Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Structure of tetralithium tetrametaphosphate pentahydrate

M. T. Averbuch-Pouchot and A. Durif

Supplement to *Acta Cryst.* (1986). C**42**, 129–131 **SUP42467**

Supplementary Table 1. Analysis of anisotropic temperature factor data - r.m.s. amplitudes (amp) [Å] and angles [°] with crystallographic axes (deviations of amp < 0.003 Å deviation of angles < 0.3 °).

For symmetrical reasons the thermal vibration ellipsoids around Pb and N are rotation ellipsoids, therefore only the direction of the rotation axis is given.

atom	amp	angle with a	b	c
Pb	0.142			
	0.142			
	0.143	54.7	54.7	54.7
N	0.139			
	0.139			
	0.148		ac Pb	
O	0.155	110.1	102.2	43.8
	0.164	129.0	39.2	93.3
	0.217	45.8	56.5	66.5

Supplementary Table 2. Structure Factors (observed and calculated), weights, differences ($F_{obs} - F_{calc}$), weights, and reflection factors.

[illegible]

[illegible] reflection rejected ($F_{obs} - F_{calc}$ / weight > 4σ)

[illegible] reflection rejected (observed intensity by less than 2 sigma)

PB(NO3)2 LEAD NITRATE SACLAY 06/84 w = 0.0103

H	K	L	F(OBS)	F(CALC)	DELTA/SIGMA	EXT. FACTOR	
1	1	1	16.375	15.809	2.7638	.9567	
0	0	2	24.153	23.896	.8647	.9161	
1	0	2	65.772	64.868	1.2776	.5767	
1	1	2	48.306	47.219	2.0652	.7562	
0	2	2	3.295	3.256	3.3818	.9988	*
1	2	2	16.648	16.977	-1.3094	.9707	
2	2	2	92.108	92.385	-.2825	.4939	
1	1	3	57.653	57.103	.8793	.7405	
2	1	3	4.742	4.756	-.0263	.9981	
0	2	3	5.475	5.693	2.0161	.9972	
1	2	3	36.843	36.295	1.3509	.8964	
2	2	3	12.554	12.025	2.0841	.9891	
1	3	3	6.325	6.027	.8406	.9974	
2	3	3	29.543	29.225	.9446	.9442	
3	3	3	45.986	46.766	-1.5774	.8752	
0	0	4	59.700	59.045	1.0103	.7641	
1	0	4	38.617	37.622	2.3130	.8983	
2	0	4	13.714	13.169	2.2395	.9879	
3	0	4	24.903	24.871	.1080	.9616	
1	1	4	44.826	44.650	.3566	.8635	
2	1	4	18.390	18.998	-.3922	.9755	
3	1	4	3.008	3.054	4.2483	.9994	*
0	2	4	27.632	26.973	2.0278	.9502	
1	2	4	26.950	26.383	1.7596	.9533	
2	2	4	12.008	10.697	5.1026	.9926	*
3	2	4	42.947	42.903	-.1174	.8970	
1	3	4	14.396	14.046	1.4492	.9878	
2	3	4	21.697	21.764	-.2345	.9724	
3	3	4	40.323	39.948	.8305	.9160	
0	4	4	94.195	94.590	-.7259	.6128	
1	4	4	13.305	13.681	-1.3400	.9896	
2	4	4	2.736 *	.535	1.8620	1.0000	* *
3	4	4	4.910	1.691	3.2374	.9999	*
4	4	4	30.430	31.171	-2.1510	.9550	
1	1	5	16.170	16.339	-.6538	.9838	
2	1	5	23.198	22.592	2.0640	.9707	
3	1	5	45.304	44.726	1.1507	.8972	
4	1	5	5.397	4.169	1.5763	.9991	
0	2	5	36.843	36.751	.2196	.9233	
1	2	5	22.788	22.552	.8257	.9708	
2	2	5	4.906	4.745	.2860	.9987	
3	2	5	11.462	10.860	1.9438	.9938	
4	2	5	51.376	51.725	-.6153	.8782	
1	3	5	42.984	42.525	.9571	.9065	
2	3	5	50.967	51.461	-.8617	.8708	
3	3	5	43.393	43.409	-.0322	.9108	
4	3	5	37.321	38.017	-1.6209	.9350	
0	4	5	26.609	26.734	-.3781	.9644	
1	4	5	14.191	13.869	1.0627	.9904	
2	4	5	11.940	11.961	-.0715	.9931	
3	4	5	5.536	2.154	3.4895	.9998	*
4	4	5	30.839	31.268	-1.1348	.9578	
1	5	5	4.560	2.675	2.6877	.9997	

