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Supporting information for article:

Reference spectra of important adsorbed organic and inorganic phosphate binding forms for soil P speciation using synchrotron-based *K*-edge XANES spectroscopy

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Table S1 Raw data (energy, signal) of normalized P *K*-edge XANES spectra of orthophosphate and inositol hexakisphosphate (IHP) retained by ferrihydrite at pH 5. P concentration after retention was 11.3 mg g⁻¹ (PO₄) and 7.9 mg g⁻¹ (IHP), respectively.

Energy / eV	Signal PO4	Signal IHP	Energy / eV	Signal PO4	Signal IHP	Energy / eV	Signal PO4	Signal IHP
2140.00	0.0036	-0.0039	2156.75	2.1625	2.2079	2173.50	1.7965	1.7627
2140.25	-0.0061	0.0033	2157.00	1.8751	1.9603	2173.75	1.7639	1.7754
2140.50	-0.0015	-0.0048	2157.26	1.7202	1.7900	2174.00	1.7619	1.7468
2140.75	-0.0025	-0.0033	2157.50	1.5962	1.6817	2174.25	1.7134	1.7325
2141.00	0.0005	-0.0002	2157.75	1.5327	1.6012	2174.50	1.6936	1.7083
2141.25	-0.0032	0.0041	2158.00	1.5042	1.5546	2174.75	1.6940	1.6793
2141.50	-0.0016	-0.0026	2158.26	1.4472	1.4883	2175.00	1.6597	1.6476
2141.75	0.0008	-0.0029	2158.50	1.4390	1.4857	2175.25	1.6343	1.6011
2142.00	0.0008	0.0018	2158.76	1.4273	1.4564	2175.50	1.6134	1.6117
2142.25	-0.0024	0.0023	2159.00	1.4130	1.4495	2175.75	1.5984	1.5836
2142.50	0.0002	-0.0069	2159.25	1.4241	1.4447	2176.00	1.5565	1.5596
2142.75	0.0037	-0.0028	2159.50	1.4262	1.4367	2176.25	1.5278	1.5284
2143.00	0.0004	-0.0064	2159.75	1.4518	1.4433	2176.50	1.5057	1.5156
2143.25	0.0005	0.0055	2160.00	1.4321	1.4531	2176.75	1.4930	1.4874
2143.50	0.0044	-0.0023	2160.25	1.4481	1.4555	2177.00	1.4455	1.4643
2143.75	0.0005	0.0046	2160.50	1.4589	1.4669	2177.25	1.4394	1.4369
2144.01	-0.0021	-0.0098	2160.76	1.4507	1.4674	2177.50	1.4188	1.4139
2144.25	0.0015	-0.0020	2161.00	1.4627	1.4769	2177.75	1.3767	1.4023
2144.50	0.0078	0.0030	2161.25	1.4785	1.4937	2178.00	1.3679	1.3760
2144.76	0.0080	0.0049	2161.50	1.5048	1.4913	2178.25	1.3523	1.3423
2145.00	0.0048	0.0010	2161.75	1.5082	1.5047	2178.50	1.3449	1.3428
2145.25	0.0048	0.0006	2162.00	1.5187	1.4926	2178.75	1.3117	1.3216
2145.50	0.0166	0.0100	2162.25	1.5166	1.5212	2179.00	1.3126	1.3118
2145.76	0.0059	0.0083	2162.50	1.5437	1.5313	2179.25	1.2802	1.3088
2146.01	0.0054	0.0065	2162.75	1.5652	1.5256	2179.50	1.2658	1.2714
2146.25	0.0139	0.0065	2163.00	1.5582	1.5327	2179.75	1.2342	1.2698
2146.50	0.0160	0.0156	2163.26	1.5695	1.5408	2180.00	1.2227	1.2485
2146.76	0.0164	0.0189	2163.50	1.5567	1.5455	2180.25	1.2131	1.2268
2147.00	0.0181	0.0194	2163.76	1.5756	1.5473	2180.50	1.1983	1.2063
2147.26	0.0225	0.0145	2164.01	1.5858	1.5822	2180.75	1.1948	1.2062
2147.51	0.0311	0.0294	2164.25	1.5906	1.5967	2181.00	1.1775	1.1925
2147.75	0.0385	0.0282	2164.50	1.6136	1.6169	2181.25	1.1673	1.1781
2148.00	0.0414	0.0434	2164.75	1.5965	1.6295	2181.50	1.1667	1.1616
2148.26	0.0492	0.0419	2165.00	1.6381	1.6290	2181.75	1.1422	1.1466
2148.51	0.0766	0.0585	2165.25	1.6421	1.6417	2182.00	1.1408	1.1404
2148.75	0.0933	0.0680	2165.50	1.6810	1.6863	2182.25	1.1356	1.1510
2149.01	0.1291	0.1004	2165.75	1.6514	1.7003	2182.50	1.1247	1.1552
2149.25	0.1693	0.1085	2166.00	1.6897	1.7226	2182.75	1.1261	1.1322
2149.51	0.2082	0.1491	2166.25	1.6954	1.7105	2183.00	1.1234	1.1149
2149.75	0.2322	0.1727	2166.50	1.7065	1.7423	2183.25	1.1202	1.1227
2150.00	0.2695	0.2033	2166.75	1.7360	1.7440	2183.50	1.1045	1.1096
2150.25	0.3064	0.2399	2167.00	1.7437	1.7697	2183.75	1.1011	1.1187
2150.50	0.3340	0.2710	2167.26	1.7579	1.7891	2184.00	1.1176	1.0923
2150.75	0.3657	0.3125	2167.50	1.7728	1.7918	2184.25	1.0947	1.1172
2151.00	0.3777	0.3445	2167.76	1.7805	1.8393	2184.50	1.0946	1.0907
2151.25	0.4152	0.3931	2168.00	1.7986	1.8355	2184.75	1.0802	1.0854
2151.50	0.4467	0.4575	2168.25	1.7960	1.8672	2185.00	1.0971	1.0852
2151.75	0.4839	0.5555	2168.50	1.8214	1.8531	2185.25	1.0799	1.0824
2152.00	0.5872	0.7235	2168.75	1.8393	1.8577	2185.50	1.0765	1.0796
2152.25	0.6967	0.9716	2169.00	1.8642	1.8712	2185.75	1.0700	1.0848
2152.50	0.8902	1.3122	2169.25	1.8510	1.8855	2186.00	1.0743	1.0695
2152.76	1.2196	1.8403	2169.50	1.8683	1.8821	2186.25	1.0791	1.0811
2153.00	1.6470	2.4664	2169.76	1.8982	1.8693	2186.50	1.0682	1.0712
2153.25	2.4276	3.2857	2170.00	1.8971	1.8987	2186.75	1.0731	1.0590
2153.50	3.3314	4.1624	2170.25	1.8847	1.9089	2187.00	1.0769	1.0710
2153.75	4.3394	4.9617	2170.50	1.9057	1.9052	2187.25	1.0593	1.0579
2154.00	5.4557	5.6853	2170.75	1.9214	1.8873	2187.50	1.0424	1.0440
2154.25	6.2085	6.1084	2171.00	1.9015	1.9005	2187.75	1.0372	1.0301
2154.50	6.7400	6.3285	2171.25	1.9090	1.9102	2188.00	1.0363	1.0495
2154.75	6.8988	6.2488	2171.50	1.9066	1.8873	2188.25	1.0417	1.0590
2155.00	6.6305	5.9277	2171.75	1.8876	1.8792	2188.50	1.0506	1.0525
2155.26	6.0152	5.3272	2172.00	1.9030	1.8449	2188.75	1.0214	1.0346
2155.50	5.2773	4.7413	2172.25	1.8800	1.8754	2189.00	1.0340	1.0313
2155.76	4.4285	4.0463	2172.50	1.8536	1.8538	2189.25	1.0532	1.0548
2156.00	3.6712	3.4822	2172.75	1.8610	1.8551	2189.50	1.0551	1.0114
2156.26	3.0290	2.9496	2173.00	1.8258	1.7962	2189.75	1.0338	1.0225
2156.50	2.5006	2.5288	2173.25	1.8153	1.8113	2190.00	1.0400	1.0238

Table S2 Raw data (energy, signal) of normalized P *K*-edge XANES spectra of orthophosphate and inositol hexakisphosphate (IHP) retained by boehmite at pH 5. P concentration after retention was 10.5 mg g⁻¹ (PO₄) and 6.8 mg g⁻¹ (IHP), respectively.

