Supporting information for

Chemical-Shift Tensors of Heavy Nuclei in Network Solids:

A DFT/ZORA Investigation of ^{207}Pb Chemical-Shift Tensors Using the Bond-Valence Method.

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Table S1. Frozen Inner Shells in FCA/DZ Basis Sets for the Elements in Outer Shells of Clusters

Elements	Frozen Core Orbitals*
O, F	1s
Si, P, Cl	[…]2p
Br	[…]3d
I, Sn	[…]4d
Pb	[…]5d

*Frozen inner shells are up to and including the listed orbitals for the given elements.

The Assignment of Modified Charges using the Bond Valence Model for β-PbO

In its crystal structure, the co-ordination numbers of both Pb and O are four for β-PbO. There are three different Pb-O bond lengths, 2.482, 2.239 and 2.219 Å respectively. From the crystallographic information and tabulated R_0 and b parameters of the Pb-O bond (1.963 and 0.49 respectively), the valence (or the total bond strength) of Pb with complete co-ordination can be calculated using equation S1,

$$S_{Pb} = 2exp\left(\frac{R_0 - R_1}{b}\right) + exp\left(\frac{R_0 - R_2}{b}\right) + exp\left(\frac{R_0 - R_3}{b}\right) \quad \textbf{(S1)}$$

where R_1, R_2 and R_3 correspond to different Pb-O bond lengths of 2.482, 2.239 and 2.219 Å. The factor of 2 in the first expression on the right-hand side of equation S1 is because there are two oxygen atoms coordinated to the lead atom with the bond length R_1. From this expression, S_{Pb} is calculated as 1.86, which is slightly lower than 2.00, the valence of the lead atom. Therefore, the R_0 parameter is adjusted to **1.999** for which the equation S1 yields to 2.00 exactly. This step is often necessary to minimize the total charge on the modified cluster.

In the next step, values of S_O are calculated for the terminal oxygen atoms in the cluster using the adjusted value of R_0. For a cluster of β-PbO which contains atoms up to the third co-ordination shell, there are ten terminal oxygen sites (Figure 1). However, there are only five **unique** sites with respect to the bond-valence model due to the symmetry of the system. As anticipated, the total bond strengths of these sites are significantly smaller than the valence of oxygen atom due to the missing co-ordination in the **cluster.** For example, in figure 1, the co-ordination number of O5 is two, and the Pb-O bond lengths are 2.482 and 2.219 Å. Using

Table S2. R_0 and b Parameters used in the Bond Valence Modelling of the Clusters of Investigated Systems

Bond type	R_0	b
α-PbO		
Pb-O	1.969	0.49
β-PbO		
Pb-O	1.999	0.49
Pb_3O_4		
Pb(II)-O	1.995	0.49
Pb(IV)-O	2.029	0.37
Pb_2SnO_4		
Pb-O	1.980	0.49
Sn-O	1.926	0.37
PbF_2		
Pb-F	2.022	0.382
$PbCl_2$		
Pb-Cl	2.447	0.40
$PbBr_2$		
Pb-Br	2.597	0.40
PbClOH		
Pb-Cl	2.583	0.40
Pb-O	1.882	0.49
PbBrOH		
Pb-Br	2.699	0.40
Pb-O	1.893	0.49
PbIOH		
Pb-I	2.900	0.386
Pb-O	1.907	0.40
$PbSiO_3$		
Si-O	1.624	0.37
Pb-O	1.997	0.49
$Pb_3(PO_4)_2$		
P-O	1.612	0.37
Pb-O	1.977	0.49

equation S1 with this co-ordination environment, S_O is calculated to be 1.01 for O5. From the S_O, the modified nuclear charge can be calculated using equation 2 and 3 in the text of the article, which results in a value of 8.99 for O5. This procedure is repeated for each terminal site in the cluster to create the proper charges for the calculation.

Table S3. Calculated NMR Chemical Shielding Parameters of First and Third Coordination Shell Clusters of Lead-Containing Systems Determined at ZORA-SO/BP86 Level of Theory

Model clusters	σ_{11} (ppm)	σ_{22} (ppm)	σ_{33} (ppm)	σ_{iso} (ppm)	Ω (ppm)	κ
α-PbO						
1-VMTA/BV	9451	9451	11269	10057	1818	1.00
3-VMTA/BV	5887	5889	8827	6868	2940	1.00
β-PbO						
1-VMTA/BV	8630	9283	11516	9810	2886	0.55
3-VMTA/BV	5655	6197	9352	7068	3697	0.71
Pb_3O_4						
1-VMTA/BV	8696	9233	11218	9716	2522	0.57
3-VMTA/BV	7350	7353	9881	8195	2531	1.00
Pb_2SnO_4 (site 1)						
1-VMTA/BV	8941	9198	11270	9803	2329	0.78
3-VMTA/BV	7146	7251	10032	8143	2885	0.93
Pb_2SnO_4 (site 2)						
1-VMTA/BV	8175	8727	11029	9311	2854	0.61
3-VMTA/BV	7187	7296	9983	8155	2796	0.92
PbF_2						
1-VMTA/BV	11746	11865	12348	11986	603	0.60
3-VMTA/BV	10784	10971	11049	10935	264	0.95
$PbCl_2$						
1-VMTA/BV	9521	9899	10276	9899	756	0.00
3-VMTA/BV	9612	9664	10177	9818	565	-0.41
$PbBr_2$						
1-VMTA/BV	8602	8940	9548	9030	946	0.29
3-VMTA/BV	9108	9118	9802	9343	694	0.81
PbClOH						
1-VMTA/BV	9226	9773	10730	9910	1503	0.27
3-VMTA/BV	8516	8903	10275	9231	1759	0.56
PbBrOH						
1-VMTA/BV	9251	9579	10341	9724	1090	0.40
3-VMTA/BV	8530	8817	10088	9145	1558	0.56
PbIOH						
1-VMTA/BV	8983	9121	9575	9227	592	0.53
3-VMTA/BV	8618	8649	9860	9043	1242	0.63
$PbSiO_3$ (site 1)						
1-VMTA/BV	9725	10093	11950	10589	2225	0.67
3-VMTA/BV	7459	7995	10331	8595	2872	0.97
$PbSiO_3$ (site 2)						
1-VMTA/BV	9270	9626	11705	10200	2435	0.71
3-VMTA/BV	7829	8249	10522	8867	2693	0.63

