Lead Soap Degradation.

Supplementary Materials

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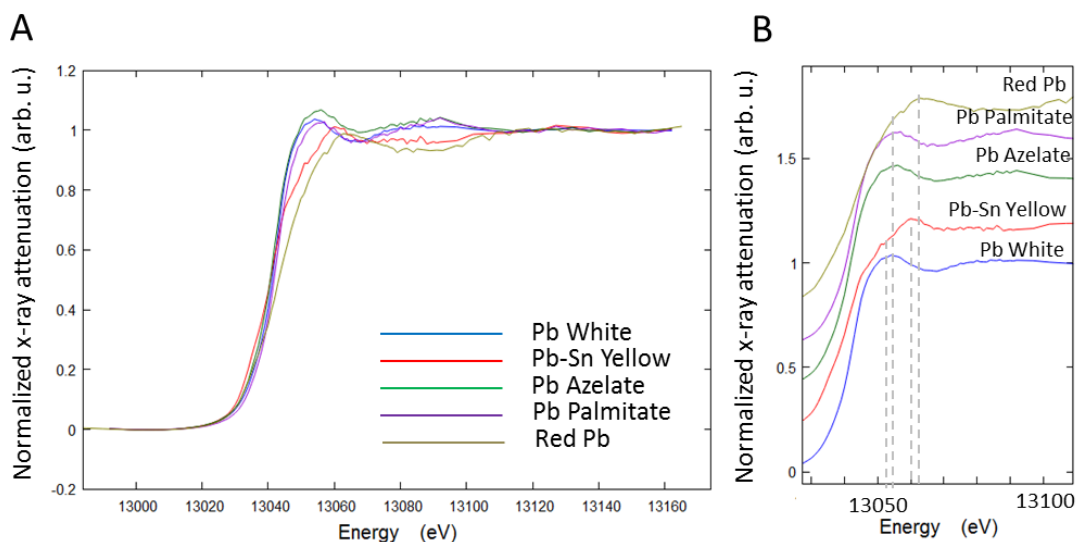


Figure S1. XANES spectra of Pb pigments and soap standards, collected in fluorescence mode around the Pb L_3 edge. (A) Full XANES spectra, (B) selected energy region of interest with stacked view.

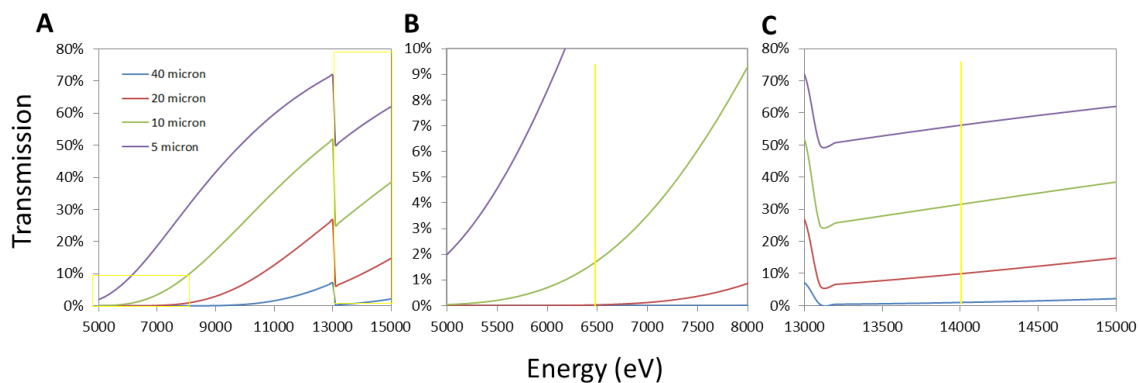


Figure S2. X-ray transmission of the PbSn yellow type I pigment with different thicknesses (5, 10, 20 and 40 microns) as a function of the X-ray photon energy: (A) energy range 5-15 keV, (B) 6.5 keV, and (C) 14 keV.

