Supplementary Information

for

$Pb_9Cu(PO_4)_6O$: A Room-Temperature Superconductor? Electronic-Structure Features Assessed via the Flat/Steep Band Model

Guoliang Liu[a,b,c], Xiyue Cheng*[a,c], Minwei Xiang[a,b,c], Zhian Li[a,b,c], and Shuiquan Deng*[a,c]

[a] State Key Laboratory of Functional Crystals and Devices, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, Fujian, P. R. China.

[b] Fujian Normal University, College of Chemistry and Materials Science.

[c] Fujian College, University of Chinese Academy of Sciences

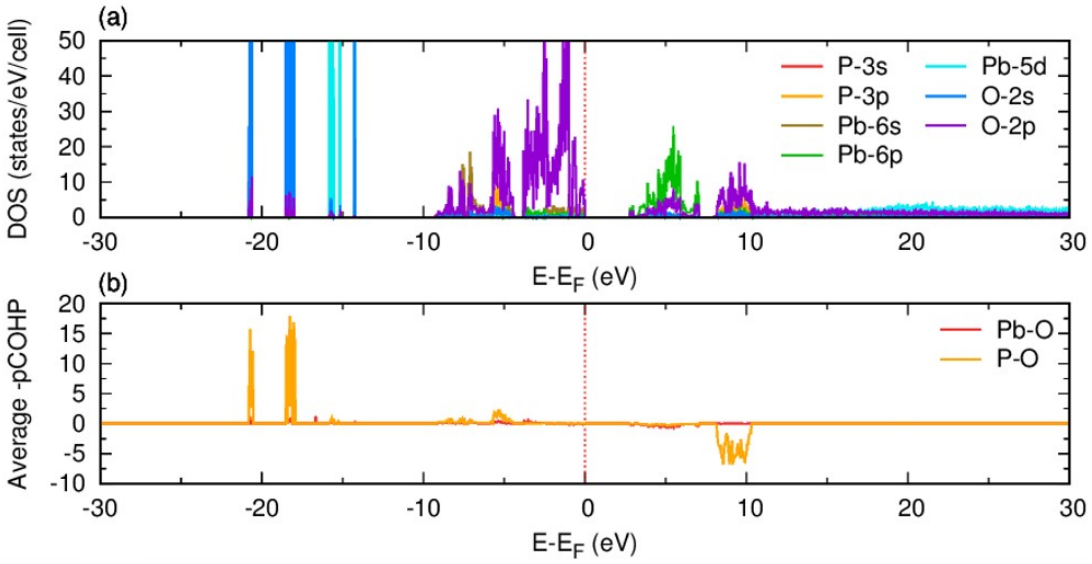

Figure S1. (a) Density of states (DOS) of defect-free $Pb_{10}(PO_4)_6O$. (b) The average -pCOHP of defect-free $Pb_{10}(PO_4)_6O$.

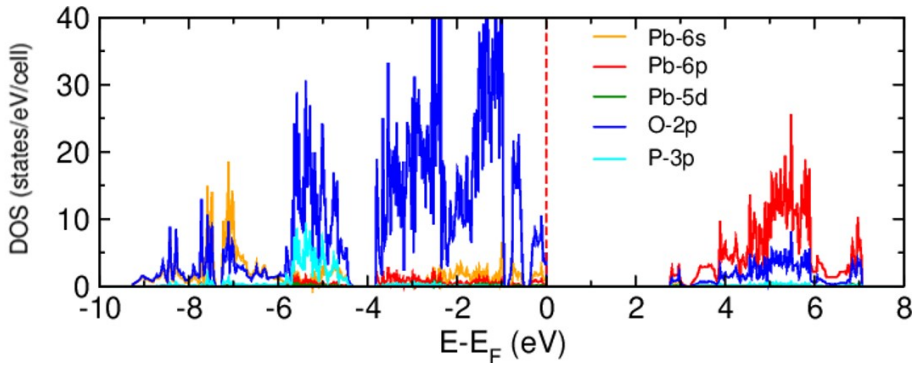

Figure S2. DOS of defect-free $Pb_{10}(PO_4)_6O$ with SOC.