$PbSiO_3$ (site 3)						
1-VMTA/BV	9742	10046	11792	10526	2050	0.70
3-VMTA/BV	7940	8532	10281	8918	2341	0.69
$Pb_3(PO_4)_2$ (site 1)						
1-VMTA/BV	12169	12225	12702	12365	533	0.79
3-VMTA/BV	11094	11159	11279	11178	185	0.49
$Pb_3(PO_4)_2$ (site 2)						
1-VMTA/BV	10797	11147	12268	11404	1471	0.52
3-VMTA/BV	10092	10556	11654	10767	1562	0.29

Table S4. Calculated NMR Chemical Shielding Parameters of Third Co-ordination Shell Clusters of Lead-Containing Systems Determined at ZORA-Scalar/BP86 Level of Theory

Model clusters	σ_{11} (ppm)	σ_{22} (ppm)	σ_{33} (ppm)	σ_{iso} (ppm)	Ω (ppm)	κ
α-PbO	5620	5621	6592	5945	972	1.00
β-PbO	5690	6027	6976	6231	1285	0.48
Pb_3O_4	6465	6752	7333	6850	869	0.34
Pb_2SnO_4 (site 1)	6455	6701	7398	6852	943	0.48
Pb_2SnO_4 (site 2)	6427	6669	7345	6814	918	0.47
PbF_2	8084	8157	8231	8157	146	0.01
$PbCl_2$	7417	7422	7630	7489	213	0.95
$PbBr_2$	7159	7204	7433	7265	275	0.67
PbClOH	7036	7286	7631	7318	595	0.16
PbBrOH	6991	7173	7551	7238	559	0.35
PbIOH	6995	7036	7512	7181	517	0.84
$PbSiO_3$ (site 1)	6742	6905	7578	7075	836	0.61
$PbSiO_3$ (site 2)	7041	7143	7759	7314	718	0.72
$PbSiO_3$ (site 3)	7065	7262	7656	7328	591	0.33
$Pb_3(PO_4)_2$ (site 1)	8152	8220	8285	8219	133	-0.02
$Pb_3(PO_4)_2$ (site 2)	7901	8115	8573	8196	672	0.36

Table S5. Calculated NMR Chemical Shielding Parameters of Fifth Co-ordination Shell Clusters of Lead-Containing Systems Determined at ZORA-SO/BP86 Level of Theory

Model clusters	σ_{11} (ppm)	σ_{22} (ppm)	σ_{33} (ppm)	σ_{iso} (ppm)	Ω (ppm)	κ
α-PbO	5914	5915	8900	6910	2986	1.00
β-PbO	6098	6172	9593	7288	3495	0.96
Pb_3O_4	6701	7374	9918	7998	3217	0.58
Pb_2SnO_4 (site 1)	6737	7175	10045	7988	3313	0.74
Pb_2SnO_4 (site 2)	6675	7300	9988	7986	3308	0.62
$PbSiO_3$ (site 1)	7748	8196	10352	8766	2604	0.66
$PbSiO_3$ (site 2)	7734	8131	10380	8748	2646	0.70
$PbSiO_3$ (site 3)	8138	8641	10334	9038	2196	0.54

Cartesian Coordinates Used in Defining Clusters

Given below are the positions of atoms in clusters discussed in the text of the article. Each position is given in Angstrøm units along each of the three axes used to define the structure.

First co-ordination shell cluster of α-PbO

Pb	0.00000000	0.00000000	0.00000000
O	1.40038000	-1.40038000	-1.18676000
O	-1.40038000	1.40038000	-1.18676000
O	1.40038000	1.40038000	-1.18676000
O	-1.40038000	-1.40038000	-1.18676000

Third co-ordination shell cluster α-PbO

Pb	0.00000000	0.00000000	0.00000000
O	4.20130000	-4.20130000	-1.18671000
O	1.40047000	-4.20117000	-1.18661000
O	-1.40047000	-4.20117000	-1.18661000
O	4.20117000	-1.40047000	-1.18661000
O	1.40038000	-1.40038000	-1.18676000
O	4.20117000	1.40047000	-1.18661000
O	-4.20130000	-4.20130000	-1.18671000
O	-1.40038000	-1.40038000	-1.18676000
O	-4.20117000	-1.40047000	-1.18661000
O	1.40038000	1.40038000	-1.18676000
O	-1.40038000	1.40038000	-1.18676000
O	4.20130000	4.20130000	-1.18671000
O	1.40047000	4.20117000	-1.18661000
O	-4.20117000	1.40047000	-1.18661000
O	-1.40047000	4.20117000	-1.18661000
O	-4.20130000	4.20130000	-1.18671000
Pb	0.00000000	-2.80092000	-2.37349000

Pb	2.80092000	0.00000000	-2.37349000
Pb	-2.80092000	0.00000000	-2.37349000
Pb	0.00000000	2.80092000	-2.37349000
Pb	2.80090000	-2.80090000	0.00024000
Pb	-2.80090000	-2.80090000	0.00024000
Pb	2.80090000	2.80090000	0.00024000
Pb	-2.80090000	2.80090000	0.00024000