Energy / eV	Signal PO4	Signal IHP	Energy / eV	Signal PO4	Signal IHP	Energy / eV	Signal PO4	Signal IHP
2140.00	-0.0087	-0.0015	2156.75	2.0136	2.0145	2173.50	1.8458	1.6925
2140.25	-0.0028	0.0057	2157.00	1.7778	1.7784	2173.75	1.8086	1.7193
2140.50	-0.0052	0.0027	2157.26	1.6030	1.6537	2174.00	1.7890	1.6823
2140.75	0.0042	-0.0085	2157.50	1.5315	1.5351	2174.25	1.7568	1.6748
2141.00	0.0012	-0.0099	2157.75	1.4606	1.4979	2174.50	1.7502	1.6356
2141.25	-0.0034	-0.0046	2158.00	1.4632	1.4299	2174.75	1.7188	1.6491
2141.50	-0.0018	0.0006	2158.26	1.4257	1.4185	2175.00	1.6964	1.6006
2141.75	-0.0001	-0.0023	2158.50	1.4371	1.3785	2175.25	1.6599	1.5923
2142.00	-0.0045	0.0024	2158.76	1.4450	1.3867	2175.50	1.6498	1.5345
2142.25	-0.0009	-0.0012	2159.00	1.4432	1.3828	2175.75	1.6277	1.5645
2142.50	-0.0029	-0.0010	2159.25	1.4325	1.3721	2176.00	1.6245	1.5166
2142.75	-0.0018	0.0031	2159.50	1.4400	1.3413	2176.25	1.5711	1.4729
2143.00	0.0001	-0.0037	2159.75	1.4381	1.3584	2176.50	1.5555	1.4890
2143.25	0.0039	-0.0048	2160.00	1.4538	1.3745	2176.75	1.5343	1.4619
2143.50	0.0041	0.0018	2160.25	1.4531	1.3863	2177.00	1.4916	1.4398
2143.75	-0.0009	0.0029	2160.50	1.4499	1.3692	2177.25	1.4669	1.4330
2144.01	0.0027	-0.0107	2160.76	1.4558	1.3717	2177.50	1.4432	1.4090
2144.25	0.0014	-0.0074	2161.00	1.4537	1.3509	2177.75	1.4304	1.3577
2144.50	0.0073	0.0030	2161.25	1.4459	1.3650	2178.00	1.3827	1.3254
2144.76	0.0015	-0.0015	2161.50	1.4487	1.3880	2178.25	1.3763	1.3140
2145.00	0.0021	-0.0061	2161.75	1.4557	1.3976	2178.50	1.3426	1.3034
2145.25	0.0091	-0.0005	2162.00	1.4470	1.3737	2178.75	1.3128	1.2662
2145.50	0.0047	-0.0002	2162.25	1.4539	1.3975	2179.00	1.3026	1.2604
2145.76	0.0065	0.0007	2162.50	1.4637	1.4132	2179.25	1.2613	1.2648
2146.01	0.0119	0.0013	2162.75	1.4742	1.4184	2179.50	1.2546	1.2253
2146.25	0.0053	0.0088	2163.00	1.4727	1.4314	2179.75	1.2629	1.2247
2146.50	0.0070	0.0133	2163.26	1.4610	1.4300	2180.00	1.2231	1.1941
2146.76	0.0165	0.0030	2163.50	1.4664	1.4302	2180.25	1.2293	1.1847
2147.00	0.0195	0.0087	2163.76	1.4774	1.4374	2180.50	1.1847	1.1760
2147.26	0.0211	0.0169	2164.01	1.4805	1.4605	2180.75	1.1722	1.1701
2147.51	0.0265	0.0158	2164.25	1.5198	1.4661	2181.00	1.1512	1.1560
2147.75	0.0257	0.0226	2164.50	1.5179	1.4967	2181.25	1.1441	1.1181
2148.00	0.0305	0.0255	2164.75	1.4965	1.4917	2181.50	1.1258	1.1410
2148.26	0.0308	0.0223	2165.00	1.4853	1.5114	2181.75	1.1015	1.1117
2148.51	0.0287	0.0298	2165.25	1.5289	1.5061	2182.00	1.0986	1.0911
2148.75	0.0366	0.0367	2165.50	1.5537	1.5363	2182.25	1.1063	1.1101
2149.01	0.0473	0.0395	2165.75	1.5616	1.5423	2182.50	1.0857	1.1002
2149.25	0.0462	0.0472	2166.00	1.6149	1.5862	2182.75	1.0900	1.0952
2149.51	0.0558	0.0521	2166.25	1.6087	1.5911	2183.00	1.0590	1.0794
2149.75	0.0663	0.0573	2166.50	1.6282	1.6081	2183.25	1.0823	1.0786
2150.00	0.0795	0.0696	2166.75	1.6445	1.6126	2183.50	1.0588	1.0569
2150.25	0.0884	0.0915	2167.00	1.6690	1.6461	2183.75	1.0541	1.0708
2150.50	0.1021	0.1109	2167.26	1.6969	1.6762	2184.00	1.0595	1.0443
2150.75	0.1201	0.1288	2167.50	1.7309	1.6955	2184.25	1.0610	1.0457
2151.00	0.1527	0.1701	2167.76	1.7692	1.7121	2184.50	1.0533	1.0577
2151.25	0.1829	0.2080	2168.00	1.7572	1.7031	2184.75	1.0238	1.0516
2151.50	0.2403	0.2797	2168.25	1.7740	1.7403	2185.00	1.0364	1.0249
2151.75	0.3053	0.3634	2168.50	1.8347	1.7652	2185.25	1.0447	1.0203
2152.00	0.4154	0.5343	2168.75	1.8301	1.7729	2185.50	1.0401	1.0258
2152.25	0.5698	0.7880	2169.00	1.8239	1.7805	2185.75	1.0168	1.0310
2152.50	0.7995	1.1376	2169.25	1.8508	1.8064	2186.00	1.0336	1.0222
2152.76	1.1562	1.6238	2169.50	1.8568	1.7852	2186.25	1.0257	1.0200
2153.00	1.6571	2.2377	2169.76	1.8606	1.7779	2186.50	0.9931	1.0093
2153.25	2.4432	3.0794	2170.00	1.8851	1.7934	2186.75	1.0102	1.0127
2153.50	3.4030	3.9498	2170.25	1.9100	1.8002	2187.00	1.0217	1.0113
2153.75	4.5144	4.8151	2170.50	1.9160	1.8020	2187.25	1.0017	1.0264
2154.00	5.6812	5.5368	2170.75	1.8853	1.8101	2187.50	1.0211	1.0332
2154.25	6.4770	5.9746	2171.00	1.9066	1.7933	2187.75	1.0199	1.0154
2154.50	7.0077	6.1733	2171.25	1.9067	1.8346	2188.00	1.0129	1.0181
2154.75	7.0078	6.0744	2171.50	1.8958	1.8093	2188.25	1.0213	0.9993
2155.00	6.6441	5.7694	2171.75	1.8989	1.8016	2188.50	1.0043	1.0021
2155.26	5.9959	5.1813	2172.00	1.8862	1.7874	2188.75	1.0231	0.9981
2155.50	5.1590	4.5432	2172.25	1.8806	1.8142	2189.00	1.0193	1.0027
2155.76	4.2089	3.8327	2172.50	1.8986	1.7664	2189.25	1.0097	1.0211
2156.00	3.4765	3.2755	2172.75	1.8702	1.7876	2189.50	1.0109	0.9941
2156.26	2.8208	2.7241	2173.00	1.8696	1.7649	2189.75	1.0171	1.0167
2156.50	2.3475	2.2987	2173.25	1.8618	1.7438	2190.00	1.0082	1.0115

Table S3 Raw data (energy, signal) of normalized P *K*-edge XANES spectra of orthophosphate (PO₄), and inositol hexakisphosphate (IHP) retained by Al-saturated montmorillonite at pH 5. P concentration after retention was 8.0 mg g⁻¹ (PO₄) and 17.8 mg g⁻¹ (IHP), respectively

Energy / eV	Signal PO4	Signal IHP	Energy / eV	Signal PO4	Signal IHP	Energy / eV	Signal PO4	Signal IHP
2140.00	0.001	0.002	2156.75	2.061	2.182	2173.50	1.870	1.791
2140.25	0.016	-0.001	2157.00	1.726	1.890	2173.75	1.829	1.793
2140.50	0.005	-0.001	2157.26	1.574	1.709	2174.00	1.833	1.761
2140.75	-0.011	0.003	2157.50	1.443	1.595	2174.25	1.819	1.726
2141.00	0.008	0.000	2157.75	1.360	1.519	2174.50	1.787	1.713
2141.25	-0.005	-0.001	2158.00	1.355	1.453	2174.75	1.784	1.694
2141.50	-0.002	0.002	2158.26	1.301	1.426	2175.00	1.747	1.655
2141.75	-0.002	0.004	2158.50	1.324	1.396	2175.25	1.706	1.664
2142.00	0.001	0.000	2158.76	1.305	1.388	2175.50	1.686	1.626
2142.25	0.009	0.000	2159.00	1.335	1.365	2175.75	1.669	1.591
2142.50	0.008	0.004	2159.25	1.354	1.369	2176.00	1.649	1.581
2142.75	0.002	0.005	2159.50	1.356	1.376	2176.25	1.605	1.548
2143.00	-0.002	-0.004	2159.75	1.331	1.383	2176.50	1.578	1.538
2143.25	-0.007	0.000	2160.00	1.332	1.389	2176.75	1.543	1.512
2143.50	-0.004	0.005	2160.25	1.359	1.401	2177.00	1.515	1.482
2143.75	-0.006	0.000	2160.50	1.410	1.398	2177.25	1.489	1.457
2144.01	0.000	0.003	2160.76	1.398	1.416	2177.50	1.480	1.444
2144.25	-0.016	0.003	2161.00	1.436	1.425	2177.75	1.419	1.412
2144.50	-0.002	0.005	2161.25	1.448	1.440	2178.00	1.400	1.397
2144.76	0.003	0.006	2161.50	1.464	1.427	2178.25	1.399	1.357
2145.00	0.020	0.010	2161.75	1.448	1.465	2178.50	1.364	1.361
2145.25	0.004	0.008	2162.00	1.449	1.471	2178.75	1.321	1.306
2145.50	0.004	0.009	2162.25	1.470	1.464	2179.00	1.308	1.295
2145.76	-0.006	0.015	2162.50	1.450	1.493	2179.25	1.285	1.278
2146.01	0.028	0.015	2162.75	1.511	1.491	2179.50	1.280	1.265
2146.25	0.008	0.012	2163.00	1.455	1.483	2179.75	1.248	1.244
2146.50	-0.004	0.016	2163.26	1.435	1.479	2180.00	1.244	1.236
2146.76	0.010	0.015	2163.50	1.452	1.497	2180.25	1.210	1.220
2147.00	0.011	0.013	2163.76	1.465	1.519	2180.50	1.204	1.208
2147.26	0.028	0.028	2164.01	1.465	1.509	2180.75	1.168	1.195
2147.51	0.020	0.027	2164.25	1.437	1.526	2181.00	1.169	1.186
2147.75	0.015	0.026	2164.50	1.435	1.537	2181.25	1.129	1.182
2148.00	0.038	0.028	2164.75	1.445	1.563	2181.50	1.141	1.163
2148.26	0.039	0.031	2165.00	1.495	1.550	2181.75	1.119	1.156
2148.51	0.051	0.043	2165.25	1.486	1.564	2182.00	1.102	1.156
2148.75	0.035	0.046	2165.50	1.474	1.570	2182.25	1.112	1.134
2149.01	0.041	0.044	2165.75	1.543	1.605	2182.50	1.098	1.134
2149.25	0.044	0.054	2166.00	1.533	1.632	2182.75	1.066	1.101
2149.51	0.043	0.063	2166.25	1.547	1.634	2183.00	1.092	1.099
2149.75	0.060	0.071	2166.50	1.605	1.658	2183.25	1.048	1.103
2150.00	0.077	0.079	2166.75	1.642	1.656	2183.50	1.076	1.094
2150.25	0.090	0.107	2167.00	1.638	1.682	2183.75	1.053	1.093
2150.50	0.080	0.104	2167.26	1.670	1.712	2184.00	1.054	1.086
2150.75	0.113	0.133	2167.50	1.675	1.731	2184.25	1.043	1.090
2151.00	0.161	0.154	2167.76	1.685	1.754	2184.50	1.038	1.062
2151.25	0.140	0.204	2168.00	1.689	1.772	2184.75	1.049	1.060
2151.50	0.188	0.264	2168.25	1.721	1.769	2185.00	1.045	1.060
2151.75	0.232	0.351	2168.50	1.746	1.785	2185.25	1.002	1.055
2152.00	0.306	0.497	2168.75	1.764	1.791	2185.50	1.047	1.053
2152.25	0.413	0.725	2169.00	1.799	1.802	2185.75	1.025	1.036
2152.50	0.590	1.034	2169.25	1.783	1.813	2186.00	0.995	1.044
2152.76	0.852	1.503	2169.50	1.851	1.813	2186.25	1.020	1.047
2153.00	1.204	2.061	2169.76	1.866	1.838	2186.50	1.018	1.046
2153.25	1.789	2.847	2170.00	1.859	1.838	2186.75	1.039	1.047
2153.50	2.597	3.658	2170.25	1.875	1.858	2187.00	1.002	1.039
2153.75	3.657	4.468	2170.50	1.854	1.860	2187.25	1.016	1.039
2154.00	5.037	5.211	2170.75	1.901	1.855	2187.50	1.014	1.018
2154.25	6.183	5.704	2171.00	1.876	1.855	2187.75	0.998	1.038
2154.50	7.201	6.030	2171.25	1.881	1.867	2188.00	0.999	1.018
2154.75	7.775	6.063	2171.50	1.928	1.847	2188.25	1.017	1.020
2155.00	7.695	5.858	2171.75	1.899	1.872	2188.50	1.027	1.037
2155.26	7.110	5.417	2172.00	1.947	1.855	2188.75	1.005	1.017
2155.50	6.253	4.863	2172.25	1.908	1.854	2189.00	0.994	1.026
2155.76	5.168	4.189	2172.50	1.919	1.849	2189.25	0.989	1.026
2156.00	4.068	3.540	2172.75	1.895	1.830	2189.50	1.035	1.006
2156.26	3.223	2.972	2173.00	1.871	1.816	2189.75	0.983	1.014
2156.50	2.516	2.521	2173.25	1.904	1.803	2190.00	1.030	1.000