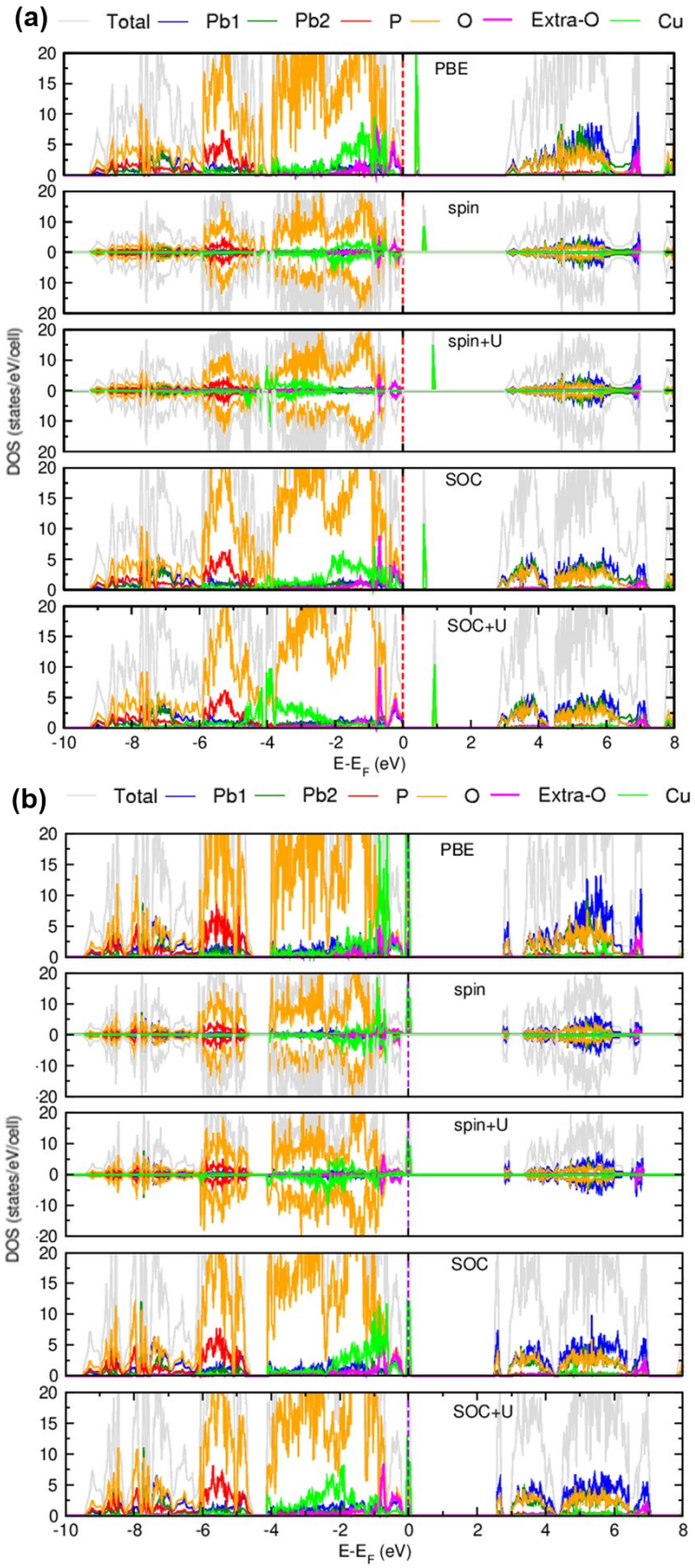

Figure S3. DOS with five distinct levels. (a) DOS of mod1-00. (b) DOS of mod2-00.

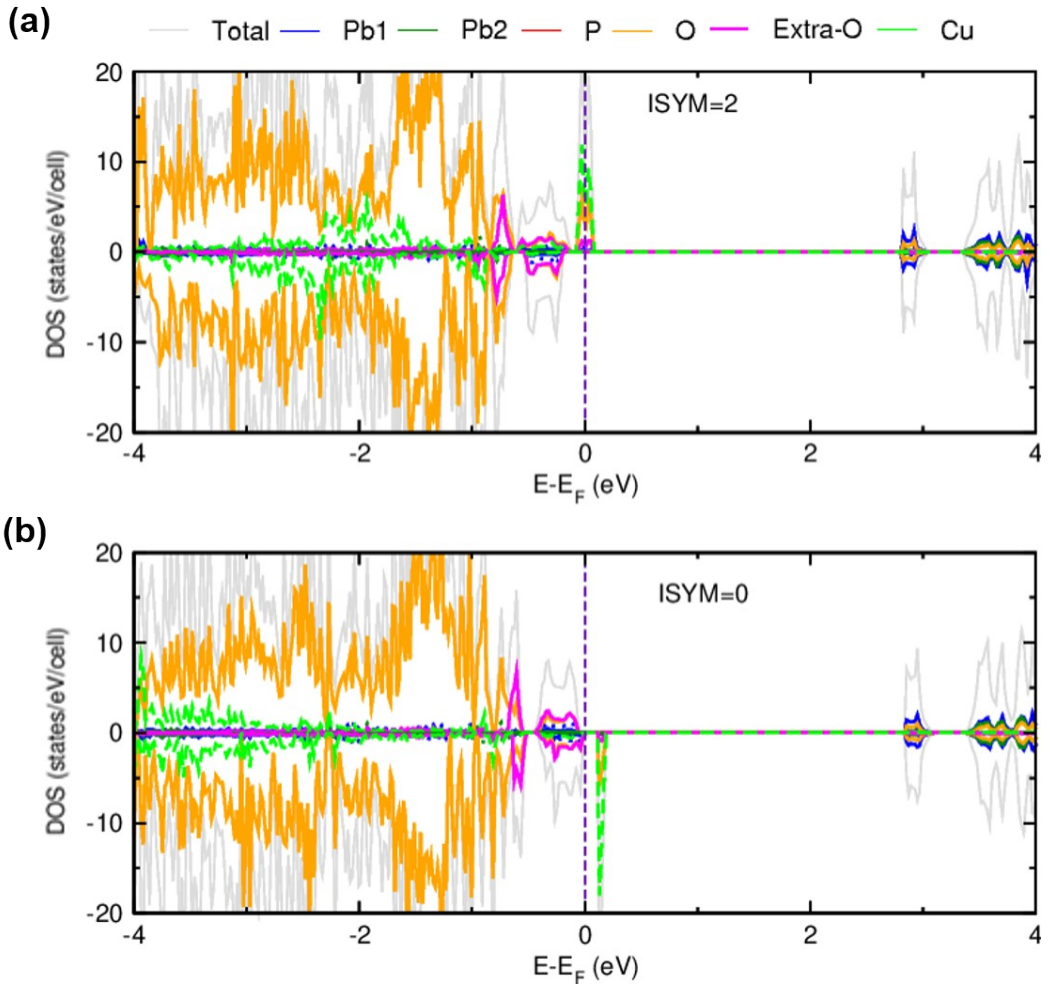

Figure S4. (a) DOS of mod2-00 (without symmetry breaking). (b) DOS of mod2-00 (with symmetry breaking).

