Tuning Optical Properties and Band Gap Energies in $Pb_3(C_6X_6)$ Extended Solid-State Structures

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Supporting Information The optimized coordinates for the solid state structures obtained using VASP, the molecular structures obtained from the Gaussian calculations, the k-points for the solid state structures, and various HSE06 band gaps at different k-points for $Pb_3(C_6S_6)$ with NWChem. The optimized unit cell coordinates for the $Pb_3C_6X_6$ solid state compounds are given in Tables S1 – 4. The optimized coordinates for the molecular structures are given in Tables S5 – 16. K-points used in the calculations are given in Table S17 with the scaling distances used to scale the band structure based on the distances in the unit cell. The NWChem band gaps in $Pb_3C_6S_6$ are given in Table S18. The first Brillouin zone is given in Figure S1.

Table S1: Cartesian coordinates and lattice vectors for $Pb_3C_6O_6$ ground state structure

ID	X	Y	Z
Pb	1.96988	3.41203	1.70356
Pb	-1.97061	3.41249	1.70356
Pb	3.94049	-0.00042	1.70356
C	3.93977	5.41938	0.00000
C	-2.72485	6.12243	0.00000
C	1.21632	0.70222	0.00000
C	-0.00002	1.40447	0.00000
C	6.66460	0.70142	0.00000
C	2.72343	6.12163	0.00000
O	-1.52755	5.43117	0.00000
O	1.52608	5.43039	0.00000
O	3.93981	4.03682	0.00000
O	5.46731	1.39268	0.00000
O	2.41367	1.39346	0.00000
O	-0.00006	2.78703	0.00000
Tv	7.880970489	-0.000845621	-0.000000751
Tv	-3.941217570	6.824698230	-0.000000301
Tv	-0.000000360	-0.000000299	3.407112519

Table S2: Cartesian coordinates and lattice vectors for $Pb_3C_6S_6$ ground state structure

ID	X	Y	Z
Pb	2.25788	3.91076	1.99032
Pb	4.51577	-0.00001	1.99032
Pb	-2.25789	3.91077	1.99032
C	4.51576	6.40291	0.00000
C	7.80298	0.70930	0.00000
C	-3.28722	7.11223	0.00000
C	0.00000	1.41862	0.00000
C	3.28720	7.11222	0.00000
C	1.22856	0.70931	0.00000
S	4.51577	4.63077	0.00000
S	6.26826	1.59537	0.00000
S	-1.75249	6.22616	0.00000
S	-0.00001	3.19076	0.00000
S	1.75248	6.22615	0.00000
S	2.76328	1.59538	0.00000
Tv	9.031546297	-0.000013263	-0.000000131
Tv	-4.515784480	7.821540893	-0.000000029
Tv	-0.000000058	-0.000000030	3.980647891

Table S3: Cartesian coordinates and lattice vectors for $Pb_3C_6Se_6$ ground state structure

ID	X	Y	Z
Pb	2.35650	4.08158	2.06537
Pb	-2.35650	4.08158	2.06537
Pb	4.71301	0.00000	2.06537
C	4.71301	6.75140	0.00000
C	-3.49038	7.45728	0.00000
C	1.22262	0.70588	0.00000
C	0.00000	1.41176	0.00000
C	8.20339	0.70588	0.00000
C	3.49038	7.45728	0.00000
Se	-1.80867	6.48635	0.00000
Se	1.80867	6.48635	0.00000
Se	4.71301	4.80953	0.00000
Se	6.52168	1.67682	0.00000
Se	2.90433	1.67682	0.00000
Se	0.00000	3.35363	0.00000
Tv	9.426011225	0.000000000	0.000000000
Tv	-4.713005613	8.163161720	0.000000000
Tv	0.000000000	0.000000000	4.130733251

Table S4: Cartesian coordinates and lattice vectors for $Pb_3C_6Te_6$ ground state structure

ID	X	Y	Z
Pb	2.49171	4.31577	2.20081
Pb	-2.49210	4.31599	2.20081
Pb	4.98381	-0.00023	2.20081
C	4.98336	7.22775	0.00000
C	-3.76858	7.93014	0.00000
C	1.21568	0.70194	0.00000
C	0.00005	1.40378	0.00000
C	8.75199	0.70139	0.00000
C	3.76773	7.92959	0.00000
Te	-1.88471	6.84250	0.00000
Te	1.88383	6.84213	0.00000
Te	4.98354	5.05251	0.00000
Te	6.86813	1.78904	0.00000
Te	3.09959	1.78940	0.00000
Te	-0.00013	3.57902	0.00000
Tv	9.967611176	-0.000450539	-0.000000987
Tv	-4.984196400	8.631983247	-0.000000527
Tv	-0.000000562	-0.000000657	4.401628609