PB(NO3)2 LEAD NITRATE SACLAY 06/74 W = 0.0103

H	K	L	F(OBS)	F(CALC)	DELTA/SIGMA	EXT. FACTOR	
2	5	5	10.164	10.189	-.0587	.9953	
3	5	5	32.136	31.826	.7963	.9569	
4	5	5	12.349	12.132	.5852	.9939	
5	5	5	19.309	19.634	-1.1390	.9846	
0	0	6	75.051	73.030	2.6038	.7539	
1	0	6	29.611	29.738	-.3657	.9542	
2	0	6	5.260	3.392	3.2083	.9994	*
3	0	6	35.515	35.793	-.4335	.9396	
4	0	6	5.142	5.773	-.8927	.9985	
5	0	6	60.587	60.759	-.2580	.8540	
1	1	6	19.17[illegible]	19.293	-.3978	.9807	
2	1	6	40.732	40.685	.1038	.9196	
3	1	6	36.093	36.566	-1.1925	.9375	
4	1	6	37.662	37.934	-.6292	.9367	
5	1	6	34.251	34.229	.0524	.9513	
0	2	6	16.511	16.474	.1299	.9862	
1	2	6	5.629	5.106	.8970	.9987	
2	2	6	59.973	60.551	-.8824	.8359	
3	2	6	5.472	5.167	.5050	.9987	
4	2	6	18.645	18.949	-.5130	.9843	
5	2	6	31.058	32.109	-1.1722	.9578	
1	3	6	29.133	29.343	-.5956	.9593	
2	3	6	6.161	5.754	.6977	.9984	
3	3	6	10.917	10.928	-.0325	.9946	
4	3	6	10.760	10.558	.5307	.9952	
5	3	6	17.876	18.045	-.5141	.9868	
0	4	6	12.527	13.271	-1.3910	.9920	
1	4	6	52.399	53.076	-1.1726	.8801	
2	4	6	33.295	33.417	-.3067	.9516	
3	4	6	10.098	10.646	-1.2399	.9951	
4	4	6	44.348	44.921	-1.1312	.9204	
5	4	6	5.049	4.832	.2204	.9991	
1	5	6	33.909	34.200	-.7168	.9513	
2	5	6	42.302	42.378	-.1579	.9276	
3	5	6	22.720	22.872	-.4545	.9789	
4	5	6	25.244	25.130	.3256	.9755	
5	5	6	22.242	22.404	-.4615	.9812	
0	6	6	54.651	54.116	.8787	.9890	
1	6	6	8.051	8.613	-.9279	.9970	
2	6	6	19.104	19.729	-1.7974	.9848	
3	6	6	16.579	16.610	-.0818	.9894	
4	6	6	5.956	2.703	3.6874	.9997	*
5	6	6	9.484	9.425	.1266	.9968	
6	6	6	43.393	43.015	.7825	.9370	
1	1	7	19.240	19.349	-.3682	.9829	
2	1	7	10.096	9.557	.7150	.9956	
3	1	7	42.233	41.957	.5740	.9263	
4	1	7	2.670	4.778	1.1844	.9990	
5	1	7	38.322	39.089	-.5824	.9412	
6	1	7	7.028	6.314	.9631	.9985	
0	2	7	27.564	27.781	-.6277	.9655	
1	2	7	38.549	38.568	-.0434	.9352	
2	2	7	10.166	9.869	.7033	.9957	