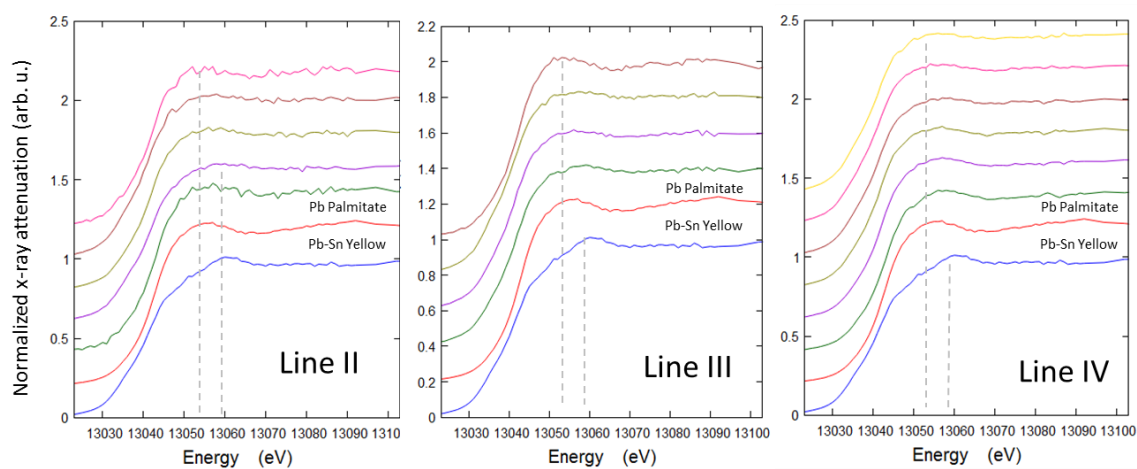


Figure S3. μ -XANES spectra acquired in the sample cross-section. The positions where the spectra were measured are indicated in Figure 4B.

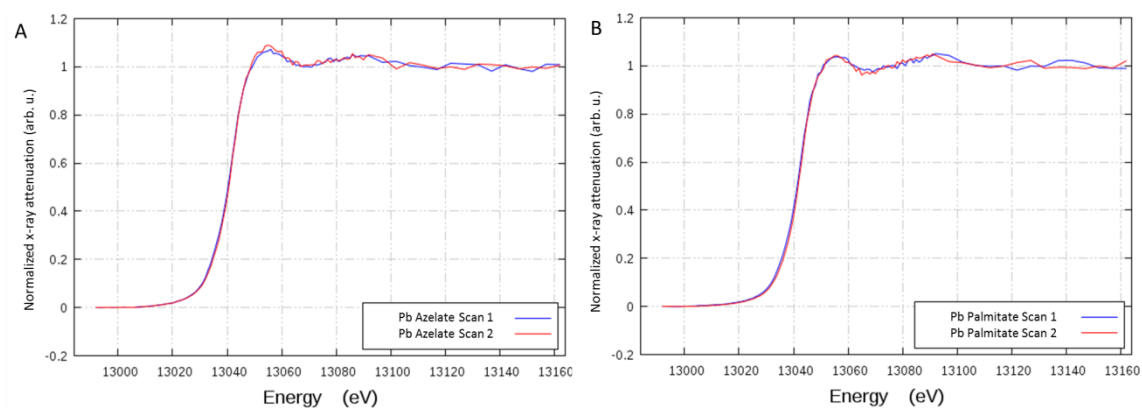


Figure S4. XANES spectra acquired consecutively in the same spot in Pb soap compounds, showing that no radiation damage is visible in the spectra.

Table S1. XANES linear combination fitting results: all combination tested, ranked by R-factor. Tests constraints: PbSn yellow must be present, weight should be between 0 and 1.