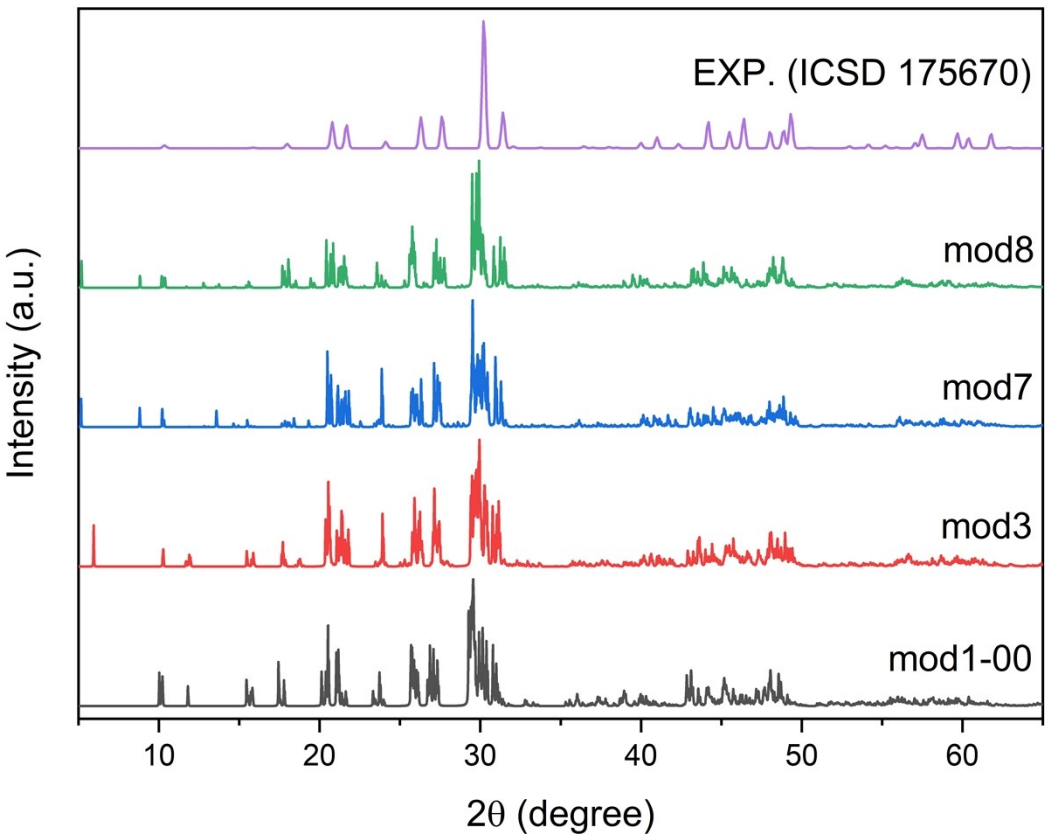

Figure S5. Simulated XRD patterns for mod1-00, mod3, mod7, mod8 and the experimentally reported XRD pattern for $Pb_{7.629}Cu_{2.371}(PO_4)_6O$ from ICSD.

Table S1. Atomic coordinates and Wyckoff positions for the undoped $Pb_{10}(PO_4)_6O$ compound. Lattice parameters: a = b = 9.865 Å, c = 7.431 Å, α = β = 90°, γ = 120°. Space group: $P6_3/m$.

Atoms	Wyckoff sites	x	y	Z	Occupation
Pb1	6h	0.00056	0.75351	0.25	1
Pb2	4f	0.66667	0.33333	-0.00353	1
P1	6h	0.6274	0.5981	0.25	1
O1	6h	0.5134	0.6639	0.25	1
O2	12i	0.7358	0.6528	0.08333	1
O3	6h	0.5306	0.4147	0.25	1
O4	4e	0	0	0.1342	0.25

Table S2. Atomic coordinates and Wyckoff positions for defect-free $Pb_{10}(PO_4)_6O$ compound. Lattice parameters: a = b = 10.021 Å, c = 7.485 Å, α = β = 90°, γ = 120°. Space group: $P3$.

Atoms	Wyckoff sites	x	y	Z	Occupation
P1	3d	0.62377	0.59502	0.25145	1
P2	3d	0.02771	0.63218	0.75179	1
Pb1	3d	0.99568	0.77103	0.25832	1
Pb2	3d	0.25759	0.99379	0.75606	1
O1	3d	0.50031	0.64584	0.25275	1
O2	3d	0.85023	0.53051	0.75124	1
O3	3d	0.73025	0.65968	0.08374	1
O4	3d	0.09035	0.73805	0.58377	1
O5	3d	0.25913	0.34841	0.91755	1
O6	3d	0.92611	0.27063	0.42026	1
O7	3d	0.5448	0.41512	0.24894	1
O8	3d	0.10393	0.52685	0.75479	1
Pb3	1c	0.66667	0.33333	0.00449	1
Pb4	1c	0.66667	0.33333	0.49572	1
Pb5	1b	0.33333	0.66667	0.49129	1
Pb6	1b	0.33333	0.66667	0.01177	1
O9	1a	0	0	0.27053	1

Table S3. The Coulomb energy and relaxed total energy of mod1-00, mod1-01, mod2-00, mod2-01, mod2-02, and mod2-03.