Table S5: Cartesian coordinates for the planar $C_{12}H_8PbO_4$ ground state structure

ID	X	Y	Z
C	0.000000	3.200815	0.749643
C	0.000000	3.200333	-0.748353
C	0.000000	4.44069	-1.42896
C	0.000000	5.646994	-0.724708
C	0.000000	5.647457	0.724445
C	0.000000	4.441613	1.429454
C	0.000000	-4.441613	1.429454
C	0.000000	-5.647457	0.724445
C	0.000000	-5.646994	-0.724708
C	0.000000	-4.44069	-1.42896
C	0.000000	-3.200333	-0.748353
C	0.000000	-3.200815	0.749643
Pb	0.000000	0.000000	0.001504
O	0.000000	-2.061607	-1.372462
O	0.000000	-2.062527	1.374482
O	0.000000	2.062527	1.374482
O	0.000000	2.061607	-1.372462
O	0.000000	4.485731	2.823094
O	0.000000	6.821276	1.363521
O	0.000000	6.820437	-1.364479
O	0.000000	4.483931	-2.822625
O	0.000000	-4.485731	2.823094
O	0.000000	-6.821276	1.363521
O	0.000000	-6.820437	-1.364479
O	0.000000	-4.483931	-2.822625
H	0.000000	5.43626	3.026024
H	0.000000	5.434325	-3.026172
H	0.000000	-5.43626	3.026024
H	0.000000	-5.434325	-3.026172
Pb	0.000000	8.604548	-0.001011
Pb	0.000000	-8.604548	-0.001011

Table S6: Cartesian coordinates for the planar $C_{12}H_8PbS_4$ ground state structure

ID	X	Y	Z
S	0.000000	2.368678	-1.682363
S	0.000000	2.369241	1.683452
S	0.000000	-2.368678	-1.682363
S	0.000000	-2.369241	1.683452
C	0.000000	-3.834335	0.720385
C	0.000000	-3.834097	-0.719759
C	0.000000	-5.075411	-1.411242
C	0.000000	-6.310719	-0.718543
C	0.000000	-6.310955	0.718384
C	0.000000	-5.075871	1.411466
C	0.000000	5.075871	1.411466
C	0.000000	6.310955	0.718384
C	0.000000	6.310719	-0.718543
C	0.000000	5.075411	-1.411242
C	0.000000	3.834097	-0.719759
C	0.000000	3.834335	0.720385
Pb	0.000000	0.000000	0.000848
S	0.000000	4.944242	-3.20668
S	0.000000	4.945233	3.206942
S	0.000000	-4.944242	-3.20668
S	0.000000	-4.945233	3.206942
S	0.000000	-7.816078	-1.670471
S	0.000000	-7.816605	1.669875
S	0.000000	7.816078	-1.670471
S	0.000000	7.816605	1.669875
H	0.000000	6.280265	-3.421577
H	0.000000	6.281316	3.421463
H	0.000000	-6.280265	3.026024
H	0.000000	-6.281316	-3.026172
Pb	0.000000	9.740141	-0.001011
Pb	0.000000	-9.740141	-0.001011

Table S7: Cartesian coordinates for the planar $C_{12}H_8PbSe_4$ ground state structure