Table S4 Raw data (energy, signal) of normalized P *K*-edge XANES spectra of orthophosphate and inositol hexakisphosphate (IHP) retained by Al-saturated soil organic matter (forest floor Waldsassen) at pH 4. P concentration after retention was 14.1 mg g⁻¹ (PO₄) and 6.0 mg g⁻¹ (IHP), respectively.

Energy / eV	Signal PO4	Signal IHP	Energy / eV	Signal PO4	Signal IHP	Energy / eV	Signal PO4	Signal IHP
2140.00	-0.0071	-0.0061	2156.75	2.3085	2.3542	2173.50	1.9238	1.8389
2140.25	-0.0172	0.0047	2157.00	1.9550	2.0271	2173.75	1.9214	1.8373
2140.50	-0.0006	0.0026	2157.26	1.7157	1.8448	2174.00	1.9140	1.8099
2140.75	-0.0011	-0.0134	2157.50	1.5786	1.6784	2174.25	1.8658	1.8131
2141.00	0.0065	-0.0056	2157.75	1.4606	1.5939	2174.50	1.8600	1.7867
2141.25	0.0047	-0.0131	2158.00	1.4399	1.5251	2174.75	1.8249	1.7365
2141.50	-0.0038	0.0133	2158.26	1.4288	1.4867	2175.00	1.8173	1.7252
2141.75	-0.0074	0.0040	2158.50	1.3859	1.4565	2175.25	1.7926	1.7013
2142.00	-0.0089	0.0011	2158.76	1.3957	1.4366	2175.50	1.7627	1.6643
2142.25	0.0086	-0.0081	2159.00	1.4050	1.4256	2175.75	1.7452	1.6483
2142.50	0.0058	-0.0042	2159.25	1.4139	1.4073	2176.00	1.6842	1.6011
2142.75	-0.0005	-0.0071	2159.50	1.4331	1.4187	2176.25	1.6606	1.6108
2143.00	0.0036	0.0003	2159.75	1.4488	1.4247	2176.50	1.6176	1.5928
2143.25	-0.0001	0.0022	2160.00	1.5056	1.4469	2176.75	1.6203	1.5337
2143.50	0.0063	0.0068	2160.25	1.5085	1.4574	2177.00	1.5819	1.5314
2143.75	-0.0082	0.0017	2160.50	1.5147	1.4613	2177.25	1.5428	1.4775
2144.01	0.0020	0.0136	2160.76	1.5475	1.4828	2177.50	1.5117	1.4664
2144.25	0.0109	0.0066	2161.00	1.5581	1.4767	2177.75	1.4973	1.4465
2144.50	0.0107	0.0051	2161.25	1.5416	1.4988	2178.00	1.4766	1.4162
2144.76	0.0135	-0.0020	2161.50	1.5646	1.5136	2178.25	1.4608	1.3949
2145.00	0.0120	0.0056	2161.75	1.5711	1.5173	2178.50	1.4195	1.3651
2145.25	0.0066	0.0076	2162.00	1.5655	1.5067	2178.75	1.3824	1.3512
2145.50	0.0089	0.0123	2162.25	1.5763	1.5232	2179.00	1.3679	1.3192
2145.76	0.0189	0.0215	2162.50	1.5578	1.5202	2179.25	1.3298	1.3087
2146.01	0.0050	0.0178	2162.75	1.5503	1.5225	2179.50	1.2934	1.3002
2146.25	0.0127	0.0226	2163.00	1.5523	1.5200	2179.75	1.3025	1.2766
2146.50	0.0151	0.0255	2163.26	1.5379	1.5364	2180.00	1.2630	1.2518
2146.76	0.0164	0.0284	2163.50	1.5550	1.5385	2180.25	1.2506	1.2535
2147.00	0.0338	0.0147	2163.76	1.5522	1.5297	2180.50	1.2261	1.2142
2147.26	0.0228	0.0289	2164.01	1.5406	1.5454	2180.75	1.2172	1.1931
2147.51	0.0380	0.0261	2164.25	1.5281	1.5312	2181.00	1.1875	1.1896
2147.75	0.0359	0.0346	2164.50	1.5353	1.5474	2181.25	1.1704	1.1755
2148.00	0.0384	0.0350	2164.75	1.5356	1.5497	2181.50	1.1977	1.1600
2148.26	0.0534	0.0389	2165.00	1.5332	1.5520	2181.75	1.1633	1.1648
2148.51	0.0464	0.0401	2165.25	1.5321	1.5843	2182.00	1.1316	1.1415
2148.75	0.0532	0.0598	2165.50	1.5315	1.5972	2182.25	1.1193	1.1381
2149.01	0.0561	0.0667	2165.75	1.5814	1.5964	2182.50	1.0968	1.1338
2149.25	0.0648	0.0653	2166.00	1.5871	1.6481	2182.75	1.1073	1.1207
2149.51	0.0702	0.0733	2166.25	1.6073	1.6460	2183.00	1.0901	1.1033
2149.75	0.0686	0.0862	2166.50	1.6211	1.6682	2183.25	1.0661	1.0985
2150.00	0.0937	0.1028	2166.75	1.6552	1.6961	2183.50	1.1050	1.0780
2150.25	0.1002	0.1113	2167.00	1.6828	1.7066	2183.75	1.0745	1.0939
2150.50	0.1104	0.1275	2167.26	1.7023	1.7139	2184.00	1.0646	1.0939
2150.75	0.1437	0.1601	2167.50	1.7252	1.7656	2184.25	1.0429	1.0831
2151.00	0.1537	0.1743	2167.76	1.7369	1.7947	2184.50	1.0679	1.0717
2151.25	0.1948	0.2182	2168.00	1.7769	1.8067	2184.75	1.0446	1.0612
2151.50	0.2204	0.2722	2168.25	1.7807	1.8176	2185.00	1.0486	1.0494
2151.75	0.2692	0.3384	2168.50	1.8282	1.8258	2185.25	1.0383	1.0506
2152.00	0.3589	0.4665	2168.75	1.8587	1.8391	2185.50	1.0521	1.0626
2152.25	0.4672	0.6323	2169.00	1.8687	1.8648	2185.75	1.0356	1.0445
2152.50	0.6541	0.9038	2169.25	1.8697	1.8849	2186.00	1.0076	1.0332
2152.76	0.9072	1.2962	2169.50	1.9113	1.8914	2186.25	1.0234	1.0387
2153.00	1.2828	1.8586	2169.76	1.9285	1.8958	2186.50	1.0105	1.0355
2153.25	1.7841	2.5374	2170.00	1.9267	1.8954	2186.75	1.0123	1.0191
2153.50	2.4616	3.3264	2170.25	1.9639	1.8890	2187.00	1.0209	1.0354
2153.75	3.4850	4.3789	2170.50	1.9759	1.8955	2187.25	1.0370	1.0210
2154.00	4.6443	5.3490	2170.75	1.9846	1.9105	2187.50	1.0137	1.0221
2154.25	5.9563	6.1729	2171.00	1.9595	1.9145	2187.75	1.0261	1.0180
2154.50	7.1637	6.7966	2171.25	1.9823	1.9053	2188.00	1.0158	1.0052
2154.75	7.8351	7.0095	2171.50	1.9938	1.9146	2188.25	1.0068	1.0242
2155.00	7.9811	6.9381	2171.75	1.9765	1.9223	2188.50	1.0249	1.0212
2155.26	7.5500	6.4685	2172.00	1.9869	1.9176	2188.75	0.9931	1.0172
2155.50	6.6065	5.7430	2172.25	1.9865	1.9018	2189.00	1.0063	1.0295
2155.76	5.5721	4.8952	2172.50	1.9878	1.9027	2189.25	1.0001	1.0219
2156.00	4.5141	4.1167	2172.75	1.9421	1.9153	2189.50	1.0115	1.0227
2156.26	3.5119	3.3423	2173.00	1.9517	1.8972	2189.75	1.0202	1.0199
2156.50	2.8159	2.7946	2173.25	1.9494	1.8504	2190.00	1.0195	1.0144

Table S5 Raw data (energy, signal) of normalized P *K*-edge XANES spectra of inositol hexakisphosphate (IHP) retained by calcite at pH 6