Model	Coulomb energy (eV)	Relaxed total energy (eV)
mod1-00	-1762.468	-266.245
mod1-01	-1762.468	-266.154
mod2-00	-1762.468	-265.890
mod2-01	-1762.468	-265.684
mod2-02	-1762.468	-265.685
mod2-03	-1762.468	-265.886

Table S4. Atomic coordinates and Wyckoff positions for mod1-00. Lattice parameters: a = 7.495 Å, b = 9.969 Å, c = 10.096 Å, α = 60.853°, β = 89.025°, γ = 88.659°. Space group: *P*1.

Atoms	Wyckoff sites	x	y	Z	Occupation
O1	1a	0.26449	0.36495	0.48155	1
O2	1a	0.75935	0.48073	0.85638	1
O3	1a	0.25252	0.14218	0.35803	1
O4	1a	0.73784	0.7051	0.46242	1
O5	1a	0.24017	0.49565	0.14525	1
O6	1a	0.75535	0.85409	0.69863	1
O7	1a	0.18256	0.28508	0.75335	1
O8	1a	0.58618	0.27541	0.09011	1
O9	1a	0.07849	0.92526	0.35231	1
O10	1a	0.58807	0.62237	0.28424	1
O11	1a	0.07328	0.72535	0.93063	1
O12	1a	0.56062	0.08502	0.66683	1
O13	1a	0.90764	0.69863	0.24391	1
O14	1a	0.41056	0.71943	0.93383	1
O15	1a	0.88122	0.12132	0.63811	1
O16	1a	0.49327	0.39112	0.65595	1
O17	1a	0.91957	0.25114	0.08035	1
O18	1a	0.41359	0.92381	0.33926	1
O19	1a	0.23523	0.57005	0.56411	1
O20	1a	0.77678	0.46619	0.11489	1
O21	1a	0.25432	0.86908	0.58632	1
O22	1a	0.82704	0.45059	0.47781	1
O23	1a	0.24289	0.53647	0.87377	1
O24	1a	0.72205	0.09017	0.43636	1
O25	1a	0.24583	0.98336	0.018	1
P1	1a	0.28965	0.40045	0.61342	1
P2	1a	0.7611	0.36912	0.02818	1
P3	1a	0.25053	0.96717	0.40991	1
P4	1a	0.76086	0.61965	0.36876	1
P5	1a	0.24284	0.61795	0.9731	1
P6	1a	0.73024	0.02864	0.6114	1
Pb1	1a	0.23745	0.21476	0.0145	1
Pb2	1a	0.7466	0.9968	0.2631	1
Pb3	1a	0.24671	0.76378	0.24337	1
Pb4	1a	0.7509	0.73081	0.01069	1
Pb5	1a	0.23428	0.99515	0.7914	1
Pb6	1a	0.00791	0.67157	0.67153	1
Pb7	1a	0.4913	0.3439	0.30274	1
Pb8	1a	0.0143	0.32289	0.35124	1
Pb9	1a	0.50523	0.64673	0.6781	1
Cu1	1a	0.68699	0.27807	0.62616	1

Table S5. Atomic coordinates and Wyckoff positions for mod2-00. Lattice parameters: a = b = 9.867 Å, c = 7.379 Å, α = β = 90°, γ = 120°. Space group: *P*3.

Atoms	Wyckoff sites	x	y	Z	Occupation
O1	3d	0.49505	0.63751	0.2492	1
O2	3d	0.83454	0.52252	0.74104	1
O3	3d	0.71317	0.6172	0.08629	1
O4	3d	0.07864	0.74658	0.58909	1
O5	3d	0.28117	0.36088	0.9247	1
O6	3d	0.9529	0.25137	0.41186	1
O7	3d	0.54925	0.41793	0.33066	1
O8	3d	0.09242	0.51762	0.72582	1
P1	3d	0.62459	0.59187	0.26946	1
P2	3d	0.016	0.62431	0.74574	1
Pb1	3d	0.00019	0.7699	0.24934	1
Pb2	3d	0.2568	0.00355	0.74389	1
O9	1a	0	0	0.1974	1
Cu1	1c	0.66667	0.33333	0.48018	1
Pb3	1c	0.66667	0.33333	0.99239	1
Pb4	1b	0.33333	0.66667	0.49017	1
Pb5	1b	0.33333	0.66667	0.00441	1

Table S6. Atomic coordinates and Wyckoff positions for mod3. Lattice parameters: a = 9.927 Å, b = 10.047 Å, c = 14.878 Å, α = 91.477°, β = 88.414°, γ = 119.880°. Space group: *P*1.