ID	X	Y	Z
C	0.000000	3.990194	0.721475
C	0.000000	3.990194	-0.706085
C	0.000000	5.239012	-1.374885
C	0.000000	6.459558	-0.695376
C	0.000000	6.459558	0.710766
C	0.000000	5.239012	1.390275
C	0.000000	-5.239012	1.390275
C	0.000000	-6.459558	0.710766
C	0.000000	-6.459558	-0.695376
C	0.000000	-5.239012	-1.374885
C	0.000000	-3.990194	-0.706085
C	0.000000	-3.990194	0.721475
Pb	0.000000	0.000000	0.007695
Se	0.000000	-2.420595	1.840996
Se	0.000000	-2.420595	-1.825606
Se	0.000000	2.420595	-1.825606
Se	0.000000	2.420595	1.840996
Se	0.000000	5.224138	3.330218
Se	0.000000	5.224138	-3.314828
Se	0.000000	8.125564	-1.68937
Se	0.000000	8.125564	1.704761
Se	0.000000	-5.224138	3.330218
Se	0.000000	-8.125564	1.704761
Se	0.000000	-8.125564	-1.68937
Se	0.000000	-5.224138	-3.314828
H	0.000000	6.606269	3.83083
H	0.000000	6.606269	-3.81544
H	0.000000	-6.606269	3.83083
H	0.000000	-6.606269	-3.81544
Pb	0.000000	10.210423	-0.026557
Pb	0.000000	-10.210423	-0.026557

Table S8: Cartesian coordinates for the planar $C_{12}H_8PbTe_4$ ground state structure

ID	X	Y	Z
C	4.405382	0.740643	0.000000
C	4.378488	-0.677891	0.000000
C	5.59526	-1.404463	0.000000
C	6.841781	-0.728076	0.000000
C	6.868852	0.697113	0.000000
C	5.648918	1.420261	0.000000
C	-5.649034	1.420111	0.000000
C	-6.868917	0.696858	0.000000
C	-6.84174	-0.728333	0.000000
C	-5.595169	-1.404601	0.000000
C	-4.378473	-0.677953	0.000000
C	-4.405444	0.740579	0.000000
Pb	0.000000	0.10264	0.000000
Te	-2.61483	1.936247	0.000000
Te	2.614745	1.936281	0.000000
Te	2.544366	-1.806058	0.000000
Te	-2.544366	-1.806067	0.000000
Te	5.433713	3.59319	0.000000
Te	5.299523	-3.567962	0.000000
Te	8.640559	-1.945983	0.000000
Te	8.711571	1.846326	0.000000
Te	-5.433957	3.593059	0.000000
Te	-5.29919	-3.568025	0.000000
Te	-8.711697	1.845921	0.000000
Te	-8.640422	-1.946395	0.000000
H	7.115768	3.839129	0.000000
H	-7.116015	3.838975	0.000000
H	-6.969947	-3.87677	0.000000
H	6.970305	-3.876636	0.000000
Pb	10.778084	-0.08909	0.000000
Pb	-10.778087	-0.089623	0.000000

Table S9: Cartesian coordinates for the torsional $C_{12}H_8PbO_4$ ground state structure

ID	X	Y	Z
Pb	0.000012	2.018521	0.000082
C	-2.714364	0.587251	0.746368
C	-2.714288	0.587161	-0.74623
C	-3.873889	0.170716	-1.42869
C	-5.012831	-0.23627	-0.722836
C	-5.012903	-0.236189	0.722841
C	-3.874041	0.170894	1.42876
C	3.873856	0.170505	1.428701
C	5.0128	-0.236419	0.722815
C	5.012888	-0.236178	-0.722861
C	3.874033	0.170981	-1.42875
C	2.71436	0.587293	-0.746325
C	2.714271	0.587047	0.746272
Pb	-7.816572	-1.18769	-0.000078
Pb	7.816579	-1.187658	-0.000015
O	-3.921545	0.170623	-2.822098
H	-4.814194	-0.157001	-3.023675
O	-6.120039	-0.617193	-1.362606
O	-6.120185	-0.616985	1.362541
O	-3.921839	0.170983	2.822165
H	-4.814492	-0.156659	3.023694
O	-1.639718	0.988994	-1.366935
O	-1.639854	0.989161	1.367132
O	1.639867	0.989267	-1.367053
O	1.6397	0.988822	1.367009
O	3.921495	0.170259	2.822109
H	4.814138	-0.157397	3.023661
O	3.921843	0.171198	-2.822153
H	4.814514	-0.156384	-3.023701
O	6.120169	-0.616932	-1.362593
O	6.120003	-0.61739	1.362554

Table S10: Cartesian coordinates for the torsional $C_{12}H_8PbS_4$ ground state structure