PB(NO3)2 LEAD NITRATE SACLAY 66/34 W = 0.0103

H	K	L	F(OBS)	F(CALC)	DELTA/SIGMA	EXT. FACTOR	
1	2	7	7.369	7.751	-.6115	.9974	
4	2	7	5.513	5.080	.4981	.9989	
0	3	7	41.019	41.791	-.3574	.9340	
1	3	7	46.508	46.521	.2793	.9103	
2	3	7	23.334	23.390	-.1671	.9769	
3	3	7	46.668	47.032	-.6891	.9126	
4	3	7	21.424	21.426	-.0072	.9819	
5	3	7	38.549	39.225	-1.4599	.9429	
6	3	7	7.542	7.150	.9745	.9981	
0	4	7	39.914	40.295	-.8202	.9343	
1	4	7	43.461	43.384	.1558	.9247	
2	4	7	22.447	22.687	-.7218	.9792	
3	4	7	15.351	15.090	.7320	.9910	
4	4	7	13.782	13.261	1.3408	.9932	
5	4	7	22.993	23.090	-.3011	.9804	
6	4	7	4.339 *	1.946	1.6123	.9999	* **
1	5	7	37.457	37.946	-1.1077	.9445	
2	5	7	6.219	6.759	-1.8463	.9982	
3	5	7	33.304	33.411	-.1146	.9582	
4	5	7	8.324	8.275	.1055	.9975	
5	5	7	31.249	32.302	-2.7090	.9630	
6	5	7	8.460	9.246	-1.3393	.9970	
0	6	7	6.257	6.268	-.0144	.9985	
1	6	7	21.014	21.119	-.2910	.9833	
3	6	7	11.328	11.334	-.0237	.9953	
4	6	7	16.579	16.566	.0403	.9902	
5	6	7	11.189	11.141	.1051	.9957	
6	6	7	8.001	7.007	2.9557	.9983	
1	7	7	9.757	9.682	.1894	.9966	
2	7	7	7.776	7.439	.5990	.9980	
3	7	7	23.402	23.452	-.1500	.9808	
5	7	7	21.628	21.902	-.7321	.9838	
6	7	7	15.283	15.198	.1885	.9923	
7	7	7	28.353	28.434	-.1322	.9738	
0	0	8	43.325	42.942	.7714	.9253	
1	0	8	38.958	39.257	-.6638	.9375	
2	0	8	3.753 *	2.101	1.3226	.9998	* **
3	0	8	4.940	3.566	1.2727	.9995	
4	0	8	15.078	15.166	-.2273	.9911	
5	0	8	43.598	43.109	.8118	.9330	
6	0	8	16.307	16.089	.6339	.9907	
7	0	8	11.121	11.011	.2409	.9958	
1	1	8	4.776	4.786	-.0149	.9990	
2	1	8	14.601	14.248	.9633	.9917	
3	1	8	57.380	57.939	-.8776	.8751	
4	1	8	16.548	16.606	.1121	.9894	
5	1	8	3.602 *	.594	2.9012	1.0000	* **
6	1	8	4.556	2.444	2.1054	.9998	
7	1	8	7.946	7.337	1.0088	.9981	
0	2	8	21.083	21.273	-.5621	.9815	
1	2	8	49.579	49.406	-1.5086	.9051	
2	2	8	35.274	35.370	-.2255	.9509	
3	2	8	35.547	36.405	-1.9957	.9493	

PB(NO3)2 LEAD NITRATE SACLAY 06/84 w = 0.0103

H	K	L	F(OBS)		F(CALC)	DELTA/SIGMA	EXT. FACTOR	
4	2	8	29.679		30.019	-.9574	.9963	
5	2	8	7.028		6.974	.0944	.9982	
6	2	8	19.309		19.424	-.3543	.9867	
7	2	8	13.168		12.798	.9414	.9944	
1	3	8	19.445		19.969	-1.5215	.9842	
2	3	8	4.592	*	1.895	2.3111	.9999	* **
3	3	8	14.874		15.366	-1.3052	.9909	
5	3	8	5.175		5.143	1.3951	.9990	
6	3	8	3.923	*	3.236	.4401	.9996	* **
7	3	8	29.133		28.831	.7882	.9721	
0	4	8	14.260		14.103	.3826	.9923	
1	4	8	31.999		32.194	-.4785	.9808	
2	4	8	16.784		16.284	1.3725	.9899	
4	4	8	26.950		26.818	.3755	.9741	
5	4	8	23.539		23.854	-.9400	.9800	
6	4	8	6.011		6.318	-.3973	.9986	
7	4	8	25.927		25.847	.2096	.9778	
1	5	8	35.683		35.842	-.3916	.9533	
2	5	8	8.256		7.914	.7339	.9977	
3	5	8	31.317		31.205	.2922	.9454	
5	5	8	12.927		12.679	.3671	.9944	
6	5	8	7.232		8.358	-1.4790	.9976	
7	5	8	27.223		26.977	.6216	.9761	
0	6	8	27.905		28.129	-.6120	.9719	
1	6	8	13.441		12.221	3.6890	.9947	*
2	6	8	15.147		15.462	-.8829	.9915	
3	6	8	23.266		23.766	-1.4174	.9804	
4	6	8	14.123		14.075	.1263	.9932	
5	6	8	26.200		26.355	-.4100	.9767	
6	6	8	16.490		16.987	-1.1639	.9881	
7	6	8	16.443		15.379	2.3344	.9923	
1	7	8	11.189		10.432	1.9286	.9962	
2	7	8	5.354		5.198	.7858	.9991	
3	7	8	4.326	*	.591	1.6990	1.0000	* **
4	7	8	8.529		7.378	1.8346	.9982	
5	7	8	6.338		4.686	1.7636	.9993	
6	7	8	6.223		4.313	2.2136	.9994	
0	8	8	12.213		12.791	-1.2191	.9945	
1	8	8	5.274		4.875	.3864	.9992	
2	8	8	24.630		24.905	-.6982	.9795	
3	8	8	6.700		6.748	-.0529	.9985	
4	8	8	10.985		10.503	.9743	.9964	
5	8	8	10.917		11.205	-.4393	.9959	
1	1	9	23.607		23.848	-.6775	.9785	
2	1	9	19.558		19.126	1.1941	.9877	
3	1	9	16.511		16.919	-1.2696	.9894	
4	1	9	13.782		12.885	2.4710	.9940	
5	1	9	4.735	*	2.649	1.3352	.9998	* **
6	1	9	6.727		6.848	-.1511	.9984	
7	1	9	38.413		38.327	.1856	.9520	
8	1	9	7.096		7.329	-.2452	.9982	
0	2	9	37.562		37.772	-.2438	.9473	
1	2	9	10.848		11.219	-.7886	.9953	