Atoms	Wyckoff sites	x	y	Z	Occupation
Pb1	1a	0.99513	0.75896	0.12059	1
Pb2	1a	0.25937	0.99817	0.37372	1
Pb3	1a	0.22224	0.21174	0.12347	1
Pb4	1a	0.0009	0.2648	0.3735	1
Pb5	1a	0.77625	0.99758	0.12733	1
Pb6	1a	0.7382	0.73602	0.37431	1
Pb7	1a	0.00225	0.78737	0.61985	1
Pb8	1a	0.25229	0.99085	0.87357	1
Pb9	1a	0.23158	0.22794	0.62063	1
Pb10	1a	0.00861	0.25789	0.87364	1
Pb11	1a	0.77178	0.01226	0.62369	1
Pb12	1a	0.66115	0.34931	0.99683	1
Pb13	1a	0.32216	0.66149	0.24722	1
Pb14	1a	0.36032	0.67284	0.00704	1
Pb15	1a	0.6657	0.3265	0.25006	1
Pb16	1a	0.6618	0.32148	0.52122	1
Pb17	1a	0.30705	0.65846	0.74432	1
Pb18	1a	0.33896	0.67333	0.5029	1
O1	1a	0.50938	0.65103	0.12925	1
O2	1a	0.84423	0.53119	0.37856	1
O3	1a	0.36509	0.85291	0.12578	1
O4	1a	0.465	0.31341	0.37266	1
O5	1a	0.1521	0.50025	0.12709	1
O6	1a	0.67661	0.15105	0.38444	1
O7	1a	0.48282	0.63204	0.62298	1
O8	1a	0.84016	0.51521	0.8632	1
O9	1a	0.35142	0.85285	0.62347	1
O10	1a	0.50593	0.33038	0.83785	1
O11	1a	0.13176	0.51223	0.62885	1
O12	1a	0.71117	0.15536	0.9029	1
O13	1a	0.73768	0.64023	0.05233	1
O14	1a	0.0898	0.73521	0.29416	1
O15	1a	0.33138	0.05523	0.04333	1
O16	1a	0.25482	0.34607	0.29234	1
O17	1a	0.96306	0.25333	0.04659	1
O18	1a	0.67429	0.92527	0.29733	1
O19	1a	0.28505	0.29665	0.94194	1
O20	1a	0.92442	0.27651	0.21236	1
O21	1a	0.63754	0.87709	0.94833	1
O22	1a	0.72431	0.64723	0.22092	1

O23	1a	0.06191	0.73425	0.95428	1
O24	1a	0.3482	0.07047	0.21178	1
O25	1a	0.73186	0.6555	0.55341	1
O26	1a	0.09732	0.72622	0.78901	1
O27	1a	0.35794	0.07942	0.53952	1
O28	1a	0.28387	0.37777	0.78412	1
O29	1a	0.90068	0.29296	0.54812	1
O30	1a	0.69084	0.94892	0.79178	1
O31	1a	0.25572	0.34682	0.45997	1
O32	1a	0.94459	0.26541	0.71058	1
O33	1a	0.63225	0.90566	0.46431	1
O34	1a	0.7214	0.70427	0.71877	1
O35	1a	0.08254	0.74211	0.46216	1
O36	1a	0.29872	0.04732	0.70454	1
O37	1a	0.53392	0.40845	0.13634	1
O38	1a	0.09986	0.52672	0.37923	1
O39	1a	0.5881	0.13083	0.11828	1
O40	1a	0.47123	0.57177	0.37595	1
O41	1a	0.87239	0.43915	0.10713	1
O42	1a	0.42349	0.8961	0.36773	1
O43	1a	0.56242	0.4318	0.65605	1
O44	1a	0.098	0.52058	0.88249	1
O45	1a	0.57567	0.12922	0.64179	1
O46	1a	0.48965	0.56279	0.89347	1
O47	1a	0.85462	0.45511	0.66338	1
O48	1a	0.44216	0.92059	0.86937	1
O49	1a	0.99426	0.98558	0.13886	1
O50	1a	0.00069	0.00973	0.59897	1
Cu1	1a	0.64527	0.74424	0.8343	1
Cu2	1a	0.69369	0.42159	0.75715	1
P1	1a	0.62416	0.58753	0.13436	1
P2	1a	0.02279	0.63166	0.37859	1
P3	1a	0.40869	0.02527	0.12461	1
P4	1a	0.36432	0.39107	0.3749	1
P5	1a	0.97936	0.36968	0.12271	1
P6	1a	0.60551	0.97462	0.37837	1
P7	1a	0.62132	0.60542	0.63666	1
P8	1a	0.01843	0.62249	0.8726	1
P9	1a	0.39877	0.02617	0.62878	1
P10	1a	0.3903	0.38997	0.86222	1
P11	1a	0.95933	0.38246	0.63964	1
P12	1a	0.62006	0.98464	0.87902	1

Table S7. Atomic coordinates and Wyckoff positions for mod4. Lattice parameters: a = b = 9.888 Å, c = 14.778 Å, α = β = 90°, γ = 120°. Space group: *P*3

Atoms	Wyckoff sites	x	y	Z	Occupation
P1	3d	0.62358	0.59525	0.12239	1
P2	3d	0.03757	0.64048	0.38534	1
P3	3d	0.61856	0.5913	0.63102	1
P4	3d	0.01334	0.62276	0.86904	1
Pb1	3d	0.99995	0.77077	0.12422	1
Pb2	3d	0.2841	0.00238	0.38565	1
Pb3	3d	0.00016	0.77056	0.6281	1
Pb4	3d	0.24929	0.9968	0.87278	1
O1	3d	0.5003	0.64922	0.12279	1
O2	3d	0.86386	0.51152	0.37782	1
O3	3d	0.48238	0.62513	0.61667	1
O4	3d	0.83218	0.52461	0.85958	1
O5	3d	0.73695	0.66799	0.04041	1
O6	3d	0.10775	0.727	0.29462	1
O7	3d	0.27069	0.3357	0.95457	1
O8	3d	0.92354	0.27612	0.21053	1
O9	3d	0.71157	0.61601	0.54068	1
O10	3d	0.0899	0.73562	0.78734	1
O11	3d	0.23124	0.29166	0.45511	1
O12	3d	0.96616	0.26111	0.70118	1
O13	3d	0.54198	0.41353	0.11614	1
O14	3d	0.13379	0.55916	0.41545	1
O15	3d	0.5534	0.41812	0.66207	1
O16	3d	0.08648	0.51387	0.8749	1
Pb5	1c	0.66667	0.33333	0.98864	1
Pb6	1c	0.66667	0.33333	0.24016	1
Pb7	1c	0.66667	0.33333	0.50656	1
Cu1	1c	0.66667	0.33333	0.74396	1
Pb8	1b	0.33333	0.66667	0.25231	1
Pb9	1b	0.33333	0.66667	0.00487	1
Pb10	1b	0.33333	0.66667	0.73657	1
Cu2	1b	0.33333	0.66667	0.50532	1
O17	1a	0	0	0.12465	1
O18	1a	0	0	0.61755	1