Fifth co-ordination shell cluster α-PbO

Pb	0.00000000	0.00000000	0.00000000
Pb	-5.71567935	-1.72821739	3.03116971
Pb	-3.94554025	0.02877063	0.33666072
Pb	-0.00000938	7.89124755	-0.67448670
Pb	-0.00000256	3.94559772	-0.33721611
O	9.96525954	0.02880240	0.33702816
Pb	-0.00000256	-3.94560281	0.33715653
Pb	-0.00000938	-7.89126622	0.67426826
Pb	7.89112235	-0.05752131	-0.67349801
O	7.99226205	2.01603104	0.33666642
O	6.01954487	4.00309996	0.33652576
O	7.99226205	-1.92966629	0.67387940
O	6.01972185	0.05757833	0.67371857
Pb	6.12097598	2.13116159	1.68389992
O	6.01954487	-3.88794244	1.01092162
Pb	6.12097598	-1.81453731	2.02109451
Pb	-3.94536412	-3.91665478	0.67381699
Pb	-7.89114112	0.05753743	0.67327662
O	4.04678307	5.99027802	0.33629652
O	2.07413165	7.97741221	0.33593234
O	4.04692012	2.04472927	0.67358744
O	2.07405969	4.03200825	0.67333960
O	4.04692012	-1.90078645	1.01076638
O	2.07393351	0.08636727	1.01063075
O	4.04678307	-5.84635372	1.34784062
O	2.07405969	-3.85929094	1.34772036
Pb	2.17546647	6.10550672	1.68340396
O	2.07413165	-7.80473526	1.68465530
Pb	2.17544383	2.15991219	2.02082347
Pb	2.17544383	-1.78570217	2.35801101
O	0.10132373	9.96482787	0.33578912
Pb	2.17546647	-5.73133634	2.69496660
O	0.10132373	6.01922763	0.67297505
O	-1.87150467	8.00618611	0.67263091
O	0.10134080	2.07337661	1.01038285
O	-1.87139345	4.06078083	1.01002272
O	0.10134080	-1.87187139	1.34753908
O	-1.87125191	0.11513791	1.34729119

O	0.10132373	-5.81775634	1.68454973
O	-1.87139345	-3.83051833	1.68440380
O	0.10132373	-9.76335661	2.02173604
O	-1.87150467	-7.77596130	2.02135456
Pb	3.94535900	3.91664972	-0.67387637
Pb	3.94553513	-0.02877570	-0.33672029
Pb	-1.77016985	6.13428062	2.02010288
O	-3.84413731	6.04782325	1.00966407
Pb	-1.77010795	2.18868547	2.35751517
O	-3.84425389	2.10227637	1.34697677
O	-5.81689911	4.08941670	1.34660131
O	-3.84425389	-1.84323934	1.68415590
O	-5.81707439	0.14389608	1.68380599
O	-3.84413731	-5.78880843	2.02120869
O	-5.81689911	-3.80162881	2.02096077
Pb	-1.77010794	-1.75692888	2.69470273
Pb	-1.77016985	-5.70256243	3.03166557
Pb	3.94535900	-3.97419856	0.00046585
O	-7.78963507	2.13112034	1.68341609
Pb	-3.94536411	3.97419347	-0.00052561
O	-7.78963507	-1.81457856	2.02061087
O	-9.76261208	0.17266925	2.02049650
Pb	-5.71567935	2.21748150	2.69397494

First co-ordination shell cluster of β-PbO

Pb	0.00000000	0.00000000	0.00000000
O	-2.37680000	-0.25384100	0.66848700
O	2.37680000	-0.25384100	0.66848700
O	0.00000000	-1.88842200	1.20482900
O	0.00000000	1.21765100	1.85587800

Third co-ordination shell cluster of β-PbO

O	0.82951757	0.10722676	7.13198000
O	-1.61342243	2.13061676	2.37729000
O	0.82951757	0.10722676	2.37740000
O	0.23180757	1.71900676	4.75426000
O	-0.30111243	-1.40739324	4.75426000
O	0.29646757	-3.01957324	2.37729000
O	-2.21137243	3.74228676	0.00000000
O	-1.61342243	2.13061676	-2.37729000
O	0.82951757	0.10722676	-2.37740000
O	0.23216757	1.71951676	0.00000000
O	-0.30147243	-1.40790324	0.00000000
O	0.29646757	-3.01957324	-2.37729000
O	2.14158757	-3.43088324	0.00000000
O	0.82951757	0.10722676	-7.13198000
O	0.23180757	1.71900676	-4.75426000

O	-0.30111243	-1.40739324	-4.75426000
Pb	1.50665757	-0.12143324	4.75426000
Pb	0.59581757	2.33386676	2.37721000
Pb	-0.97861243	-1.17924324	2.37772000
Pb	-1.97787243	1.51572676	0.00000000
Pb	1.50628757	-0.12194324	0.00000000
Pb	0.59581757	2.33386676	-2.37721000
Pb	-0.97861243	-1.17924324	-2.37772000
Pb	-0.06758243	-3.63462324	0.00000000
Pb	1.50665757	-0.12143324	-4.75426000

Fifth co-ordination shell cluster of β-PbO

O	0.74864420	-0.21110556	11.88618000
O	-0.71673580	2.60245444	7.13191000
O	0.74910420	-0.21118556	7.13136000
O	0.82358420	1.50716444	9.50904000
O	-0.88145580	-1.16772556	9.50851000
O	-0.95641580	-2.88556556	7.13191000
O	0.98881420	5.27688444	2.37768000
O	-0.64179580	4.31979444	4.75427000
O	-0.71673580	2.60245444	2.37762000
O	0.74860420	-0.21116556	2.37715000
O	0.82410420	1.50670444	4.75427000
O	-0.88146580	-1.16822556	4.75427000
O	-0.95645580	-2.88561556	2.37712000
O	0.50894420	-5.69868556	2.37709000
O	0.58439420	-3.98136556	4.75477000
O	0.98881420	5.27688444	-2.37768000
O	1.06426420	6.99420444	0.00000000
O	-0.64127580	4.32026444	0.00000000
O	-0.71673580	2.60245444	-2.37762000
O	0.74860420	-0.21116556	-2.37715000
O	0.82362420	1.50722444	0.00000000
O	-0.88095580	-1.16774556	0.00000000
O	-0.95645580	-2.88561556	-2.37712000
O	0.50894420	-5.69868556	-2.37709000
O	0.58394420	-3.98079556	0.00000000
O	-1.12162580	-6.65571556	0.00000000
O	-0.64179580	4.31979444	-4.75427000
O	-0.71673580	2.60245444	-7.13191000
O	0.74910420	-0.21118556	-7.13136000
O	0.82410420	1.50670444	-4.75427000
O	-0.88146580	-1.16822556	-4.75427000
O	-0.95641580	-2.88556556	-7.13191000
O	0.58439420	-3.98136556	-4.75477000
O	0.74864420	-0.21110556	-11.88618000
O	0.82358420	1.50716444	-9.50904000