Energy / eV	Signal IHP	Energy / eV	Signal IHP	Energy / eV	Signal IHP	Energy / eV	Signal IHP	Energy / eV	Signal IHP
2140.00	-0.0056	2150.00	0.1252	2160.00	1.4888	2170.00	2.0550	2180.00	1.4668
2140.25	-0.0125	2150.25	0.1507	2160.25	1.4746	2170.25	2.0433	2180.25	1.4468
2140.50	-0.0038	2150.50	0.1576	2160.50	1.4737	2170.50	2.0304	2180.50	1.4340
2140.75	-0.0062	2150.75	0.1814	2160.75	1.4881	2170.75	2.0294	2180.75	1.4355
2141.00	-0.0065	2151.00	0.2412	2161.00	1.4779	2171.00	2.0515	2181.00	1.4062
2141.25	-0.0090	2151.25	0.2820	2161.25	1.4780	2171.25	2.0022	2181.25	1.4154
2141.50	-0.0131	2151.50	0.3846	2161.50	1.4837	2171.50	2.0127	2181.50	1.3957
2141.75	-0.0033	2151.75	0.5211	2161.75	1.5156	2171.75	2.0186	2181.75	1.3923
2142.00	-0.0064	2152.00	0.7434	2162.00	1.5239	2172.00	1.9979	2182.00	1.3711
2142.25	0.0031	2152.25	1.0361	2162.25	1.5530	2172.25	1.9778	2182.25	1.3535
2142.50	-0.0065	2152.50	1.5348	2162.50	1.5572	2172.50	1.9648	2182.50	1.3408
2142.75	0.0010	2152.75	2.1078	2162.75	1.5538	2172.75	1.9864	2182.75	1.3265
2143.00	-0.0004	2153.00	2.8811	2163.00	1.5670	2173.00	1.9689	2183.00	1.3463
2143.25	-0.0045	2153.25	3.7760	2163.25	1.5579	2173.25	1.9380	2183.25	1.3330
2143.50	0.0082	2153.50	4.6245	2163.50	1.5754	2173.50	1.9334	2183.50	1.3469
2143.75	-0.0010	2153.75	5.3946	2163.75	1.6155	2173.75	1.9302	2183.75	1.3304
2144.01	-0.0019	2154.00	5.8116	2164.01	1.6158	2174.00	1.8872	2184.00	1.3308
2144.25	0.0059	2154.25	5.9288	2164.25	1.6400	2174.25	1.8767	2184.25	1.3332
2144.50	0.0075	2154.50	5.8648	2164.50	1.6701	2174.50	1.8578	2184.50	1.3059
2144.76	0.0089	2154.75	5.6172	2164.75	1.6684	2174.75	1.8381	2184.75	1.3087
2145.00	0.0101	2155.00	5.1510	2165.00	1.7122	2175.00	1.8205	2185.00	1.3001
2145.25	0.0064	2155.25	4.6665	2165.25	1.7476	2175.25	1.8274	2185.25	1.2949
2145.50	0.0156	2155.50	4.1286	2165.50	1.7361	2175.50	1.7760	2185.50	1.3083
2145.76	0.0195	2155.75	3.7171	2165.75	1.7815	2175.75	1.7671	2185.75	1.3202
2146.01	0.0240	2156.00	3.4147	2166.00	1.8024	2176.00	1.7305	2186.00	1.2968
2146.25	0.0233	2156.25	3.1325	2166.25	1.8439	2176.25	1.6994	2186.25	1.3064
2146.50	0.0237	2156.50	2.9036	2166.50	1.8509	2176.50	1.6951	2186.50	1.3113
2146.76	0.0260	2156.75	2.7254	2166.75	1.8894	2176.75	1.6723	2186.75	1.3214
2147.00	0.0301	2157.00	2.5477	2167.00	1.8932	2177.00	1.6602	2187.00	1.2960
2147.26	0.0353	2157.25	2.3711	2167.25	1.9401	2177.25	1.6538	2187.25	1.2968
2147.51	0.0423	2157.50	2.1770	2167.50	1.9561	2177.50	1.6240	2187.50	1.2991
2147.75	0.0388	2157.75	2.0699	2167.75	1.9868	2177.75	1.6052	2187.75	1.2860
2148.00	0.0482	2158.00	1.9368	2168.00	1.9782	2178.00	1.5907	2188.00	1.3023
2148.26	0.0449	2158.25	1.8183	2168.25	1.9955	2178.25	1.5589	2188.25	1.3047
2148.51	0.0686	2158.50	1.7380	2168.50	2.0056	2178.50	1.5798	2188.50	1.3102
2148.75	0.0662	2158.75	1.6263	2168.75	2.0069	2178.75	1.5357	2188.75	1.3001
2149.01	0.0667	2159.00	1.5830	2169.00	1.9780	2179.00	1.5042	2189.00	1.3164
2149.25	0.0913	2159.25	1.5472	2169.25	2.0452	2179.25	1.4900	2189.25	1.3061
2149.51	0.0995	2159.50	1.5085	2169.50	2.0501	2179.50	1.5035	2189.50	1.3102
2149.75	0.0946	2159.75	1.4833	2169.75	2.0457	2179.75	1.4747	2189.75	1.3042

Table S6 Raw data (energy, signal) of normalized P *K*-edge XANES spectra of Ca phytate and Fe phytate.

Energy / eV	Signal Ca phytate	Signal Fe phytate	Energy / eV	Signal Ca phytate	Signal Fe phytate	Energy / eV	Signal Ca phytate	Signal Fe phytate
2140.20	-0.001	-0.010	2156.96	2.458	2.124	2173.70	1.758	1.755
2140.45	0.000	-0.002	2157.20	2.304	1.874	2173.95	1.745	1.743
2140.70	0.013	-0.001	2157.45	2.152	1.740	2174.20	1.707	1.755
2140.95	0.009	0.003	2157.70	2.001	1.657	2174.45	1.702	1.698
2141.20	0.004	0.005	2157.95	1.892	1.606	2174.70	1.668	1.676
2141.46	0.001	-0.013	2158.21	1.798	1.522	2174.95	1.644	1.687
2141.70	0.003	-0.012	2158.45	1.695	1.517	2175.20	1.642	1.643
2141.95	0.003	-0.010	2158.70	1.616	1.481	2175.45	1.610	1.608
2142.20	0.002	0.008	2158.95	1.557	1.514	2175.70	1.565	1.593
2142.45	0.002	0.007	2159.20	1.553	1.509	2175.95	1.558	1.590
2142.70	0.002	-0.002	2159.45	1.493	1.521	2176.20	1.537	1.541
2142.96	0.001	-0.003	2159.71	1.481	1.501	2176.45	1.507	1.522
2143.20	0.003	0.015	2159.95	1.490	1.515	2176.70	1.493	1.495
2143.46	0.018	0.003	2160.20	1.471	1.510	2176.95	1.482	1.479
2143.70	0.013	0.012	2160.45	1.461	1.502	2177.20	1.476	1.478
2143.95	0.004	-0.008	2160.71	1.446	1.504	2177.45	1.451	1.453
2144.20	0.009	-0.001	2160.95	1.429	1.481	2177.70	1.454	1.416
2144.45	0.013	0.004	2161.21	1.428	1.508	2177.95	1.383	1.385
2144.71	0.012	0.002	2161.46	1.462	1.512	2178.20	1.385	1.385
2144.95	0.019	0.011	2161.70	1.456	1.511	2178.45	1.364	1.379
2145.20	0.010	0.018	2161.95	1.481	1.505	2178.70	1.337	1.355
2145.45	0.016	0.002	2162.21	1.496	1.527	2178.95	1.313	1.335
2145.71	0.019	0.012	2162.45	1.472	1.522	2179.20	1.298	1.315
2145.95	0.027	0.016	2162.71	1.498	1.553	2179.45	1.298	1.268
2146.20	0.026	0.025	2162.96	1.540	1.556	2179.70	1.258	1.267
2146.45	0.026	0.031	2163.20	1.516	1.553	2179.95	1.273	1.270
2146.70	0.038	0.020	2163.46	1.525	1.586	2180.20	1.264	1.256
2146.96	0.043	0.047	2163.70	1.550	1.577	2180.45	1.247	1.249
2147.21	0.025	0.023	2163.96	1.599	1.594	2180.70	1.225	1.232
2147.45	0.030	0.043	2164.21	1.594	1.617	2180.95	1.196	1.213
2147.70	0.031	0.045	2164.45	1.607	1.637	2181.20	1.205	1.176
2147.95	0.052	0.048	2164.71	1.616	1.677	2181.45	1.168	1.190
2148.20	0.050	0.059	2164.95	1.665	1.663	2181.70	1.166	1.199
2148.46	0.044	0.058	2165.20	1.676	1.681	2181.95	1.167	1.182
2148.70	0.047	0.080	2165.45	1.706	1.660	2182.20	1.144	1.190
2148.96	0.064	0.119	2165.71	1.718	1.703	2182.45	1.135	1.157
2149.20	0.068	0.153	2165.95	1.742	1.746	2182.70	1.123	1.148
2149.45	0.081	0.201	2166.20	1.729	1.748	2182.95	1.104	1.122
2149.70	0.101	0.269	2166.46	1.751	1.744	2183.20	1.130	1.130
2149.95	0.118	0.282	2166.70	1.800	1.775	2183.45	1.096	1.118
2150.20	0.137	0.334	2166.95	1.814	1.793	2183.70	1.073	1.122
2150.45	0.148	0.371	2167.20	1.840	1.792	2183.95	1.070	1.116
2150.70	0.166	0.401	2167.45	1.813	1.821	2184.20	1.092	1.108
2150.96	0.210	0.434	2167.70	1.823	1.832	2184.45	1.073	1.095
2151.20	0.283	0.447	2167.95	1.871	1.852	2184.70	1.050	1.074
2151.45	0.392	0.478	2168.21	1.887	1.841	2184.95	1.067	1.094
2151.70	0.556	0.515	2168.45	1.889	1.856	2185.20	1.070	1.084
2151.95	0.820	0.599	2168.70	1.910	1.883	2185.45	1.053	1.082
2152.20	1.212	0.759	2168.95	1.881	1.885	2185.70	1.062	1.082
2152.46	1.711	0.995	2169.21	1.891	1.875	2185.95	1.061	1.086
2152.70	2.410	1.390	2169.45	1.912	1.925	2186.20	1.044	1.079
2152.95	3.176	1.837	2169.70	1.908	1.922	2186.45	1.039	1.061
2153.21	4.071	2.473	2169.95	1.928	1.947	2186.70	1.029	1.084
2153.46	4.965	3.309	2170.20	1.903	1.935	2186.95	1.034	1.070
2153.70	5.540	4.124	2170.45	1.886	1.897	2187.20	1.030	1.077
2153.96	5.869	5.032	2170.70	1.914	1.898	2187.45	1.039	1.075
2154.20	5.976	5.653	2170.95	1.925	1.897	2187.70	1.023	1.043
2154.46	5.738	6.080	2171.20	1.898	1.886	2187.95	1.024	1.053
2154.70	5.424	6.259	2171.45	1.889	1.854	2188.20	1.029	1.063
2154.96	4.906	6.222	2171.70	1.853	1.900	2188.45	1.016	1.028
2155.20	4.447	5.835	2171.95	1.869	1.871	2188.70	1.041	1.042
2155.46	4.025	5.269	2172.20	1.851	1.846	2188.95	1.014	1.047
2155.70	3.571	4.581	2172.45	1.847	1.834	2189.20	1.020	1.035
2155.96	3.254	3.907	2172.70	1.814	1.850	2189.45	1.009	1.016
2156.20	3.037	3.294	2172.95	1.813	1.818	2189.70	1.022	1.033
2156.46	2.848	2.735	2173.20	1.815	1.834	2189.95	1.055	1.002
2156.71	2.665	2.365	2173.45	1.762	1.803	2190.00	1.030	1.000

Table S7 Raw data (energy, signal) of normalized P *K*-edge XANES spectra of Al phytate and free inositol hexakisphosphate (IHP).