Point a

rfactor	chinu	chisqr	nvarys	scaleby	PbSn Yellow		PbAzellate		Pb Palmitate		Pb White		Red Pb	
					weight	error	weight	error	weight	error	weight	error	weight	error
0.001416	0.0001606	0.01189	2	1	0.722413	0.097624	0.261328	0.057983			0.016259	0.068027		
0.001417	0.0001586	0.0119	1	1	0.725764	0.037589	0.274236	0.020973						
0.00142	0.0001633	0.01192	3	1	0.73228	0.058091	0.250978	0.082676			0.016742	0.12955	7.00058E-09	0.039462
0.00144	0.0001634	0.01209	2	1	0.702545	0.06872	0.297455	0.035624	1.571E-08	0.043735				
0.001447	0.0001641	0.01215	2	1	0.752102	0.05848	0.247898	0.028214					9.74451E-09	0.032912
0.001469	0.0001713	0.01233	4	1	0.702504	0.221714	0.168212	0.097491	2.08815E-09	0.133853	0.129283	0.125836	1.7761E-08	0.074292
0.001804	0.000202	0.01515	1	1	0.698178	0.041762					0.301822	0.027767		
0.001815	0.0002059	0.01524	2	1	0.716472	0.109774			4.22811E-09	0.07412	0.283528	0.070824		
0.001832	0.0002079	0.01538	2	1	0.727942	0.059452					0.272058	0.031663	1.02822E-08	0.031484
0.003292	0.0003686	0.02764	1	1	0.781982	0.039251			0.218017982	0.223983				
0.003298	0.0003742	0.02769	2	1	0.795962	0.067605			0.204038231	0.039903			1.30268E-08	0.037915
0.004649	0.0005202	0.03901	1	1	1	0.054183							1.85661E-10	0.044303

Point b:

rfactor	chinu	chisqr	nvarys	scaleby	PbSn Yellow		PbAzellate		Pb Palmitate		Pb White		Red Pb	
					weight	error	weight	error	weight	error	weight	error	weight	error
0.003219	0.000377	0.02863	1	1	0.583558	0.032315	0.416442	0.032315					2.90335E-08	0.050204
0.003219	0.000382	0.02863	2	1	0.586052	0.084839	0.413948	0.103742						
0.003223	0.000382	0.02866	2	1	0.593474	0.039077	0.406526	0.11655			7.93966E-08	0.104941		
0.003499	0.000421	0.03112	3	1	0.546492	0.237282	0.292198	0.101086	6.48E-09	0.114155	0.161309438	0.179109		
0.003591	0.000432	0.03194	3	1	0.549706	0.202793	0.25288	0.134412			0.197414286	0.134046	4.76499E-09	0.064164
0.003813	0.000465	0.03392	4	1	0.580728	0.365195	0.224091	0.160484	0.025734	0.220517	0.169447179	0.207458	1.77516E-08	0.122362
0.004159	0.0005	0.03699	3	1	0.595069	0.254101	0.29885	0.163736	0.106081	0.153356			1.38015E-08	0.115182
0.004643	0.000543	0.04129	1	1	0.563661	0.045527					0.436339394	0.045527		
0.004714	0.000559	0.04192	2	1	0.612901	0.073222					0.387098818	0.051914	2.13793E-08	0.051638
0.005385	0.000647	0.04788	3	1	0.620555	0.34537			0.078544	0.226186	0.300901198	0.240831	2.35735E-10	0.095645
0.008132	0.000951	0.0723	1	1	0.719104	0.063043			0.280896	0.063043				
0.00827	0.000981	0.07354	2	1	0.64723	0.094839			0.35277	0.112974			9.29183E-09	0.06139
0.010259	0.0012	0.09119	1	1	1	0							0	0.079159

Point b':