O	-0.88145580	-1.16772556	-9.50851000
Pb	1.28436420	-0.68473556	9.50854000
Pb	1.39838420	1.93201444	7.13189000
Pb	-1.41670580	-0.69417556	7.13139000
Pb	-1.17703580	4.79383444	2.37715000
Pb	-1.29153580	2.17666444	4.75427000
Pb	1.28388420	-0.68421556	4.75427000
Pb	1.39842420	1.93207444	2.37715000
Pb	-1.41670580	-0.69417556	2.37715000
Pb	-1.53121580	-3.31041556	4.75477000
Pb	1.15871420	-3.55599556	2.37764000
Pb	1.52403420	4.80327444	0.00000000
Pb	-1.17703580	4.79383444	-2.37715000
Pb	-1.29102580	2.17714444	0.00000000
Pb	1.28436420	-0.68473556	0.00000000
Pb	1.39842420	1.93207444	-2.37715000
Pb	-1.41670580	-0.69417556	-2.37715000
Pb	-1.53077580	-3.31098556	0.00000000
Pb	1.04468420	-6.17275556	0.00000000
Pb	1.15871420	-3.55599556	-2.37764000
Pb	-1.29153580	2.17666444	-4.75427000
Pb	1.28388420	-0.68421556	-4.75427000
Pb	1.39838420	1.93201444	-7.13189000
Pb	-1.41670580	-0.69417556	-7.13139000
Pb	-1.53121580	-3.31041556	-4.75477000
Pb	1.28436420	-0.68473556	-9.50854000

First co-ordination shell cluster of Pb_3O_4

Pb	3.10600000	-7.56700000	-17.64300000
O	2.60700000	-8.06600000	-19.74300000
O	2.27500000	-9.42800000	-16.77600000
O	5.08500000	-8.76600000	-17.97200000
O	0.39800000	-7.58200000	-17.95400000

Third co-ordination shell cluster of Pb_3O_4

O	6.03100000	-7.16900000	-15.31700000
O	-1.59400000	-8.40700000	-20.37100000
O	-1.92700000	-9.76900000	-17.40400000
O	6.36400000	-5.80700000	-18.28400000
O	6.60100000	-11.03100000	-17.02600000
O	6.93300000	-9.66900000	-19.99300000
O	2.94000000	-6.70400000	-22.71000000
O	-0.37400000	-5.88300000	-15.44600000
O	-0.04100000	-4.52100000	-18.41300000
O	1.94200000	-10.79000000	-13.80900000
O	7.37200000	-12.72900000	-19.53400000
O	-1.88900000	-3.61900000	-16.39100000

O	-0.43800000	-8.98400000	-15.06200000
O	8.28000000	-7.17200000	-20.51100000
O	0.22700000	-6.26000000	-20.99600000
O	7.61500000	-9.89600000	-14.57700000
O	2.60700000	-8.06600000	-19.74300000
O	2.27500000	-9.42800000	-16.77600000
O	5.08500000	-8.76600000	-17.97200000
O	0.39800000	-7.58200000	-17.95400000
O	4.68400000	-9.66500000	-14.80000000
O	5.35000000	-6.94100000	-20.73400000
Pb	6.64900000	-7.73800000	-19.13900000
Pb	6.31600000	-9.10000000	-16.17200000
Pb	0.17400000	-9.59900000	-17.09000000
Pb	0.50700000	-8.23700000	-20.05700000
Pb	3.10600000	-7.56700000	-17.64300000
Pb	5.66900000	-11.21000000	-19.02800000
Pb	3.10100000	-11.15400000	-15.66100000
Pb	-1.30500000	-6.06300000	-17.44700000
Pb	3.76700000	-8.43000000	-21.59500000
O	7.87900000	-8.07100000	-17.33900000
O	0.28200000	-10.25400000	-19.19300000
O	1.11900000	-8.85100000	-22.08500000
O	0.45300000	-11.57500000	-16.15100000

Fifth co-ordination shell cluster of Pb_3O_4

O	-5.44600000	-31.64300000	-21.59900000
O	-5.48700000	-31.66400000	-18.31700000
O	5.18100000	-28.39500000	-21.44700000
O	5.14100000	-28.41600000	-18.16600000
O	2.62400000	-27.89500000	-26.39800000
O	-5.58800000	-29.03500000	-13.37900000
O	-6.01500000	-20.96400000	-23.17900000
O	-6.09600000	-21.00600000	-16.61700000
O	0.74700000	-35.72900000	-23.18900000
O	0.66600000	-35.77100000	-16.62600000
O	-5.42600000	-28.95200000	-26.50400000
O	2.46200000	-27.97700000	-13.27300000
O	-8.69500000	-21.01400000	-21.57200000
O	-5.52700000	-31.68400000	-15.03600000
O	-8.73500000	-21.03500000	-18.29100000
O	-2.90900000	-27.68800000	-28.10600000
O	-5.40600000	-31.62200000	-24.88000000
O	-4.74100000	-23.45000000	-24.82000000
O	5.22200000	-28.37400000	-24.72800000
O	-4.86300000	-23.51200000	-14.97600000
O	5.10000000	-28.43600000	-14.88400000
O	-3.11200000	-27.79200000	-11.70000000