Energy / eV	Signal Al phytate	Signal IHP	Energy / eV	Signal Al phytate	Signal IHP	Energy / eV	Signal Al phytate	Signal IHP
2140.03	0.002	-0.037	2156.79	2.189	2.191	2173.53	1.822	1.742
2140.28	0.009	0.018	2157.03	1.924	1.970	2173.78	1.807	1.699
2140.53	-0.007	-0.022	2157.28	1.765	1.822	2174.03	1.805	1.713
2140.78	-0.009	-0.012	2157.53	1.640	1.725	2174.28	1.754	1.691
2141.03	0.001	0.019	2157.78	1.588	1.630	2174.53	1.756	1.659
2141.28	-0.001	0.011	2158.03	1.519	1.580	2174.78	1.737	1.605
2141.54	-0.003	-0.008	2158.29	1.494	1.566	2175.03	1.669	1.597
2141.78	-0.003	-0.003	2158.53	1.450	1.494	2175.28	1.643	1.614
2142.03	-0.011	0.002	2158.78	1.448	1.457	2175.53	1.667	1.563
2142.28	0.000	0.007	2159.03	1.424	1.427	2175.78	1.575	1.514
2142.53	-0.001	-0.007	2159.28	1.437	1.405	2176.03	1.570	1.507
2142.78	0.008	0.010	2159.53	1.425	1.414	2176.28	1.534	1.493
2143.04	0.002	0.039	2159.79	1.452	1.423	2176.53	1.534	1.515
2143.28	0.014	0.016	2160.03	1.450	1.378	2176.78	1.474	1.451
2143.54	0.017	0.003	2160.28	1.442	1.393	2177.03	1.488	1.452
2143.78	0.002	0.000	2160.53	1.487	1.388	2177.28	1.474	1.464
2144.03	-0.009	-0.014	2160.79	1.482	1.408	2177.53	1.445	1.371
2144.28	0.011	0.022	2161.03	1.506	1.412	2177.78	1.419	1.373
2144.53	-0.006	0.011	2161.29	1.487	1.368	2178.03	1.380	1.392
2144.79	0.017	0.027	2161.54	1.480	1.421	2178.28	1.385	1.378
2145.03	0.023	0.024	2161.78	1.495	1.404	2178.53	1.370	1.332
2145.28	0.018	0.034	2162.04	1.535	1.452	2178.78	1.391	1.323
2145.53	0.020	0.026	2162.29	1.514	1.443	2179.03	1.326	1.277
2145.79	0.016	0.013	2162.53	1.533	1.445	2179.28	1.277	1.277
2146.03	0.013	0.043	2162.79	1.566	1.443	2179.53	1.310	1.263
2146.28	0.025	0.042	2163.04	1.551	1.465	2179.78	1.304	1.257
2146.53	0.019	0.065	2163.28	1.585	1.452	2180.03	1.290	1.257
2146.78	0.021	0.038	2163.54	1.586	1.475	2180.28	1.254	1.211
2147.04	0.025	0.069	2163.78	1.578	1.491	2180.53	1.259	1.217
2147.29	0.021	0.032	2164.04	1.566	1.480	2180.78	1.242	1.203
2147.53	0.035	0.018	2164.29	1.624	1.476	2181.03	1.223	1.210
2147.78	0.034	0.041	2164.53	1.614	1.527	2181.28	1.238	1.143
2148.03	0.047	0.039	2164.79	1.627	1.531	2181.53	1.188	1.142
2148.28	0.038	0.058	2165.04	1.642	1.529	2181.78	1.182	1.164
2148.53	0.044	0.049	2165.28	1.678	1.560	2182.03	1.223	1.110
2148.78	0.052	0.081	2165.53	1.689	1.593	2182.28	1.187	1.133
2149.04	0.060	0.069	2165.79	1.687	1.580	2182.53	1.179	1.126
2149.28	0.075	0.068	2166.03	1.737	1.610	2182.78	1.166	1.140
2149.53	0.069	0.122	2166.28	1.720	1.619	2183.03	1.153	1.138
2149.78	0.079	0.084	2166.54	1.743	1.642	2183.28	1.120	1.115
2150.03	0.091	0.097	2166.78	1.751	1.660	2183.53	1.118	1.106
2150.28	0.109	0.122	2167.03	1.788	1.677	2183.78	1.134	1.069
2150.53	0.145	0.151	2167.28	1.775	1.660	2184.03	1.095	1.089
2150.78	0.159	0.174	2167.53	1.793	1.757	2184.28	1.103	1.123
2151.03	0.176	0.191	2167.78	1.839	1.775	2184.53	1.075	1.047
2151.28	0.220	0.235	2168.03	1.800	1.766	2184.78	1.095	1.060
2151.53	0.272	0.301	2168.29	1.836	1.819	2185.03	1.092	1.065
2151.78	0.355	0.443	2168.53	1.870	1.801	2185.28	1.052	1.053
2152.03	0.477	0.556	2168.78	1.860	1.802	2185.53	1.073	1.067
2152.28	0.711	0.857	2169.03	1.858	1.811	2185.78	1.078	1.077
2152.54	1.003	1.171	2169.29	1.881	1.846	2186.03	1.060	1.069
2152.78	1.481	1.640	2169.53	1.894	1.868	2186.28	1.044	1.051
2153.03	2.076	2.246	2169.78	1.880	1.833	2186.53	1.036	1.066
2153.28	2.811	3.029	2170.03	1.882	1.868	2186.78	1.048	1.064
2153.54	3.717	4.028	2170.28	1.858	1.855	2187.03	1.064	1.053
2153.78	4.622	5.086	2170.53	1.893	1.842	2187.28	1.060	1.024
2154.04	5.481	5.886	2170.78	1.852	1.828	2187.53	1.071	1.050
2154.28	6.027	6.347	2171.03	1.869	1.899	2187.78	1.061	1.063
2154.54	6.376	6.437	2171.28	1.931	1.897	2188.03	1.052	1.015
2154.78	6.392	6.364	2171.53	1.889	1.858	2188.29	1.022	1.025
2155.04	6.189	5.828	2171.78	1.873	1.821	2188.53	1.024	1.040
2155.28	5.771	5.222	2172.03	1.877	1.822	2188.78	1.016	1.016
2155.54	5.170	4.532	2172.28	1.887	1.835	2189.03	1.021	1.034
2155.78	4.343	3.899	2172.53	1.855	1.815	2189.28	1.031	1.010
2156.04	3.641	3.296	2172.78	1.858	1.809	2189.53	1.011	1.013
2156.28	3.047	2.791	2173.03	1.861	1.760	2189.78	1.019	1.025
2156.54	2.518	2.457	2173.28	1.826	1.782	2190.03	1.027	1.015

Table S8 Raw data (energy, signal) of amorphous AlPO₄ and crystalline AlPO₄ (berlinite).

Energy / eV	Signal AlPO ₄ amo	Signal AlPO ₄ crys	Energy / eV	Signal AlPO ₄ amo	Signal AlPO ₄ crys	Energy / eV	Signal AlPO ₄ amo	Signal AlPO ₄ crys
2140.00	-0.005	-0.013	2156.75	1.919	2.184	2173.50	1.965	2.003
2140.25	-0.006	-0.005	2157.01	1.731	1.840	2173.75	1.918	2.013
2140.50	-0.003	0.017	2157.25	1.645	1.600	2174.00	1.932	2.004
2140.75	-0.001	0.004	2157.50	1.560	1.505	2174.25	1.864	1.947
2141.00	-0.004	0.009	2157.75	1.520	1.420	2174.50	1.836	1.926
2141.25	0.001	-0.018	2158.00	1.519	1.426	2174.75	1.802	1.912
2141.51	0.009	-0.007	2158.26	1.502	1.458	2175.00	1.781	1.901
2141.75	0.010	-0.006	2158.50	1.508	1.427	2175.25	1.736	1.864
2142.00	0.008	0.002	2158.75	1.494	1.463	2175.50	1.736	1.820
2142.25	0.005	0.010	2159.00	1.487	1.432	2175.75	1.693	1.800
2142.50	-0.008	0.004	2159.25	1.484	1.424	2176.00	1.645	1.730
2142.75	-0.002	0.024	2159.50	1.481	1.471	2176.25	1.615	1.732
2143.01	0.003	-0.001	2159.76	1.499	1.458	2176.50	1.618	1.712
2143.25	0.004	0.004	2160.00	1.526	1.410	2176.75	1.549	1.626
2143.51	-0.001	0.019	2160.25	1.554	1.436	2177.00	1.517	1.592
2143.75	0.004	0.010	2160.50	1.540	1.393	2177.25	1.509	1.565
2144.00	0.008	-0.001	2160.76	1.517	1.430	2177.50	1.461	1.543
2144.25	0.018	0.014	2161.00	1.525	1.445	2177.75	1.448	1.502
2144.50	0.019	0.008	2161.26	1.538	1.457	2178.00	1.401	1.469
2144.76	0.015	0.022	2161.51	1.536	1.479	2178.25	1.385	1.436
2145.00	0.013	0.011	2161.75	1.529	1.505	2178.50	1.369	1.416
2145.25	0.012	0.006	2162.00	1.567	1.558	2178.75	1.341	1.410
2145.50	0.011	0.007	2162.26	1.543	1.608	2179.00	1.312	1.350
2145.76	0.009	0.009	2162.50	1.560	1.642	2179.25	1.306	1.353
2146.01	0.022	0.014	2162.76	1.550	1.674	2179.50	1.260	1.331
2146.25	0.026	0.034	2163.01	1.554	1.677	2179.75	1.256	1.349
2146.50	0.022	0.013	2163.25	1.585	1.675	2180.00	1.260	1.287
2146.75	0.029	0.014	2163.51	1.577	1.708	2180.25	1.233	1.327
2147.00	0.032	0.034	2163.75	1.562	1.697	2180.50	1.200	1.304
2147.26	0.028	0.019	2164.01	1.573	1.721	2180.75	1.192	1.254
2147.50	0.031	0.009	2164.26	1.562	1.712	2181.00	1.179	1.289
2147.75	0.035	0.023	2164.50	1.546	1.703	2181.25	1.169	1.309
2148.00	0.036	0.041	2164.76	1.555	1.724	2181.50	1.150	1.269
2148.26	0.048	0.016	2165.00	1.558	1.711	2181.75	1.150	1.265
2148.50	0.048	0.023	2165.25	1.552	1.650	2182.00	1.129	1.194
2148.75	0.045	0.048	2165.50	1.577	1.648	2182.25	1.119	1.219
2149.01	0.051	0.040	2165.76	1.600	1.610	2182.50	1.139	1.236
2149.25	0.065	0.051	2166.00	1.607	1.616	2182.75	1.125	1.226
2149.50	0.079	0.072	2166.25	1.602	1.616	2183.00	1.107	1.201
2149.76	0.085	0.063	2166.51	1.625	1.592	2183.25	1.091	1.201
2150.00	0.091	0.089	2166.75	1.654	1.593	2183.50	1.068	1.152
2150.25	0.097	0.096	2167.00	1.675	1.592	2183.75	1.086	1.200
2150.50	0.113	0.107	2167.25	1.691	1.559	2184.00	1.081	1.148
2150.76	0.132	0.110	2167.50	1.734	1.561	2184.25	1.097	1.148
2151.00	0.161	0.129	2167.75	1.767	1.563	2184.50	1.096	1.134
2151.25	0.194	0.135	2168.00	1.804	1.550	2184.75	1.059	1.130
2151.50	0.243	0.179	2168.26	1.834	1.583	2185.00	1.063	1.112
2151.75	0.318	0.204	2168.50	1.844	1.617	2185.25	1.098	1.121
2152.01	0.430	0.252	2168.75	1.851	1.656	2185.50	1.065	1.092
2152.25	0.567	0.328	2169.00	1.890	1.711	2185.75	1.071	1.096
2152.51	0.813	0.468	2169.26	1.910	1.766	2186.00	1.063	1.085
2152.75	1.170	0.596	2169.50	1.951	1.844	2186.25	1.071	1.087
2153.00	1.685	0.832	2169.75	1.957	1.872	2186.50	1.048	1.096
2153.25	2.429	1.196	2170.00	1.991	1.912	2186.75	1.021	1.083
2153.51	3.492	1.621	2170.25	1.996	1.948	2187.00	1.023	1.071
2153.75	4.769	2.200	2170.50	2.003	1.954	2187.25	1.033	1.048
2154.01	6.274	2.754	2170.75	1.996	1.946	2187.50	1.035	1.077
2154.25	7.317	3.510	2171.00	1.988	2.004	2187.75	1.011	1.055
2154.51	7.998	4.382	2171.25	1.993	1.982	2188.00	1.006	1.053
2154.75	8.073	5.224	2171.50	1.998	1.978	2188.25	1.021	1.073
2155.01	7.559	5.822	2171.75	2.011	1.971	2188.50	1.026	1.097
2155.25	6.659	5.985	2172.00	2.003	1.993	2188.75	1.014	1.057
2155.51	5.488	5.720	2172.25	2.005	2.016	2189.00	1.019	1.044
2155.75	4.345	5.090	2172.50	1.992	2.000	2189.25	1.026	1.037
2156.01	3.400	4.376	2172.75	1.990	2.030	2189.50	1.029	1.071
2156.25	2.713	3.468	2173.00	1.969	2.028	2189.75	1.019	1.064
2156.50	2.209	2.766	2173.25	1.957	1.989	2190.00	1.016	1.048