Table S8. Atomic coordinates and Wyckoff positions for mod5. Lattice parameters: a = b = 9.875 Å, c = 14.848 Å, α = β = 90°, γ = 120°. Space group: *P*3

Atoms	Wyckoff sites	x	y	Z	Occupation
Pb1	3d	0.00106	0.77	0.12644	1
Pb2	3d	0.26011	0.00018	0.37712	1
Pb3	3d	0.00197	0.7726	0.63104	1
Pb4	3d	0.2788	0.00016	0.86394	1
P1	3d	0.62552	0.59608	0.12744	1
P2	3d	0.0245	0.63157	0.37918	1
P3	3d	0.6123	0.58735	0.63712	1
P4	3d	0.02683	0.631	0.86496	1
O1	3d	0.50565	0.65457	0.1253	1
O2	3d	0.84419	0.52839	0.38438	1
O3	3d	0.47755	0.62587	0.63752	1
O4	3d	0.85185	0.50055	0.86788	1
O5	3d	0.72942	0.64869	0.04122	1
O6	3d	0.07637	0.74729	0.29801	1
O7	3d	0.29092	0.38463	0.95752	1
O8	3d	0.92812	0.26327	0.21089	1
O9	3d	0.68904	0.61096	0.5427	1
O10	3d	0.04968	0.7664	0.80046	1
O11	3d	0.26674	0.36172	0.46527	1
O12	3d	0.95755	0.25557	0.70288	1
O13	3d	0.53981	0.41408	0.13332	1
O14	3d	0.10011	0.52536	0.36678	1
O15	3d	0.54976	0.41449	0.66824	1
O16	3d	0.12693	0.55542	0.83173	1
Pb5	1c	0.66667	0.33333	0.99719	1
Pb6	1c	0.66667	0.33333	0.25042	1
Pb7	1c	0.66667	0.33333	0.51081	1
Cu1	1c	0.66667	0.33333	0.74893	1
Pb8	1b	0.33333	0.66667	0.24542	1
Pb9	1b	0.33333	0.66667	0.99916	1
Pb10	1b	0.33333	0.66667	0.51552	1
Cu2	1b	0.33333	0.66667	0.74243	1
O17	1a	0	0	0.12376	1
O18	1a	0	0	0.60817	1

Table S9. Atomic coordinates and Wyckoff positions for mod6. Lattice parameters: a = b = 9.906 Å, c = 14.938 Å, α = β = 90°, γ = 120°. Space group: *P*3

Atoms	Wyckoff sites	x	y	Z	Occupation
Pb1	3d	0.99879	0.77078	0.12369	1
Pb2	3d	0.28116	0.99486	0.38776	1
Pb3	3d	0.00335	0.77445	0.62536	1
Pb4	3d	0.27795	0.9963	0.86401	1
P1	3d	0.62638	0.59603	0.12612	1
P2	3d	0.03864	0.63774	0.38937	1
P3	3d	0.61208	0.59903	0.62674	1
P4	3d	0.03682	0.63689	0.86449	1
O1	3d	0.50474	0.65123	0.12448	1
O2	3d	0.86714	0.50383	0.38034	1
O3	3d	0.49446	0.66109	0.62812	1
O4	3d	0.86423	0.50516	0.87105	1
O5	3d	0.7336	0.654	0.04149	1
O6	3d	0.11078	0.71893	0.2987	1
O7	3d	0.2816	0.386	0.9558	1
O8	3d	0.92557	0.26696	0.21059	1
O9	3d	0.7253	0.66509	0.54492	1
O10	3d	0.05549	0.76744	0.7985	1
O11	3d	0.23119	0.28314	0.45309	1
O12	3d	0.93337	0.27875	0.71054	1
O13	3d	0.5425	0.41338	0.12736	1
O14	3d	0.13478	0.56243	0.4278	1
O15	3d	0.53091	0.41765	0.62348	1
O16	3d	0.13463	0.5605	0.83025	1
Pb5	1c	0.66667	0.33333	0.00544	1
Pb6	1c	0.66667	0.33333	0.24923	1
Pb7	1c	0.66667	0.33333	0.5049	1
Pb8	1c	0.66667	0.33333	0.74976	1
Pb9	1b	0.33333	0.66667	0.24801	1
Pb10	1b	0.33333	0.66667	0.00179	1
Cu1	1b	0.33333	0.66667	0.73765	1
Cu2	1b	0.33333	0.66667	0.51913	1
O17	1a	0	0	0.1168	1
O18	1a	0	0	0.63092	1

Table S10. Atomic coordinates and Wyckoff positions for mod7. Lattice parameters: a = 7.454 Å, b = 10.041 Å, c = 17.146 Å, α = 89.932°, β = 91.516°, γ = 91.225°. Space group: *P*1.