rfactor	chinu	chisqr	nvarys	scaleby	PbSn Yellow		PbAzellate		Pb Palmitate		Pb White		Red Pb	
					weight	error	weight	error	weight	error	weight	error	weight	error
0.001514	0.000196	0.01487	1	1	0.449049	0.02329	0.550951	0.02329						
0.001515	0.000198	0.01487	2	1	0.452842	0.028153	0.547158	0.080664			1.23E-07	0.075592		
0.001515	0.000201	0.01488	3	1	0.452528	0.064464	0.545977	0.120161			0.001494	0.091465	1.19657E-08	0.043785
0.001521	0.000199	0.01493	2	1	0.435712	0.061296	0.564288	0.071209					4.79938E-10	0.036243
0.001537	0.000201	0.0151	2	1	0.423883	0.029015	0.576117	0.056552	7.77101E-09	0.048541				
0.001667	0.000221	0.01637	3	1	0.384103	0.030688	0.501366	0.156967	1.51006E-08	0.082736	0.114531	0.129814		
0.001723	0.000229	0.01691	3	1	0.392745	0.095545	0.578196	0.161094	2.4073E-08	0.103708			0.029059015	0.077892
0.002535	0.000341	0.02488	4	1	0.43308	0.313119	0.259828	0.137466	0.095290416	0.188866	0.211802	0.177611	1.57194E-08	0.104827
0.003221	0.000416	0.03159	1	1	0.404992	0.039826					0.595008	0.039826		
0.003221	0.000421	0.03159	2	1	0.408136	0.146606			1.9105E-08	0.105999	0.591864	0.101279		
0.00323	0.000428	0.03168	3	1	0.423494	0.104226			5.00184E-08	0.183904	0.576505	0.237583	1.18739E-08	0.077768
0.003326	0.000435	0.03262	2	1	0.467785	0.070816					0.532214	0.045807	2.96941E-08	0.045548
0.007552	0.000975	0.07409	1	1	0.541577	0.063835			0.45842349	0.063835				
0.007675	0.001004	0.07528	2	1	0.612103	0.090147			0.387896798	0.065355			3.82368E-10	0.06209
0.012692	0.001636	0.12436	1	1	1	0							0	0.115166

Point b'':

					PbSn Yellow		PbAzellate		Pb White		Red Pb		Pb Red	
rfactor	chinu	chisqr	nvarys	scaleby	weight	error	weight	error	weight	error	weight	error	weight	error
0.011982	0.001476	0.11216	1	1	0.314909	0.095078	0.685091	0.063957						
0.011988	0.001496	0.11221	2	1	0.326946	0.077307	0.673054	0.230575			3.92144E-08	0.207601		
0.011989	0.001517	0.11222	3	1	0.30184	0.177035	0.69816	0.330009			1.62362E-08	0.251192	8.67368E-09	0.12028
0.012071	0.001527	0.11299	3	1	0.266915	0.080585	0.733081	0.41234	1.7181E-09	0.217421	3.36042E-06	0.340967		
0.012097	0.00151	0.11323	2	1	0.260435	0.168762	0.739565	0.20624					7.74528E-11	0.099818
0.012314	0.001558	0.11526	3	1	0.256651	0.249371	0.732786	0.420418	1.2716E-08	0.270621			0.010563	0.203296
0.014639	0.001877	0.13703	4	1	0.427992	0.735802	0.347924	0.322554	0.0018948	0.443272	0.222189827	0.416974	1.63015E-08	0.245993
0.018899	0.002328	0.17691	1	1	0.36837	0.117595					0.631630382	0.094229		
0.018944	0.002364	0.17733	2	1	0.328141	0.181786					0.671859473	0.230669	3.75933E-09	0.106221
0.019115	0.002418	0.17892	3	1	0.299345	0.247727			2.3357E-08	0.437212	0.698150599	0.535441	0.002503947	0.184861
0.027321	0.003365	0.25574	1	1	0.672005	0.13786			0.32799501	0.118558				
0.02765	0.003451	0.25882	2	1	0.558519	0.177928			0.44148072	0.242854			8.3546E-10	0.115168
0.030072	0.003704	0.28149	1	1	1	0.137612							7.02654E-12	0.118269

Point c:

					PbSn Yellow		PbAzellate		Pb Palmitate		Pb White		Red Pb	
rfactor	chinu	chisqr	nvarys	scaleby	weight	error	weight	error	weight	error	weight	error	weight	error
0.001038	0.0001472	0.01104	2	1	0.061878	0.024246	0.664653	0.196805			0.273469	0.065116		
0.001041	0.0001496	0.01107	3	1	0.072742	0.055609	0.670301	0.211293			0.256957	0.07887	5.09735E-10	0.037779
0.001067	0.0001554	0.01134	4	1	0.08749	0.087619	0.623807	0.092813	2.25166E-08	0.127549	0.288703	0.223281	2.20255E-08	0.07079
0.001122	0.0001612	0.01193	3	1	0.121119	0.026194	0.709653	0.227739	1.09322E-08	0.070649	0.169228	0.11083		
0.001283	0.0001794	0.01363	1	1	0.118206	0.022299	0.881794	0.185477						
0.001283	0.0001819	0.01364	2	1	0.122351	0.027572	0.877649	0.191817	1.4702E-08	0.046141				
0.001285	0.0001846	0.01366	3	1	0.109936	0.085818	0.890064	0.234174	2.5008E-08	0.093131			2.30072E-10	0.069963
0.001297	0.0001838	0.01378	2	1	0.138484	0.05888	0.861516	0.196431					3.37617E-09	0.034842
0.001438	0.0002038	0.01528	2	1	0.862325	0.043241			0.767928561	0.029439			-0.63025343	0.131723
0.002803	0.0004026	0.02979	3	1	0.139012	0			-0.13901239	0.046141	1	0	1.14909E-08	0
0.003024	0.0004229	0.03214	1	1	0.00029	0.040163					0.99971	0.040163		
0.003034	0.00043	0.03225	2	1	0.020431	0.149827			1.56234E-08	0.107119	0.979569	0.102354		
0.011159	0.0015607	0.11862	1	1	0.143617	0.08075			0.856383272	0.26556				
0.027673	0.0038705	0.29416	1	1	1	0.21167							9.1112E-09	0.120891

Point d:

					PbSn Yellow		PbAzellate		Pb Palmitate		Pb White		Red Pb	
rfactor	chinu	chisqr	nvarys	scaleby	weight	error	weight	error	weight	error	weight	error	weight	error
0.000765	0.000098	0.00705	3	1	5.33979E-08	0.06255	0.208843	0.072499	0.552806	0.067905			0.238351	0.129967
0.000771	0.0001	0.00711	4	1	1.92363E-08	0.070352	0.20516	0.074506	0.530289	0.102483	0.023188	0.096366	0.241364	0.18276
0.00084	0.000108	0.00774	3	1	0.079672365	0.052238			0.680543	0.092235	0.087441	0.098199	0.152343	0.15489
0.000849	0.000107	0.00782	2	1	0.116843513	0.03136			0.760435	0.021356			0.122721	0.067463
0.001274	0.000159	0.01174	1	1	0.256782051	0.025754			0.743218	0.103811				
0.001274	0.000163	0.01175	3	1	0.260174679	0.026355	2.99E-08	0.062947	0.739825	0.132496	2.1E-08	0.111544		
0.001275	0.000161	0.01175	2	1	0.262878718	0.102668			0.737121	0.065572	1.19E-08	0.062656		
0.001744	0.00022	0.01609	2	1	4.73737E-09	0.055504					0.719139	0.032604	0.280861	0.085179
0.001767	0.000226	0.0163	3	1	6.85245E-08	0.068413	0.303255	0.097342			0.348392	0.097071	0.348353	0.163371
0.002518	0.000318	0.02323	2	1	5.39795E-08	0.077471	0.607022	0.039286					0.392978	0.103233
0.004868	0.000607	0.0449	1	1	0.385347137	0.048116					0.614653	0.106097		
0.008048	0.001003	0.07422	1	1	0.560451338	0.052733	0.439549	0.090154						
0.015589	0.001942	0.14371	1	1	0.973622721	0.085618							0.026377	0.102187

Table S2. XANES linear combination fitting results: best fit results for points a, b, b', b'', c and d, with volume fraction of standards, statistical error, and R-factors

Location	PbSn Yellow	error	PbAzellate	error	Pb Palmitate	error	Pbwhite	error	Pb Red	error	rfactor
a	0.722413114	0.097624	0.26132811	0.057983			0.016258775	0.068027			0.001416
b	0.583558022	0.032315	0.416441978	0.032315							0.003219
b'	0.449049185	0.02329	0.550950815	0.02329							0.001514
b''	0.314909059	0.095078	0.685090941	0.063957							0.011982
c	0.061877635	0.024246	0.664653499	0.196805			0.273468867	0.065116			0.001038
d	5.33979E-08	0.06255	0.20884347	0.072499	0.552805884	0.067905			0.238350593	0.129967	0.000765