O	0.47400000	-32.79400000	-23.17400000
O	-0.31100000	-28.16800000	-26.43600000
O	0.39300000	-32.83600000	-16.61100000
O	-0.47300000	-28.25100000	-13.31100000
O	-4.17200000	-33.64000000	-19.95500000
O	-10.46600000	-19.42600000	-19.94300000
O	7.10700000	-27.13100000	-16.49200000
O	-7.02500000	-33.38400000	-23.27000000
O	-7.10600000	-33.42500000	-16.70800000
O	7.18800000	-27.09000000	-23.05500000
O	6.91200000	-30.00500000	-19.79500000
O	-4.43600000	-19.22300000	-21.50800000
O	-1.57400000	-34.12000000	-18.28500000
O	-1.53300000	-34.09900000	-21.56600000
O	-4.47700000	-19.24400000	-18.22700000
O	-4.68100000	-26.10000000	-26.47700000
O	-3.16300000	-21.70900000	-23.14900000
O	-4.84300000	-26.18200000	-13.35200000
O	-3.24400000	-21.75000000	-16.58600000
O	-9.87600000	-26.92500000	-19.98300000
O	1.20800000	-23.28900000	-19.82300000
O	5.31200000	-34.92500000	-19.84600000
O	1.67600000	-23.35100000	-16.53600000
O	-9.95800000	-27.45500000	-16.70500000
O	1.75800000	-23.31000000	-23.09800000
O	-9.87700000	-27.41300000	-23.26800000
O	-7.23800000	-27.38400000	-21.59400000
O	-2.95000000	-27.70900000	-24.82500000
O	-2.99100000	-27.73000000	-21.54400000
O	-4.78200000	-23.47100000	-21.53900000
O	1.26800000	-25.93900000	-21.48000000
O	-3.07200000	-27.77100000	-14.98100000
O	-3.03100000	-27.75000000	-18.26200000
O	0.88200000	-30.20700000	-18.23000000
O	-4.82200000	-23.49200000	-18.25800000
O	0.92300000	-30.18600000	-21.51100000
O	1.22800000	-25.95900000	-18.19900000
O	-7.27800000	-27.40500000	-18.31300000
O	2.54200000	-28.42500000	-23.12100000
O	-6.09700000	-21.49400000	-19.90200000
O	-4.95700000	-29.01400000	-23.21700000
O	-5.03800000	-29.05500000	-16.65400000
O	-0.39200000	-27.72100000	-16.58900000
O	-5.31200000	-26.12000000	-16.63900000
O	-4.76200000	-26.14100000	-19.91500000
O	2.46100000	-28.46600000	-16.55800000

O	2.54300000	-27.93600000	-19.83600000
O	0.94200000	-32.85600000	-19.88600000
O	-5.50700000	-28.99300000	-19.94200000
O	-0.31100000	-27.68000000	-23.15100000
O	-5.23100000	-26.07900000	-23.20200000
O	-0.39200000	-28.21000000	-19.87400000
O	0.84200000	-30.22800000	-14.94800000
O	-7.31900000	-27.42500000	-15.03100000
O	1.30900000	-25.91800000	-24.76100000
O	2.71400000	-34.44500000	-21.51600000
O	1.18700000	-25.98000000	-14.91700000
O	-7.19700000	-27.36300000	-24.87500000
O	2.67300000	-34.46600000	-18.23400000
O	0.96300000	-30.16600000	-24.79200000
Pb	0.59000000	-34.27200000	-21.54100000
Pb	1.09500000	-28.06200000	-21.49500000
Pb	-4.65000000	-21.36800000	-18.24200000
Pb	-5.19500000	-27.59800000	-15.00600000
Pb	-5.15500000	-27.57800000	-18.28800000
Pb	1.05500000	-28.08300000	-18.21400000
Pb	1.01400000	-28.10400000	-14.93300000
Pb	0.55000000	-34.29300000	-18.25900000
Pb	-4.60900000	-21.34700000	-21.52300000
Pb	-5.11400000	-27.55700000	-21.56900000
Pb	-5.07400000	-27.53600000	-24.85000000
Pb	1.13600000	-28.04200000	-24.77700000
Pb	3.63100000	-33.30000000	-19.85600000
Pb	-6.66200000	-30.73600000	-16.68500000
Pb	0.05200000	-25.03200000	-16.56600000
Pb	4.38200000	-27.13500000	-16.52600000
Pb	-3.68800000	-24.44000000	-16.60900000
Pb	-8.03700000	-26.12300000	-16.67300000
Pb	-2.15400000	-26.62600000	-13.32200000
Pb	-1.99200000	-26.54400000	-26.44700000
Pb	2.01700000	-31.15500000	-16.58100000
Pb	-2.31300000	-29.05200000	-16.62100000
Pb	4.22300000	-29.56100000	-19.82500000
Pb	0.13300000	-24.99000000	-23.12900000
Pb	2.53900000	-25.21000000	-19.81900000
Pb	4.46300000	-27.09300000	-23.08900000
Pb	-7.77700000	-19.87000000	-19.91200000
Pb	-8.19600000	-28.54900000	-19.97200000
Pb	-3.60600000	-24.39800000	-23.17100000
Pb	-6.09400000	-24.22000000	-19.91900000
Pb	-7.95600000	-26.08200000	-23.23600000
Pb	-2.07300000	-26.58500000	-19.88400000

Pb	-6.58100000	-30.69500000	-23.24800000
Pb	2.09800000	-31.11400000	-23.14300000
Pb	-0.38900000	-30.93500000	-19.89100000
Pb	-4.17500000	-30.91500000	-19.93700000
Pb	-2.23100000	-29.01100000	-23.18300000
O	0.19800000	-35.70900000	-19.91400000
O	-3.16200000	-21.22100000	-19.86400000

First co-ordination shell cluster of Pb_2SnO_4 (site 1)

O	8.44900000	-18.42600000	-14.07800000
O	11.37200000	-18.17700000	-15.31700000
O	6.64700000	-17.02600000	-15.60900000
Pb	9.40800000	-16.92900000	-15.28300000
O	8.78900000	-17.80800000	-17.14400000

Third co-ordination shell cluster of Pb_2SnO_4 (site 1)