ID	X	Y	Z
Pb	-0.000493	0.000092	1.050278
C	-3.400423	-0.721109	-0.131534
C	-3.400465	0.721263	-0.131502
C	-4.638526	1.40987	-0.157581
C	-5.877079	0.717124	-0.194096
C	-5.877037	-0.717121	-0.194104
C	-4.638439	-1.409792	-0.157624
C	4.63869	-1.409828	-0.156493
C	5.877269	-0.717143	-0.19342
C	5.877286	0.717105	-0.193489
C	4.638728	1.409826	-0.156613
C	3.400687	0.721198	-0.130003
C	3.40067	-0.721164	-0.129942
Pb	-9.313099	-0.000096	-0.255728
Pb	9.313206	-0.000061	-0.256314
H	5.847672	3.419892	-0.180801
H	5.847578	-3.419927	-0.180599
H	-5.847519	3.419918	-0.180898
H	-5.847307	-3.419912	-0.181075
S	-4.5125	-3.205837	-0.140228
S	-7.379642	-1.668113	-0.229205
S	-7.37974	1.668029	-0.229187
S	-4.512697	3.205922	-0.140097
S	-1.931265	1.685072	-0.130051
S	-1.931159	-1.684829	-0.130156
S	1.931476	-1.684961	-0.1277
S	1.931522	1.685036	-0.127834
S	4.512877	3.205879	-0.139283
S	4.51279	-3.205876	-0.139041
S	7.379869	-1.668113	-0.228967
S	7.379909	1.668035	-0.229105

Table S11: Cartesian coordinates for the torsional $C_{12}H_8PbSe_4$ ground state structure

ID	X	Y	Z
Pb	0.000076	-0.000312	-0.557217
C	3.479345	-0.379772	0.617741
C	3.539494	0.993858	0.239169
C	4.78113	1.543054	-0.155669
C	5.970417	0.772104	-0.134569
C	5.908242	-0.596865	0.253613
C	4.650334	-1.164587	0.587942
C	-4.781221	-1.54302	-0.155837
C	-5.970477	-0.772021	-0.134641
C	-5.908207	0.596949	0.253519
C	-4.650259	1.164626	0.587758
C	-3.479299	0.379755	0.617494
C	-3.539543	-0.993876	0.238941
Pb	9.490361	-0.22658	-0.445528
Pb	-9.490394	0.226808	-0.445358
H	6.122641	3.546166	-0.979006
H	5.777462	-3.439233	0.808744
H	-6.122849	-3.54596	-0.979328
H	-5.777326	3.439288	0.80874
Se	7.61925	1.643333	-0.666365
Se	7.469561	-1.736616	0.371113
Se	4.659771	3.412099	-0.704296
Se	4.355773	-3.045707	1.026483
Se	2.005418	2.146936	0.244689
Se	1.855519	-1.227877	1.231705
Se	-1.855398	1.227819	1.231298
Se	-2.005537	-2.147058	0.244453
Se	-4.355579	3.045708	1.026239
Se	-4.66001	-3.412051	-0.704515
Se	-7.469473	1.736772	0.371112
Se	-7.619388	-1.643201	-0.666257

Table S12: Cartesian coordinates for the torsional $C_{12}H_8PbTe_4$ ground state structure

ID	X	Y	Z
Pb	0.002187	0.001747	0.114532
C	-3.730454	0.161614	1.159865
C	-3.723331	-1.185008	0.718146
C	-4.874603	-1.7096	0.086014
C	-5.969073	-0.87146	-0.246222
C	-5.976351	0.477345	0.203481
C	-4.877463	0.959229	0.962354
C	4.876265	1.709972	0.084632
C	5.969094	0.869748	-0.247545
C	5.975653	-0.477988	0.205383
C	4.876668	-0.957253	0.965766
C	3.731044	-0.15759	1.163325
C	3.725071	1.188216	0.719107
Pb	-9.228572	0.467261	-2.056051
Pb	9.225614	-0.475284	-2.057413
H	-6.443514	-3.948303	-0.493586
H	-6.442599	3.106432	1.879078
H	6.449156	3.945273	-0.49718
H	6.437013	-3.110842	1.878752
Te	-7.472178	-1.706604	-1.566659
Te	-7.532137	1.900428	-0.292967
Te	-4.74925	-3.84647	-0.289869
Te	-4.751884	2.926531	1.887007
Te	-2.006708	-2.472935	0.925698
Te	-2.012993	1.06852	2.1269
Te	2.013352	-1.05947	2.13436
Te	2.010121	2.478675	0.924952
Te	4.746864	-2.924054	1.891811
Te	4.754427	3.846749	-0.293879
Te	7.532562	-1.901803	-0.285631
Te	7.468748	1.69964	-1.575191