Atoms	Wyckoff sites	x	y	Z	Occupation
Pb1	1a	-0.00351	-0.01826	-0.33778	1
Pb2	1a	-0.48216	-0.4962	-0.15271	1
Pb3	1a	-0.01297	-0.01336	-0.66275	1
Pb4	1a	-0.50808	0.00049	-0.67408	1
Pb5	1a	-0.99605	-0.48155	-0.17237	1
Pb6	1a	-0.51333	0.00362	-0.33044	1
Pb7	1a	-0.24893	0.22337	-0.99691	1
Pb8	1a	-0.76777	0.61289	-0.619	1
Pb9	1a	-0.24029	0.36987	-0.64944	1
Pb10	1a	-0.77711	0.74682	-0.99588	1
Pb11	1a	-0.25266	0.36213	-0.37072	1
Pb12	1a	-0.75073	-0.39177	-0.38724	1
Pb13	1a	-0.27817	-0.24246	-0.50403	1
Pb14	1a	-0.7571	-0.8626	-0.1281	1
Pb15	1a	-0.26719	-0.11046	-0.11105	1
Pb16	1a	-0.75719	0.2723	-0.50636	1
Pb17	1a	-0.2492	0.87962	-0.88319	1
Pb18	1a	-0.74266	0.12181	-0.8755	1
P1	1a	-0.25724	-0.28849	-0.31947	1
P2	1a	-0.72798	-0.60054	-0.00135	1
P3	1a	-0.30519	0.66296	-0.69691	1
P4	1a	-0.76877	0.28871	-0.69754	1
P5	1a	-0.20751	0.59061	-0.97588	1
P6	1a	-0.75083	-0.67565	-0.29365	1
P7	1a	-0.23186	0.21343	-0.81822	1
P8	1a	-0.76301	-0.1085	-0.51764	1
P9	1a	-0.2459	0.18127	-0.19969	1
P10	1a	-0.74167	-0.20896	-0.17848	1
P11	1a	-0.25635	0.11464	-0.48628	1
P12	1a	-0.75356	-0.16791	-0.80577	1
Cu1	1a	-0.54432	0.56705	-0.85334	1
Cu2	1a	-0.96123	0.43575	-0.8423	1
O1	1a	-0.2473	-0.40693	-0.26104	1
O2	1a	-0.71903	0.43466	-0.91087	1
O3	1a	-0.28211	-0.18565	-0.67547	1
O4	1a	-0.78943	0.4059	-0.75631	1
O5	1a	-0.22334	-0.44195	-0.06448	1
O6	1a	-0.76118	0.17673	-0.31794	1
O7	1a	-0.25663	0.11915	-0.74786	1
O8	1a	-0.76126	-0.08084	-0.42841	1

O9	1a	-0.25274	-0.67135	-0.17518	1
O10	1a	-0.74856	-0.08387	-0.23229	1
O11	1a	-0.25864	0.0918	-0.57529	1
O12	1a	-0.75226	0.68718	-0.83762	1
O13	1a	-0.08223	-0.27265	-0.36742	1
O14	1a	-0.54596	-0.64671	-0.03226	1
O15	1a	-0.12378	0.59158	-0.68225	1
O16	1a	-0.59255	0.30132	-0.64864	1
O17	1a	-0.08814	0.72059	-0.96604	1
O18	1a	-0.58508	-0.60083	-0.32664	1
O19	1a	-0.92625	0.2824	-0.63878	1
O20	1a	-0.39656	0.62461	-0.94594	1
O21	1a	-0.92156	-0.59716	-0.31829	1
O22	1a	-0.41346	-0.31386	-0.38117	1
O23	1a	-0.86836	-0.71366	-0.01785	1
O24	1a	-0.44056	0.59316	-0.64153	1
O25	1a	-0.07932	0.16969	-0.87263	1
O26	1a	-0.60321	-0.19933	-0.53809	1
O27	1a	-0.07471	0.1124	-0.16649	1
O28	1a	-0.57586	-0.20216	-0.12072	1
O29	1a	-0.08298	0.1897	-0.45582	1
O30	1a	-0.5804	-0.08404	-0.8258	1
O31	1a	-0.91114	-0.21444	-0.12561	1
O32	1a	-0.4178	0.19732	-0.4585	1
O33	1a	-0.90989	-0.0918	-0.84757	1
O34	1a	-0.40518	0.22106	-0.86964	1
O35	1a	-0.94076	-0.18124	-0.5455	1
O36	1a	-0.41169	0.09797	-0.17227	1
O37	1a	-0.28517	-0.15513	-0.27532	1
O38	1a	-0.77763	-0.46945	-0.04681	1
O39	1a	-0.36443	0.64815	-0.78439	1
O40	1a	-0.77129	0.15164	-0.7427	1
O41	1a	-0.12019	0.47272	-0.9316	1
O42	1a	-0.73687	-0.6696	-0.20058	1
O43	1a	-0.17414	0.35499	-0.78402	1
O44	1a	-0.74806	0.02324	-0.56577	1
O45	1a	-0.24657	0.17331	-0.29182	1
O46	1a	-0.73885	-0.33982	-0.22637	1
O47	1a	-0.26626	-0.02608	-0.44417	1
O48	1a	-0.77319	-0.16578	-0.71587	1
O49	1a	-0.30157	0.99423	-0.99574	1
O50	1a	-0.77696	0.49827	-0.50259	1

Table S11. Atomic coordinates and Wyckoff positions for mod8. Lattice parameters: a = 7.453 Å, b = 10.020 Å, c = 17.034 Å, α = 90.843°, β = 89.333°, γ = 90.523°. Space group: *P*1.