O	6.26000000	-14.04600000	-16.66500000
O	5.92000000	-14.66400000	-13.60000000
O	12.98200000	-19.59100000	-17.03800000
O	12.64200000	-20.20900000	-13.97200000
O	9.12900000	-17.18900000	-20.20900000
O	8.10900000	-19.04400000	-11.01200000
O	13.72800000	-18.56500000	-11.90600000
O	6.56600000	-20.31100000	-13.05300000
O	5.95600000	-17.66100000	-12.58600000
O	14.40800000	-17.32900000	-18.03800000
O	7.24600000	-19.07400000	-19.18400000
O	6.63600000	-16.42400000	-18.71700000
O	4.65000000	-12.63200000	-14.94500000
O	13.36900000	-22.57000000	-15.98200000
O	8.78900000	-17.80800000	-17.14400000
O	8.44900000	-18.42600000	-14.07800000
O	11.37200000	-18.17700000	-15.31700000
O	6.64700000	-17.02600000	-15.60900000
O	14.02100000	-17.60200000	-14.90800000
O	6.55500000	-19.70900000	-16.16100000
Pb	11.77400000	-20.88300000	-15.81800000
Pb	5.05200000	-15.33800000	-15.44600000
Pb	9.40800000	-16.92900000	-15.28300000
Pb	9.31700000	-19.93900000	-12.67200000
Pb	9.99700000	-18.70200000	-18.80400000
O	11.66500000	-17.21300000	-18.31900000
O	10.98500000	-18.45000000	-12.18700000
O	12.41000000	-16.18800000	-13.18700000
O	4.75300000	-18.30900000	-17.69200000
O	4.41300000	-18.92700000	-14.62600000
O	12.75100000	-15.57000000	-16.25300000

Sn	6.77100000	-18.05800000	-17.41800000
Sn	12.86600000	-17.58000000	-16.64500000
Sn	6.43100000	-18.67700000	-14.35200000
Sn	12.52600000	-18.19800000	-13.58000000

Fifth co-ordination shell cluster of Pb_2SnO_4 (site 1)

O	9.68300000	27.78400000	21.17600000
O	9.66100000	26.63800000	27.36300000
O	7.95900000	17.35700000	25.63800000
O	-1.86500000	24.43100000	26.91500000
O	7.98000000	18.50300000	19.45200000
O	-1.84400000	25.57700000	20.72800000
O	1.81800000	19.05700000	27.53200000
O	1.85000000	20.77600000	18.25200000
O	12.84600000	20.94800000	27.92000000
O	3.77500000	28.64100000	19.71500000
O	3.74300000	26.92200000	28.99500000
O	12.87800000	22.66700000	18.64000000
O	7.51100000	21.88500000	29.67500000
O	7.55400000	24.17700000	17.30100000
O	14.86200000	27.67400000	24.37300000
O	7.62200000	17.99300000	22.55500000
O	-1.94000000	24.66700000	23.75800000
O	3.75300000	27.49500000	25.90200000
O	12.85600000	21.52100000	24.82600000
O	3.76400000	28.06800000	22.80800000
O	12.86700000	22.09400000	21.73300000
O	2.71600000	29.32100000	27.83600000
O	14.40300000	20.58400000	19.85900000
O	14.38100000	19.43800000	26.04600000
O	2.73800000	30.46600000	21.64900000
O	5.39000000	29.31000000	24.64300000
O	-4.63900000	17.86200000	22.48900000
O	14.95100000	22.63600000	23.44000000
O	12.11500000	28.26300000	22.87300000
O	12.10500000	27.69000000	25.96600000
O	2.78000000	17.46700000	22.44100000
O	10.23200000	29.83600000	24.75700000
O	-2.54400000	18.97700000	21.10300000
O	4.80700000	24.76600000	15.80100000
O	-2.55500000	18.40400000	24.19600000
O	4.75400000	21.90200000	31.26800000
O	2.85500000	17.23200000	25.59800000
O	2.87600000	18.37700000	19.41100000
O	2.66900000	21.35900000	29.56100000
O	2.71200000	23.65100000	17.18700000
O	0.80700000	24.07800000	25.25900000

O	8.48400000	20.86800000	21.49100000
O	4.79600000	24.19300000	18.89500000
O	4.76400000	22.47400000	28.17500000
O	9.16900000	24.84600000	22.23000000
O	4.77500000	23.04700000	25.08100000
O	1.82800000	19.63000000	24.43800000
O	8.47300000	20.29500000	24.58400000
O	4.78500000	23.62000000	21.98800000
O	0.81700000	24.65000000	22.16500000
O	9.15800000	24.27300000	25.32300000
O	1.83900000	20.20300000	21.34500000
O	2.90200000	25.19300000	23.87200000
O	7.53300000	23.03100000	23.48800000
O	10.10900000	22.11000000	23.32600000
O	2.69000000	22.50500000	23.37400000
O	0.20300000	18.38800000	22.60300000
O	10.02000000	27.14800000	24.25900000
O	7.45700000	23.26600000	20.33200000
O	3.23900000	24.55700000	26.95500000
O	7.43600000	22.12100000	26.51900000
O	10.18500000	21.87500000	26.48300000
O	2.35300000	23.14100000	20.29100000
O	10.20600000	23.02000000	20.29600000
O	2.33200000	21.99500000	26.47800000
O	3.26100000	25.70300000	20.76900000
O	10.08800000	20.96400000	29.51300000
O	2.92300000	26.33800000	17.68600000
O	2.88100000	24.04700000	30.05900000
O	10.13100000	23.25600000	17.14000000
Pb	8.24000000	25.67600000	23.98000000
Pb	9.40200000	19.46500000	22.83400000
Pb	5.45400000	23.19100000	17.11200000
Pb	12.76300000	26.68900000	24.18300000
Pb	4.68200000	26.66500000	24.15100000
Pb	12.20900000	23.09600000	23.51600000
Pb	5.43300000	22.04500000	23.29800000
Pb	0.91000000	21.03300000	23.09500000
Pb	0.16000000	25.65200000	23.94800000
Pb	-1.89700000	17.40200000	22.41300000
Pb	5.41200000	20.90000000	29.48500000
Pb	2.27900000	26.59900000	27.33000000
Pb	10.62200000	24.59600000	26.98800000
Pb	-0.34900000	23.87400000	20.41800000
Pb	5.96200000	24.97000000	20.64200000
Pb	3.29200000	19.95300000	26.10300000
Pb	7.02000000	20.54500000	19.82600000