PB(NO3)2 LEAD NITRATE SACLAY 06/84 w = 0.0103

H	K	L	F(OBS)		F(CALC)	DELTA/SIGMA	EXT. FACTOR	
3	2	0	11.567		11.553	.2942	.9951	
4	2	0	18.080		18.252	-.5114	.9881	
5	2	0	27.496		26.993	1.3568	.9748	
6	2	0	11.940		12.114	-.3576	.9950	
7	2	0	4.328	*	3.454	.3660	.9996	* **
8	2	0	5.950		4.681	1.0149	.9992	
1	3	0	9.484		9.791	-.8055	.9965	
2	3	0	32.272		32.689	-1.0787	.9615	
3	3	0	51.239		51.486	-.4323	.9089	
4	3	0	27.769		28.324	-1.5238	.9720	
5	3	0	13.577		13.795	-.5530	.9934	
6	3	0	7.437		6.965	.7794	.9984	
7	3	0	6.175		5.463	.7434	.9990	
8	3	0	9.415		9.430	-.0198	.9971	
0	4	0	25.381		24.579	2.3239	.9783	
1	4	0	14.737		14.341	1.2207	.9926	
2	4	0	25.586		25.860	-.7817	.9763	
3	4	0	3.616	*	1.074	1.2338	1.0000	* **
4	4	0	11.258		10.758	1.1228	.9960	
5	4	0	15.929		16.176	-.9026	.9911	
6	4	0	5.963		2.245	3.2198	.9998	*
1	5	0	7.164		6.783	.7002	.9984	
2	5	0	4.747		2.769	1.8648	.9997	
3	5	0	21.287		21.660	-1.0495	.9839	
4	5	0	10.848		10.168	1.3684	.9965	
5	5	0	5.515		5.290	.3257	.9991	
6	5	0	23.880		23.639	.5725	.9820	
0	6	0	3.591	*	2.437	.1898	.9996	* **
1	6	0	25.814		26.668	.4234	.9759	
2	6	0	21.424		21.486	-.1730	.9844	
3	6	0	4.169	*	4.582	-.2897	.9993	* **
4	6	0	10.849		10.196	1.7895	.9890	
5	6	0	4.537	*	.947	1.7426	1.0000	* **
6	6	0	23.880		23.667	.4993	.9819	
1	7	0	34.251		33.933	.7666	.9621	
2	7	0	16.102		16.226	-.2648	.9913	
3	7	0	7.232		6.504	.8785	.9986	
5	7	0	18.595		18.035	1.4574	.9895	
0	8	0	16.784		16.983	-.4483	.9906	
1	8	0	7.096		7.424	-.3352	.9982	
2	8	0	7.028		8.652	-1.8257	.9976	
3	8	0	14.806		14.649	.3168	.9930	
0	0	10	18.012		1.640	28.6329	.9999	*
1	0	10	34.560		34.555	.2568	.9581	
2	0	10	38.517		38.397	.4919	.9489	
3	0	10	23.607		23.185	1.2029	.9813	
4	0	10	52.263		51.955	.5243	.9112	
5	0	10	26.577		26.145	1.3754	.9771	
7	0	10	4.735	*	1.033	1.7065	1.0000	* **
1	1	10	12.640		12.499	.5853	.9944	
2	1	10	23.334		23.541	-.6181	.9805	
3	1	10	4.326	*	.157	2.4436	1.0000	* **
4	1	10	17.396		17.400	-.0039	.9896	