Atoms	Wyckoff sites	x	y	Z	Occupation
Cu1	1a	-0.83398	-0.42062	-0.36658	1
Cu2	1a	-0.14317	-0.21985	-0.47002	1
P1	1a	-0.2133	-0.2952	-0.32611	1
P2	1a	-0.75457	-0.61844	-0.01206	1
P3	1a	-0.26052	0.67011	-0.69303	1
P4	1a	-0.75813	0.2992	-0.68253	1
P5	1a	-0.25101	0.61391	-0.98718	1
P6	1a	-0.72769	-0.68598	-0.29505	1
P7	1a	-0.2596	0.21916	-0.80865	1
P8	1a	-0.77287	-0.0945	-0.51556	1
P9	1a	-0.25489	0.17317	-0.20233	1
P10	1a	-0.75143	-0.23222	-0.19888	1
P11	1a	-0.24573	0.1083	-0.48939	1
P12	1a	-0.75694	-0.16472	-0.80641	1
Pb1	1a	-0.25749	0.23617	-0.99676	1
Pb2	1a	-0.77791	-0.37998	-0.59596	1
Pb3	1a	-0.27281	0.38324	-0.62347	1
Pb4	1a	-0.74859	-0.2635	-0.00662	1
Pb5	1a	-0.26304	0.36087	-0.37708	1
Pb6	1a	-0.73825	-0.86762	-0.12688	1
Pb7	1a	-0.25376	-0.1102	-0.11557	1
Pb8	1a	-0.78573	0.28319	-0.49593	1
Pb9	1a	-0.25831	-0.11166	-0.88687	1
Pb10	1a	-0.75105	0.13381	-0.86368	1
Pb11	1a	-0.98427	-0.00544	-0.3262	1
Pb12	1a	-0.48936	-0.48581	-0.17779	1
Pb13	1a	-0.02133	-0.0084	-0.67165	1
Pb14	1a	-0.50615	0.51068	-0.82723	1
Pb15	1a	-0.00682	0.50829	-0.82978	1
Pb16	1a	-0.51297	-0.02044	-0.65958	1
Pb17	1a	-0.00506	-0.50652	-0.16113	1
Pb18	1a	-0.49572	-0.01024	-0.34447	1
O1	1a	-0.23062	-0.42057	-0.27436	1
O2	1a	-0.76056	0.4073	-0.92276	1
O3	1a	-0.26594	-0.18356	-0.66241	1
O4	1a	-0.75896	0.41326	-0.74276	1
O5	1a	-0.24888	-0.42623	-0.0759	1
O6	1a	-0.73461	0.16661	-0.32249	1
O7	1a	-0.26056	0.09697	-0.75501	1
O8	1a	-0.76003	-0.07098	-0.42644	1

O9	1a	-0.25237	-0.68251	-0.16939	1
O10	1a	-0.74956	-0.09881	-0.244	1
O11	1a	-0.25229	0.09706	-0.57981	1
O12	1a	-0.75651	0.69519	-0.84797	1
O13	1a	-0.01557	-0.27408	-0.3584	1
O14	1a	-0.59666	-0.71042	-0.0365	1
O15	1a	-0.09479	0.59458	-0.6627	1
O16	1a	-0.59154	0.3045	-0.62962	1
O17	1a	-0.08199	0.698	-0.96651	1
O18	1a	-0.55336	-0.61405	-0.31804	1
O19	1a	-0.92252	0.30719	-0.62606	1
O20	1a	-0.41708	0.70148	-0.96773	1
O21	1a	-0.88923	-0.60908	-0.3273	1
O22	1a	-0.31835	-0.31103	-0.40484	1
O23	1a	-0.92497	-0.68714	-0.04506	1
O24	1a	-0.4273	0.58706	-0.66681	1
O25	1a	-0.09305	0.22409	-0.86357	1
O26	1a	-0.61594	-0.17745	-0.54888	1
O27	1a	-0.089	0.09211	-0.17731	1
O28	1a	-0.58639	-0.2387	-0.1436	1
O29	1a	-0.08152	0.19121	-0.46087	1
O30	1a	-0.59254	-0.07959	-0.83383	1
O31	1a	-0.91927	-0.2444	-0.14467	1
O32	1a	-0.41272	0.18169	-0.45524	1
O33	1a	-0.92304	-0.08155	-0.82941	1
O34	1a	-0.42739	0.22312	-0.86147	1
O35	1a	-0.94677	-0.17918	-0.53678	1
O36	1a	-0.422	0.09311	-0.17346	1
O37	1a	-0.26486	-0.16709	-0.28055	1
O38	1a	-0.73377	-0.48025	-0.05572	1
O39	1a	-0.2546	0.66835	-0.78518	1
O40	1a	-0.76393	0.16125	-0.72874	1
O41	1a	-0.25692	0.48764	-0.93467	1
O42	1a	-0.74155	-0.68044	-0.20226	1
O43	1a	-0.25899	0.35337	-0.75809	1
O44	1a	-0.78214	0.03801	-0.56118	1
O45	1a	-0.25678	0.175	-0.29454	1
O46	1a	-0.74054	-0.3574	-0.25586	1
O47	1a	-0.24384	-0.03294	-0.45087	1
O48	1a	-0.75436	-0.17942	-0.71558	1
O49	1a	-0.26023	-0.99468	-0.00131	1
O50	1a	-0.83281	-0.47538	-0.47302	1