Table S13: Cartesian coordinates for the C_6H_5OH ground state structure

ID	X	Y	Z
C	1.149136	1.23159	0.000000
C	-0.256676	1.218101	0.000004
C	-0.95136	-0.022071	0.000001
C	-0.216012	-1.239904	0.000002
C	1.187228	-1.204904	0.000003
C	1.877486	0.025943	-0.000005
H	1.679041	2.193999	-0.000003
H	-0.824125	2.158825	0.000007
H	-0.761157	-2.192191	0.000002
H	1.749959	-2.148447	0.000002
H	2.974278	0.043946	-0.000008
O	-2.361752	-0.121048	-0.000005
H	-2.662794	0.859726	0.000003
C	1.149136	1.23159	0.000000

Table S14: Cartesian coordinates for the C_6H_5SH ground state structure

ID	X	Y	Z
C	1.200133	-1.613822	0.000000
C	1.214746	-0.20683	0.000000
C	0.000000	0.526924	0.000000
C	-1.226145	-0.190815	0.000000
C	-1.232086	-1.595945	0.000000
C	-0.020147	-2.316281	0.000000
H	2.151392	-2.163505	0.000000
H	2.175999	0.324686	0.000000
H	-2.176804	0.359146	0.000000
H	-2.190236	-2.133308	0.000000
H	-0.027807	-3.413607	0.000000
H	1.300766	2.461985	0.000000
S	-0.05327	2.309076	0.000000
C	1.200133	-1.613822	0.000000

Table S15: Cartesian coordinates for the C_6H_5SeH ground state structure

ID	X	Y	Z
C	1.200133	-1.613822	0.000000
C	1.214746	-0.20683	0.000000
C	-0.711296	2.423129	0.000000
C	-1.027646	1.058712	0.000000
C	0.000000	0.103257	0.000000
C	1.340287	0.522279	0.000000
H	1.646346	1.887956	0.000000
H	0.623941	2.845692	0.000000
H	-1.513799	3.155311	0.000000
H	-2.068494	0.750242	0.000000
H	2.145365	-0.207515	0.000000
H	2.686309	2.201847	0.000000
Se	0.864149	3.904226	0.000000
C	-1.80768	-1.669637	0.000000

Table S16: Cartesian coordinates for the C_6H_5TeH ground state structure

ID	X	Y	Z
C	-1.105249	2.730248	0.000000
C	-1.178588	1.331339	0.000000
C	0.000000	0.568396	0.000000
C	1.246232	1.215993	0.000000
C	1.310261	2.614891	0.000000
C	0.136274	3.378627	0.000000
H	-2.022693	3.312156	0.000000
H	-2.15093	0.848823	0.000000
H	2.170746	0.64434	0.000000
H	2.279407	3.105731	0.000000
H	0.188137	4.462936	0.000000
H	-1.687985	-1.655882	0.000000
Te	-0.023659	-1.572213	0.000000
C	-1.105249	2.730248	0.000000

Table S17: Table of k-points

The points of high symmetry in the first Brillouin zone used in the calculations are:

Γ = (0, 0, 0)

A = (0, 0, ½)

M = (½, 0, 0)

K = (⅓, ⅓, 0)

H = (⅓,⅓, ½)

L = (½, 0, ½)

Each vector was divided into 20 points.

Once the band structure was obtained the distances were scaled in units of 4π/a√3, 4π/a√3, 2π/c along the three primitive reciprocal vectors $\underline{b}$ the points. The real space lattice vectors *a1* to *a3* and reciprocal space lattice vectors *b1* to *b3* are:

$$a1 = \left(\frac{1}{2}a, -\frac{1}{2}3^{\frac{1}{2}}a, 0\right)$$

$$a2 = \left(\frac{1}{2}a, \frac{1}{2}3^{\frac{1}{2}}a, 0\right)$$

$$a3 = (0,0,c)$$

$$b1 = (2\pi a)\left(1, -3^{-\frac{1}{2}}, 0\right)$$

$$b2 = (2\pi a)\left(1, 3^{-\frac{1}{2}}\right)$$

$$b3 = \left(\frac{2\pi}{c}\right)(0,0,1)$$

and basis vectors *B1* and *B2* are:

$$B1 = \frac{2}{3}a_1 + \frac{1}{3}a_2 + \frac{1}{4}a_3$$

$$B2 = \frac{1}{3}a_1 + \frac{2}{3}a_2 + \frac{3}{4}a_3$$

where a and c are the lattice parameters of the unit cell

Table S18: NWChem Band Gaps (eV) for $Pb_3C_6S_6$

k_x	k_y	k_z	**Band Energy**
0.213	0.123	0.293	**1.9**
0.071	0.123	0.293	1.7
-0.071	0.123	0.293	1.7
0.142	0.000	0.293	1.7
0.000	0.000	0.290	2.5
0.142	0.000	-0.293	1.5
0.071	-0.123	0.293	1.7
0.071	0.123	-0.293	1.5
0.213	0.123	-0.293	1.7
0.213	0.123	0.000	3.0
0.071	0.123	0.000	2.3
0.071	-0.123	0.000	2.2
0.142	0.000	0.000	2.3
0.000	0.000	0.000	2.0

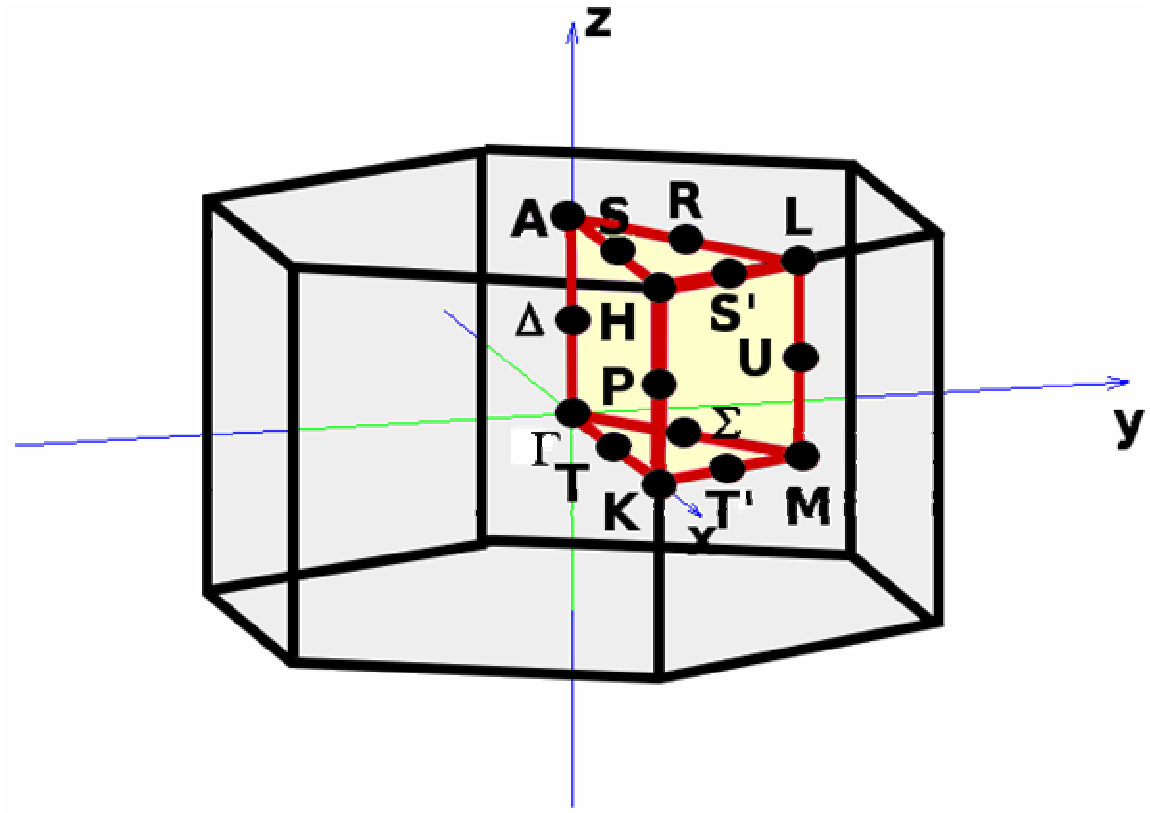

Figure S1 First Brillouin Zone for the Pb3C6X6 crystal structures