Pb	11.70100000	21.31700000	19.98500000
Pb	5.94100000	23.82400000	26.82900000
Pb	11.68000000	20.17100000	26.17200000
Pb	6.99900000	19.39900000	26.01300000
Pb	10.64300000	25.74200000	20.80100000
Pb	-0.37000000	22.72800000	26.60400000
Pb	2.30000000	27.74500000	21.14300000
Pb	3.31300000	21.09900000	19.91600000
O	10.59000000	30.34600000	21.65400000
O	10.56900000	29.20000000	27.84000000
O	0.12800000	18.62300000	19.44700000
O	0.10600000	17.47700000	25.63400000
O	9.17900000	25.41900000	19.13700000
O	9.14700000	23.70000000	28.41700000
O	8.46300000	19.72200000	27.67800000
O	8.49400000	21.44100000	18.39800000
O	0.79600000	23.50500000	28.35200000
O	0.82800000	25.22300000	19.07200000
O	8.13700000	28.72100000	26.14400000
O	8.14700000	29.29400000	23.05000000
O	1.14300000	15.65200000	23.69900000
O	1.15400000	16.22500000	20.60600000
Sn	1.49700000	18.21400000	20.97500000
Sn	2.81200000	24.70800000	18.98300000
Sn	2.80100000	24.13500000	22.07700000
Sn	8.83700000	23.43000000	18.76700000
Sn	8.82600000	22.85700000	21.86100000
Sn	10.13100000	28.77800000	22.96200000
Sn	1.48600000	17.64100000	24.06900000
Sn	2.79100000	23.56200000	25.17000000
Sn	2.78000000	22.99000000	28.26300000
Sn	8.81600000	22.28400000	24.95400000
Sn	8.80500000	21.71100000	28.04700000
Sn	10.12100000	28.20600000	26.05500000

First co-ordination shell cluster of Pb_2SnO_4 (site 2)

O	19.22900000	-3.08400000	14.52400000
O	21.09800000	-2.37200000	16.56000000
O	16.44800000	-3.67200000	15.91200000
Pb	18.29900000	-2.44400000	16.45900000
O	19.15400000	-4.26900000	17.43700000

Third co-ordination shell cluster of Pb_2SnO_4 (site 2)

O	14.98900000	-4.78300000	13.72500000
O	14.91500000	-5.96800000	16.63800000
O	19.08000000	-5.45400000	20.35100000
O	19.30300000	-1.89900000	11.61100000

O	13.71600000	-3.28900000	15.99900000
O	21.38500000	-4.91700000	15.53200000
O	21.18400000	-0.42500000	19.05200000
O	21.25800000	0.75900000	16.13900000
O	13.79500000	-2.43200000	12.95200000
O	13.64700000	-4.80100000	18.77900000
O	21.37700000	-3.57600000	19.47400000
O	21.52600000	-1.20700000	13.64800000
O	22.71600000	1.87100000	18.32700000
O	14.83000000	-7.91500000	14.14600000
O	19.15400000	-4.26900000	17.43700000
O	19.22900000	-3.08400000	14.52400000
O	21.09800000	-2.37200000	16.56000000
O	16.44800000	-3.67200000	15.91200000
O	16.36800000	-4.52900000	18.95900000
O	16.51700000	-2.15900000	13.13200000
Pb	18.33100000	-3.52600000	12.62300000
Pb	18.18200000	-5.89500000	18.45000000
Pb	18.29900000	-2.44400000	16.45900000
Pb	16.23900000	-6.25900000	14.85500000
Pb	22.50800000	-0.71600000	17.26900000
O	15.17500000	-2.17700000	18.18600000
O	23.32900000	-3.02000000	14.65500000
O	15.24900000	-0.99200000	15.27300000
O	23.25500000	-4.20400000	17.56800000
O	21.10600000	-3.71200000	12.61800000
O	20.95700000	-6.08200000	18.44500000
Sn	15.11900000	-2.88800000	14.49900000
Sn	15.04500000	-4.07300000	17.41200000
Sn	21.27900000	-3.05200000	14.58900000
Sn	21.20500000	-4.23700000	17.50300000

Fifth co-ordination shell cluster of Pb_2SnO_4 (site 2)

O	19.14000000	-12.91600000	15.32800000
O	19.10200000	-12.45000000	12.21700000
O	32.17000000	-1.46200000	16.88400000
O	25.73100000	-8.12100000	22.32800000
O	25.54100000	-5.79100000	6.77300000
O	32.13200000	-0.99600000	13.77300000
O	27.89400000	-3.61500000	19.79500000
O	27.59500000	-11.74800000	18.58100000
O	17.49400000	-6.99200000	19.41700000
O	27.48100000	-10.35000000	9.24800000
O	27.78000000	-2.21700000	10.46200000
O	17.38000000	-5.59400000	10.08400000
O	21.40000000	-10.91300000	10.82900000
O	21.47600000	-11.84500000	17.05100000

O	32.48100000	-7.09500000	14.44600000
O	16.37800000	-12.59600000	13.81900000
O	21.98700000	-1.90200000	15.35200000
O	27.69800000	-7.41200000	8.09500000
O	20.10400000	-5.44800000	8.48200000
O	27.85000000	-9.27600000	20.53900000
O	20.25600000	-7.31100000	20.92600000
O	28.65200000	-12.49600000	10.50300000
O	34.11600000	0.10600000	15.50500000
O	15.61400000	-4.47100000	11.86400000
O	15.69000000	-5.40200000	18.08600000
O	25.96600000	-12.82200000	13.66800000
O	15.47200000	-7.62800000	14.57400000
O	28.72800000	-13.42800000	16.72500000
O	21.25900000	-14.07100000	13.53900000
O	26.69500000	-0.65300000	15.48200000
O	17.45600000	-6.52600000	16.30600000
O	27.51900000	-10.81600000	12.35900000
O	17.41800000	-6.06000000	13.19500000
O	27.55700000	-11.28200000	15.47000000
O	26.72300000	-1.46900000	18.54100000
O	26.64700000	-0.53700000	12.31800000
O	32.51000000	-7.91100000	17.50500000
O	21.59700000	-1.40400000	12.25000000
O	32.43400000	-6.97900000	11.28300000
O	21.67300000	-2.33600000	18.47200000
O	22.81700000	-5.93800000	8.37500000
O	22.97000000	-7.80100000	20.81900000
O	27.81800000	-2.68300000	13.57300000
O	21.30300000	-8.41000000	12.79500000
O	25.57900000	-6.25700000	9.88400000
O	25.69300000	-7.65500000	19.21700000
O	25.65500000	-7.18900000	16.10600000
O	27.85600000	-3.14900000	16.68400000
O	25.61700000	-6.72300000	12.99500000
O	21.34100000	-8.87600000	15.90600000
O	29.75800000	-7.24200000	16.04800000
O	21.73200000	-4.37300000	13.39500000
O	29.72000000	-6.77600000	12.93700000
O	21.77000000	-4.83900000	16.50600000
O	22.86500000	-6.05400000	11.53800000
O	27.45900000	-8.77900000	17.43700000
O	27.99200000	-6.11800000	17.82900000
O	22.94100000	-6.98600000	17.76100000
O	27.91500000	-5.18600000	11.60700000
O	27.38300000	-7.84700000	11.21500000