PB(NO3)2 LEAD NITRATE SACLAY 06/84 W = 0.0103

H	K	L	F(OBS)		F(CALC)	DELTA/SIGMA	EXT. FACTOR	
[illegible]	1	10	18.831		19.366	1.2209	.9867	
[illegible]	1	10	23.264		23.294	-.0722	.9821	
7	1	10	13.033		13.198	-.3222	.9943	
0	2	10	20.573		21.739	-3.2276	.9833	*
1	2	10	6.407		6.259	.2450	.9986	
2	2	10	4.626		3.942	.6340	.9995	
3	2	10	3.616	*	1.107	1.7266	1.0000	* **
4	2	10	3.425	*	.155	1.9171	1.0000	* **
5	2	10	14.942		14.291	1.5325	.9932	
6	2	10	16.170		16.349	-.4098	.9912	
7	2	10	6.257	*	1.050	3.2282	1.0000	* **
1	3	10	10.644		9.965	1.6453	.9965	
2	3	10	13.509		13.319	.4840	.9939	
3	3	10	5.103		3.773	1.2694	.9995	
4	3	10	4.237	*	4.735	-.3491	.9992	* **
5	3	10	9.620		9.126	.7864	.9972	
6	3	10	4.994	*	2.348	1.6938	.9998	* **
0	4	10	52.195		52.367	-.2944	.9099	
1	4	10	24.085		24.455	-1.1052	.9796	
2	4	10	14.191		13.676	1.3225	.9936	
3	4	10	11.872		12.641	-1.6259	.9946	
5	4	10	14.191		13.439	1.7057	.9940	
6	4	10	39.952		39.616	.7515	.9500	
1	5	10	11.258		11.092	.3732	.9958	
2	5	10	31.044		31.201	-.3859	.9678	
4	5	10	15.102		15.934	.6330	.9917	
5	5	10	13.919		13.811	.2074	.9938	
0	6	10	5.922		5.054	.7942	.9992	
1	6	10	5.172		1.369	3.2001	.9999	*
2	6	10	15.351		14.752	1.3648	.9928	
3	6	10	6.482		6.066	.4342	.9988	
4	6	10	33.022		33.256	-.5300	.9645	
2	7	10	8.254		7.961	.3556	.9979	
1	1	11	25.244		25.039	.5975	.9789	
2	1	11	11.735		10.712	2.1644	.9961	
3	1	11	4.837	*	1.974	2.0987	.9999	* **
5	1	11	21.424		21.022	.9741	.9856	
0	2	11	14.464		14.267	.4890	.9931	
1	2	11	15.692		15.219	1.3440	.9922	
2	2	11	5.295		5.142	.1547	.9991	
3	2	11	5.254		3.417	1.5725	.9996	
4	2	11	27.532		27.483	.3783	.9753	
5	2	11	11.739		10.851	1.4921	.9962	
1	3	11	9.006		8.808	.3625	.9974	
2	3	11	21.901		21.957	-.1425	.9840	
3	3	11	20.332		20.623	-.7590	.9860	
4	3	11	13.350		14.493	-1.2719	.9931	
5	3	11	22.799	*	22.656	.3100	.9834	
0	4	11	4.735	*	4.221	.2367	.9994	* **
1	4	11	4.496	*	.322	2.9276	1.0000	* **
2	4	11	4.574	*	.524	2.2779	1.0000	* **
3	4	11	9.143		8.593	.7609	.9976	
4	4	11	27.564		26.756	1.9102	.9769	

PB(NO3)2 LEAD NITRATE SACLAY 06/84 w = 0.0103

H	K	L	F(OBS)	F(CALC)	DELTA/SIGMA	EXT. FACTOR
1	5	11	16.352	16.721	.2697	.9909
2	5	11	8.362	7.776	.8134	.9980
3	5	11	13.441	13.730	-.5200	.9939
0	6	11	32.954	33.344	-.8089	.9645
0	0	12	11.940	10.206	3.1231	.9965
1	0	12	15.078	14.264	2.0697	.9933
2	0	12	7.345	7.420	.5013	.9982
3	0	12	15.829	16.614	-1.6385	.9910
1	1	12	12.590	12.240	1.0037	.9951
2	1	12	7.300	7.420	-.1365	.9982
3	1	12	11.121	11.392	-.7455	.9956
0	2	12	17.398	17.093	.7243	.9905
1	2	12	13.309	12.918	.8694	.9945
2	2	12	24.016	23.809	.5188	.9817
3	2	12	21.014	20.470	1.0497	.9865
1	3	12	4.059	4.069	.9972	.9993