Table S9 Raw data (energy, signal) of amorphous FePO₄ and Ca₅OH(PO₄)₃ (hydroxy apatite).

Energy / eV	Signal FePO4 amo	Signal Apatite	Energy / eV	Signal FePO4 amo	Signal Apatite	Energy / eV	Signal FePO4 amo	Signal Apatite
2140.00	-0.001	-0.002	2156.76	2.298	2.937	2173.50	1.772	1.719
2140.25	-0.023	-0.002	2157.00	1.959	2.802	2173.75	1.759	1.698
2140.50	0.001	0.000	2157.25	1.741	2.670	2174.00	1.683	1.702
2140.75	0.008	0.002	2157.51	1.619	2.515	2174.25	1.688	1.676
2141.00	0.001	0.005	2157.75	1.511	2.319	2174.50	1.670	1.628
2141.25	-0.001	0.003	2158.00	1.503	2.136	2174.75	1.632	1.629
2141.50	0.007	-0.009	2158.25	1.426	1.919	2175.00	1.616	1.597
2141.75	0.019	-0.011	2158.50	1.444	1.767	2175.25	1.599	1.582
2142.00	0.006	0.004	2158.75	1.377	1.581	2175.50	1.546	1.560
2142.25	0.012	0.015	2159.00	1.366	1.470	2175.75	1.555	1.537
2142.50	0.016	0.010	2159.25	1.379	1.392	2176.00	1.521	1.515
2142.76	0.012	0.008	2159.51	1.368	1.279	2176.25	1.494	1.502
2143.00	-0.003	-0.005	2159.75	1.336	1.234	2176.50	1.480	1.466
2143.25	0.016	0.013	2160.00	1.369	1.196	2176.75	1.441	1.435
2143.50	0.000	0.003	2160.25	1.354	1.163	2177.00	1.453	1.406
2143.75	0.007	-0.005	2160.50	1.360	1.158	2177.25	1.427	1.404
2144.00	0.006	0.014	2160.75	1.348	1.131	2177.50	1.396	1.374
2144.26	0.017	0.004	2161.00	1.359	1.186	2177.75	1.371	1.362
2144.50	0.008	0.014	2161.25	1.389	1.197	2178.00	1.346	1.330
2144.75	0.009	0.015	2161.50	1.370	1.213	2178.25	1.322	1.304
2145.00	0.018	0.022	2161.75	1.407	1.232	2178.50	1.330	1.274
2145.25	0.019	0.007	2162.00	1.400	1.266	2178.75	1.269	1.255
2145.50	-0.005	0.017	2162.25	1.392	1.307	2179.00	1.270	1.254
2145.76	0.008	0.021	2162.50	1.428	1.348	2179.25	1.255	1.213
2146.00	0.017	0.031	2162.75	1.404	1.344	2179.50	1.259	1.200
2146.26	0.012	0.011	2163.00	1.413	1.367	2179.75	1.227	1.191
2146.50	0.033	0.025	2163.25	1.447	1.423	2180.00	1.215	1.169
2146.75	0.026	0.027	2163.50	1.427	1.448	2180.25	1.196	1.144
2147.01	0.020	0.021	2163.75	1.461	1.479	2180.50	1.159	1.124
2147.25	0.026	0.042	2164.00	1.479	1.504	2180.75	1.175	1.132
2147.51	0.043	0.033	2164.25	1.460	1.515	2181.00	1.153	1.107
2147.76	0.013	0.033	2164.50	1.501	1.559	2181.25	1.153	1.107
2148.00	0.036	0.050	2164.75	1.515	1.565	2181.50	1.126	1.088
2148.26	0.058	0.043	2165.00	1.503	1.562	2181.75	1.120	1.082
2148.51	0.092	0.043	2165.25	1.524	1.588	2182.00	1.121	1.083
2148.75	0.111	0.052	2165.50	1.535	1.584	2182.25	1.144	1.085
2149.00	0.125	0.043	2165.75	1.546	1.564	2182.50	1.136	1.072
2149.26	0.199	0.060	2166.00	1.573	1.586	2182.75	1.083	1.059
2149.51	0.226	0.069	2166.25	1.604	1.591	2183.00	1.092	1.023
2149.76	0.292	0.084	2166.50	1.574	1.601	2183.25	1.087	1.044
2150.01	0.324	0.087	2166.75	1.629	1.626	2183.50	1.078	1.037
2150.26	0.365	0.103	2167.00	1.629	1.631	2183.75	1.106	1.035
2150.51	0.421	0.128	2167.25	1.648	1.648	2184.00	1.116	1.026
2150.75	0.430	0.145	2167.50	1.635	1.675	2184.25	1.051	1.017
2151.00	0.475	0.176	2167.75	1.686	1.690	2184.50	1.075	1.022
2151.26	0.462	0.213	2168.00	1.678	1.669	2184.75	1.064	0.997
2151.50	0.477	0.261	2168.25	1.737	1.705	2185.00	1.076	1.007
2151.75	0.448	0.324	2168.50	1.707	1.702	2185.25	1.057	1.037
2152.00	0.479	0.473	2168.75	1.734	1.756	2185.50	1.063	1.007
2152.25	0.503	0.642	2169.00	1.753	1.741	2185.75	1.083	1.005
2152.50	0.576	0.948	2169.25	1.748	1.776	2186.00	1.032	1.027
2152.75	0.699	1.354	2169.50	1.773	1.783	2186.25	1.069	1.017
2153.00	0.958	2.007	2169.75	1.800	1.816	2186.50	1.058	0.988
2153.25	1.296	2.916	2170.00	1.781	1.821	2186.75	1.059	0.996
2153.50	1.824	3.928	2170.25	1.802	1.841	2187.00	1.041	1.024
2153.76	2.598	5.079	2170.50	1.805	1.831	2187.25	1.031	1.016
2154.00	3.619	5.735	2170.75	1.790	1.847	2187.50	1.041	1.003
2154.25	4.907	5.899	2171.00	1.813	1.864	2187.75	1.016	1.017
2154.50	6.141	5.587	2171.25	1.808	1.836	2188.00	1.043	1.024
2154.75	7.036	5.063	2171.50	1.856	1.839	2188.25	1.017	1.011
2155.00	7.339	4.481	2171.75	1.842	1.842	2188.50	1.031	1.035
2155.26	7.114	4.019	2172.00	1.826	1.813	2188.75	1.036	0.992
2155.50	6.389	3.618	2172.25	1.829	1.832	2189.00	1.022	1.026
2155.75	5.416	3.339	2172.50	1.839	1.784	2189.25	1.037	1.017
2156.00	4.476	3.180	2172.75	1.811	1.778	2189.50	1.026	1.037
2156.25	3.512	3.085	2173.00	1.797	1.755	2189.75	1.022	1.006
2156.50	2.803	2.982	2173.25	1.748	1.747	2190.00	1.027	1.000

Table S10 Raw data (energy, signal) of CaHPO₄ (monetite) and Ca(H₂PO₄)₂.

Energy / eV	Signal CaHPO4	Signal Ca(H2PO4)2	Energy / eV	Signal CaHPO4	Signal Ca(H2PO4)2	Energy / eV	Signal CaHPO4	Signal Ca(H2PO4)2
2140.00	0.002	-0.002	2156.73	2.339	1.899	2173.52	1.851	1.639
2140.29	-0.003	0.004	2157.03	2.278	1.757	2173.77	1.825	1.640
2140.50	-0.006	0.004	2157.27	2.232	1.689	2174.00	1.820	1.615
2140.79	0.003	-0.011	2157.52	2.176	1.615	2174.27	1.794	1.597
2141.00	-0.008	0.004	2157.77	2.136	1.578	2174.51	1.779	1.573
2141.29	0.003	-0.002	2158.02	2.024	1.523	2174.77	1.743	1.567
2141.51	0.003	0.004	2158.28	1.933	1.468	2175.02	1.727	1.549
2141.77	0.005	0.004	2158.50	1.862	1.425	2175.30	1.702	1.537
2142.02	0.003	0.010	2158.76	1.751	1.339	2175.50	1.666	1.525
2142.26	0.002	0.004	2159.03	1.685	1.327	2175.77	1.665	1.494
2142.53	0.008	-0.009	2159.28	1.598	1.284	2176.03	1.615	1.464
2142.77	-0.002	0.010	2159.52	1.548	1.235	2176.27	1.609	1.464
2143.02	0.006	-0.003	2159.75	1.517	1.222	2176.52	1.594	1.421
2143.25	-0.002	0.010	2159.95	1.451	1.211	2176.79	1.553	1.409
2143.53	0.012	-0.003	2160.27	1.420	1.180	2177.00	1.557	1.397
2143.77	0.007	0.003	2160.52	1.390	1.180	2177.26	1.532	1.360
2144.02	0.000	-0.009	2160.78	1.374	1.181	2177.54	1.486	1.318
2144.24	0.010	0.009	2161.02	1.368	1.175	2177.75	1.486	1.324
2144.54	0.009	0.009	2161.25	1.388	1.181	2178.02	1.450	1.294
2144.75	0.005	0.016	2161.52	1.403	1.213	2178.28	1.439	1.269
2145.02	0.011	0.003	2161.77	1.428	1.238	2178.51	1.409	1.282
2145.27	0.014	-0.003	2162.02	1.468	1.269	2178.76	1.378	1.258
2145.51	0.009	0.009	2162.28	1.513	1.307	2179.00	1.362	1.258
2145.80	0.008	0.003	2162.51	1.557	1.338	2179.31	1.362	1.221
2146.01	0.023	0.009	2162.76	1.592	1.369	2179.51	1.336	1.209
2146.25	0.013	0.021	2163.01	1.637	1.407	2179.77	1.306	1.203
2146.53	0.014	0.015	2163.30	1.682	1.451	2180.02	1.290	1.191
2146.79	0.017	0.021	2163.51	1.712	1.439	2180.26	1.269	1.161
2147.02	0.017	0.015	2163.77	1.742	1.451	2180.50	1.254	1.149
2147.24	0.027	0.015	2164.02	1.736	1.452	2180.79	1.228	1.118
2147.56	0.032	0.021	2164.27	1.756	1.489	2181.01	1.213	1.119
2147.74	0.027	0.027	2164.50	1.741	1.465	2181.27	1.187	1.107
2148.02	0.037	0.021	2164.80	1.745	1.453	2181.50	1.166	1.107
2148.28	0.042	0.033	2165.00	1.709	1.472	2181.78	1.156	1.064
2148.52	0.042	0.039	2165.29	1.674	1.460	2182.02	1.150	1.077
2148.75	0.047	0.027	2165.50	1.658	1.454	2182.26	1.150	1.059
2149.01	0.057	0.052	2165.78	1.622	1.454	2182.48	1.144	1.047
2149.27	0.062	0.039	2166.01	1.612	1.442	2182.75	1.114	1.041
2149.54	0.067	0.064	2166.28	1.586	1.449	2183.05	1.098	1.029
2149.76	0.082	0.058	2166.51	1.591	1.443	2183.24	1.098	1.023
2150.03	0.087	0.076	2166.77	1.575	1.468	2183.53	1.087	1.023
2150.26	0.097	0.070	2167.03	1.565	1.475	2183.76	1.072	1.018
2150.52	0.137	0.101	2167.25	1.585	1.500	2184.03	1.071	0.999
2150.79	0.147	0.113	2167.50	1.579	1.519	2184.25	1.071	0.994
2151.01	0.167	0.132	2167.81	1.578	1.550	2184.52	1.055	1.000
2151.28	0.218	0.169	2168.01	1.603	1.557	2184.75	1.070	0.994
2151.51	0.268	0.200	2168.27	1.618	1.600	2185.06	1.054	0.982
2151.76	0.349	0.255	2168.50	1.638	1.644	2185.27	1.064	0.989
2152.03	0.490	0.354	2168.79	1.647	1.663	2185.52	1.028	1.008
2152.26	0.666	0.447	2169.03	1.672	1.682	2185.70	1.043	0.977
2152.52	0.994	0.670	2169.25	1.687	1.689	2186.07	1.042	0.978
2152.78	1.402	0.948	2169.49	1.722	1.726	2186.25	1.037	0.978
2153.02	1.952	1.282	2169.77	1.747	1.751	2186.53	1.037	0.997
2153.27	2.647	1.777	2170.04	1.756	1.721	2186.76	1.041	0.991
2153.49	3.414	2.408	2170.25	1.791	1.746	2187.04	1.046	0.985
2153.80	4.366	3.367	2170.52	1.821	1.746	2187.26	1.035	0.980
2154.01	4.905	4.128	2170.77	1.846	1.740	2187.51	1.040	0.986
2154.27	5.358	4.908	2171.05	1.875	1.735	2187.77	1.039	0.993
2154.53	5.459	5.459	2171.25	1.875	1.753	2188.04	1.039	0.987
2154.76	5.307	5.620	2171.51	1.890	1.717	2188.26	1.064	0.993
2155.03	4.903	5.379	2171.77	1.889	1.723	2188.53	1.038	0.994
2155.26	4.424	4.971	2172.03	1.904	1.699	2188.77	1.038	0.988
2155.54	3.788	4.291	2172.26	1.898	1.687	2189.00	1.037	0.988
2155.75	3.354	3.617	2172.51	1.908	1.718	2189.29	1.027	1.001
2156.03	2.905	2.974	2172.69	1.883	1.688	2189.50	1.036	0.995
2156.28	2.597	2.473	2173.03	1.892	1.663	2189.78	1.041	1.014
2156.52	2.440	2.183	2173.27	1.882	1.645	2190.01	1.041	1.002

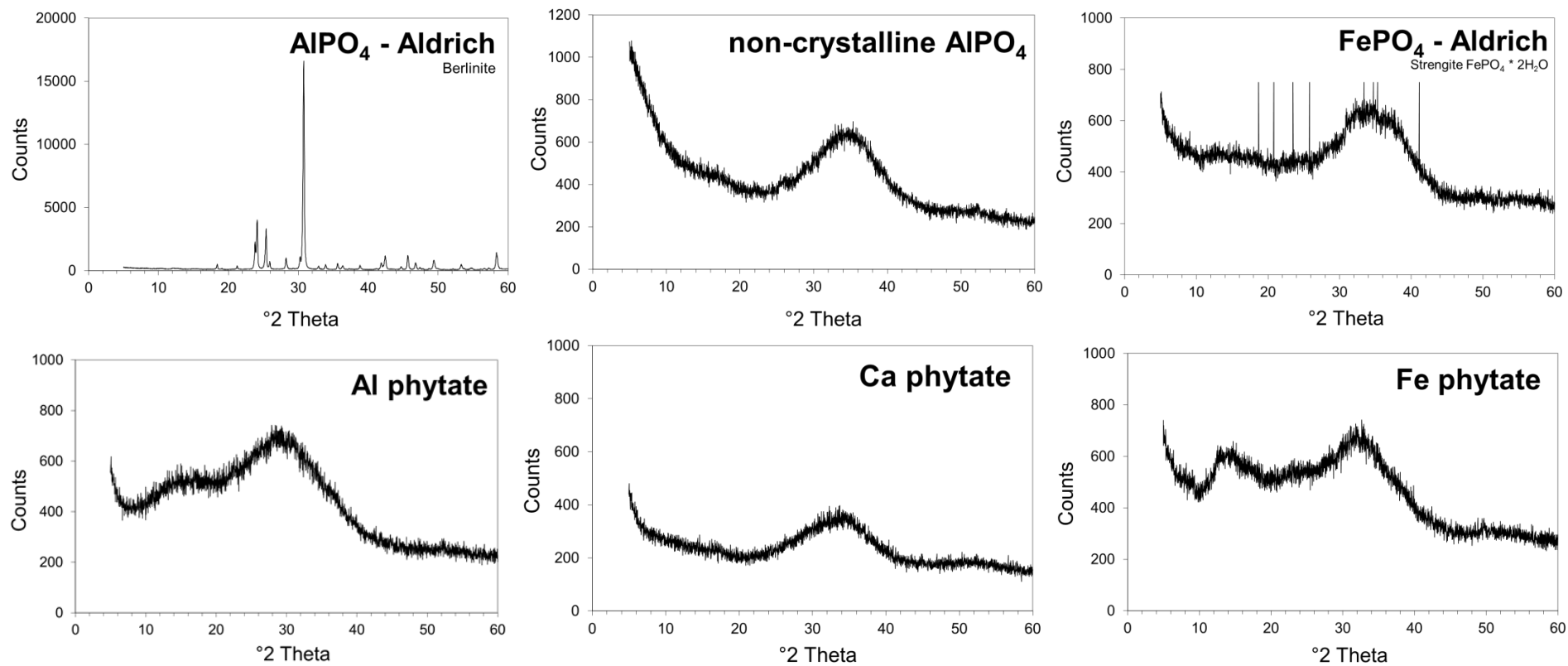


Figure S1 X-ray diffraction spectra for different P compounds investigated in our study.

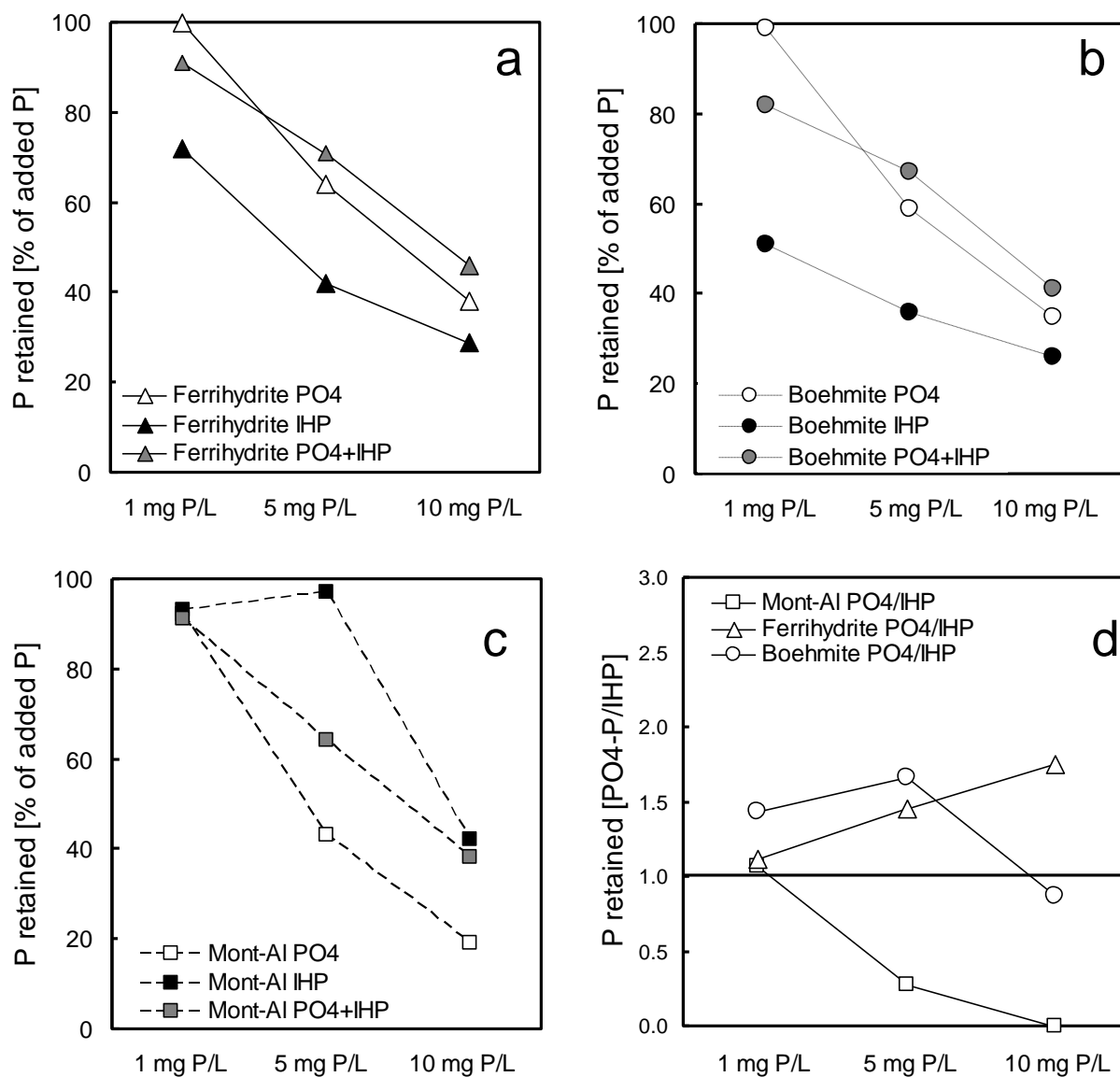


Figure S2 Percentage of retained P after addition of equal amounts of orthophosphate P (NaH_2PO_4), inositol hexakisphosphate (IHP) P, and a 1:1 molar orthophosphate:IHP mixture (initial solution concentrations 1, 5, and 10 mg P L^{-1} ; 100 mL; background 0.1 M NaCl; initial pH 5.0) to 30 mg (a) ferrihydrite, (b) boehmite, and (c) Al-saturated montmorillonite (“Mont-Al”). Additionally shown is (d) the ratio of retained orthophosphate P and IHP-P for the experimental variant with orthophosphate/IHP mixture.

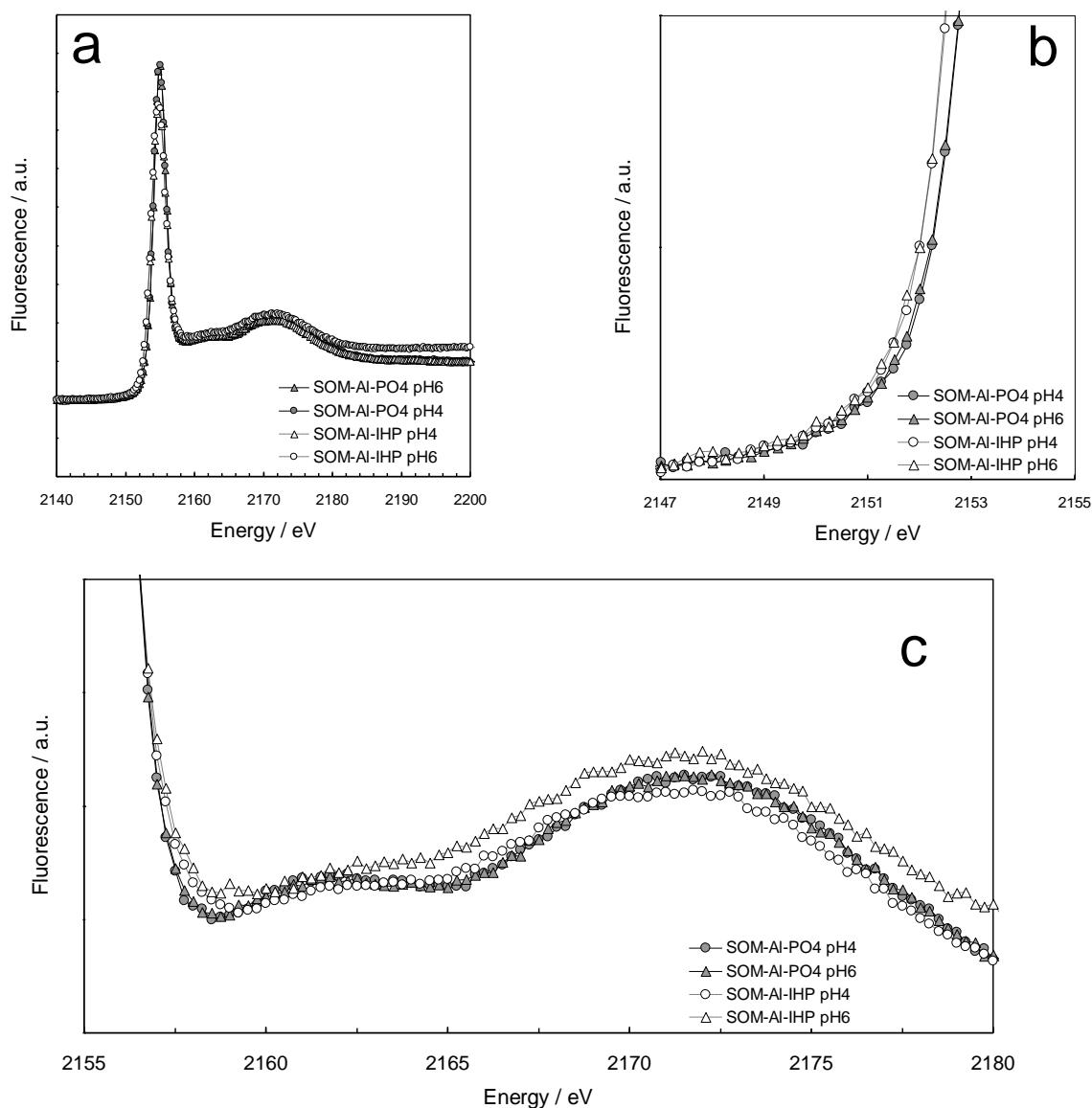


Figure S3 Phosphorus *K*-edge XANES spectra of orthophosphate and inositol hexakisphosphate (IHP) retained by Al-saturated soil organic matter (SOM from O layer of forest soil Waldsassen, Germany) at initial pH values of 4.0 and 6.0, respectively. (a) entire spectra, (b) close-up view of pre-edge region, (c) close-up view of post-edge region.

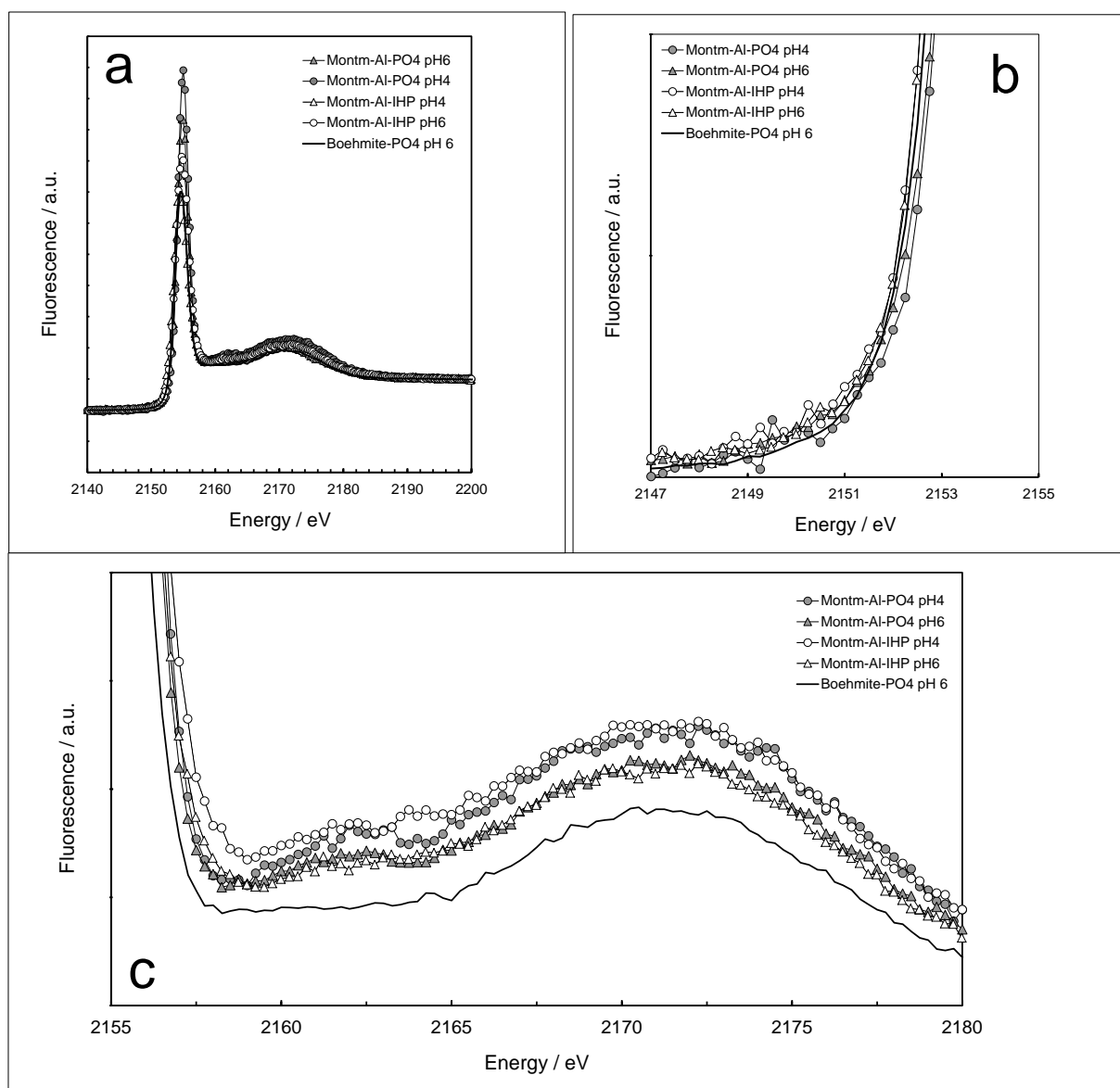


Figure S4 Phosphorus *K*-edge XANES spectra of orthophosphate and inositol hexakisphosphate (IHP) retained by Al-saturated montmorillonite at initial pH values of 4.0 and 6.0, respectively. (a) entire spectra, (b) close-up view of pre-edge region, (c) close-up view of post-edge oscillation region.