O	20.13200000	-6.26300000	11.54100000
O	20.20800000	-7.19500000	17.76300000
O	20.18000000	-6.38000000	14.70400000
O	21.08600000	-11.34700000	13.94900000
O	29.40800000	-1.14300000	15.37500000
O	27.60100000	-5.62100000	14.72700000
O	27.77400000	-8.34400000	14.31700000
O	22.89300000	-6.87000000	14.59700000
O	23.24300000	-12.96900000	15.27000000
O	23.20500000	-12.50300000	12.15900000
O	28.24700000	1.35400000	14.17300000
O	28.28500000	0.88800000	17.28400000
Pb	22.98400000	-4.23500000	18.17200000
Pb	30.68200000	-5.46700000	11.53100000
Pb	26.60400000	-3.28700000	11.90700000
Pb	24.61700000	-7.56500000	11.29100000
Pb	28.69500000	-9.74600000	10.91400000
Pb	20.08900000	-9.01400000	11.12900000
Pb	20.16500000	-9.94600000	17.35100000
Pb	18.45600000	-5.68400000	18.01000000
Pb	24.69300000	-8.49700000	17.51300000
Pb	28.77100000	-10.67800000	17.13600000
Pb	30.75800000	-6.39900000	17.75300000
Pb	26.68000000	-4.21900000	18.12900000
Pb	22.90800000	-3.30300000	11.95000000
Pb	18.38000000	-4.75200000	11.78800000
Pb	31.31400000	0.11200000	15.54000000
Pb	22.56900000	-9.62300000	14.18900000
Pb	18.28400000	-11.34200000	13.98400000
Pb	24.79900000	-5.61500000	14.76200000
Pb	30.57600000	-8.35000000	14.28100000
Pb	24.72300000	-4.68300000	8.54000000
Pb	20.50400000	-3.62600000	15.11200000
Pb	24.87500000	-6.54700000	20.98400000
Pb	26.29000000	-10.06900000	14.07600000
Pb	18.27400000	-7.63400000	14.53900000
Pb	29.08400000	-3.89600000	14.96700000
O	29.45600000	-1.25900000	18.53800000
O	20.94400000	-14.50500000	16.65900000
O	20.86800000	-13.57400000	10.43700000
O	29.38000000	-0.32700000	12.31600000
O	21.37900000	-9.34200000	19.01700000
O	21.26500000	-7.94400000	9.68400000
O	21.69400000	-3.90700000	10.28400000
O	21.80800000	-5.30500000	19.61700000
O	29.68200000	-6.31000000	9.82600000

O	29.79600000	-7.70800000	19.15900000
O	27.52500000	-4.68900000	8.50500000
O	27.67700000	-6.55300000	20.94900000
Sn	21.47900000	-5.92600000	9.98400000
Sn	27.63000000	-6.28300000	9.85500000
Sn	21.51700000	-6.39200000	13.09500000
Sn	21.55600000	-6.85800000	16.20600000
Sn	21.15300000	-12.47600000	12.18800000
Sn	21.19100000	-12.94200000	15.29900000
Sn	28.03300000	-0.66500000	13.87300000
Sn	28.07100000	-1.13100000	16.98400000
Sn	27.66800000	-6.74900000	12.96600000
Sn	27.70600000	-7.21500000	16.07700000
Sn	21.59400000	-7.32300000	19.31700000
Sn	27.74500000	-7.68100000	19.18800000

First co-ordination shell cluster of PbF_2

F	-8.12500000	-21.51200000	14.84800000
F	-10.57000000	-21.74600000	12.94100000
F	-10.91900000	-19.20100000	10.98800000
F	-7.85600000	-18.52000000	10.92900000
F	-9.10800000	-17.55200000	12.90500000
F	-7.78200000	-18.51300000	14.83600000
Pb	-8.53800000	-19.86500000	12.89900000
F	-6.12200000	-20.44400000	12.85400000
F	-10.84500000	-19.19300000	14.89500000
F	-8.19900000	-21.51900000	10.94200000

Third co-ordination shell cluster of PbF_2

F	-8.20300000	-25.08500000	14.85600000
F	-8.76500000	-14.55300000	12.89300000
F	-8.27700000	-25.09200000	10.95000000
F	-6.46600000	-23.44300000	12.86600000
F	-8.35000000	-25.09900000	7.04300000
F	-8.12900000	-25.07800000	18.76300000
F	-8.69100000	-14.54600000	16.80000000
F	-8.83800000	-14.56000000	8.98700000
F	-10.84100000	-15.62700000	10.98000000
F	-10.76800000	-15.62000000	14.88700000
F	-3.75100000	-20.21700000	10.85500000
F	-3.67700000	-20.21000000	14.76200000
F	-14.77500000	-21.65000000	14.97400000
F	-6.39300000	-14.32600000	10.89400000
F	-6.32000000	-14.31800000	14.80100000
F	-14.84900000	-21.65700000	11.06700000
F	-3.85200000	-16.05600000	14.75700000
F	-3.92500000	-16.06300000	10.85100000

F	-10.32200000	-25.89300000	16.85200000
F	-10.39600000	-25.90000000	12.94500000
F	-10.47000000	-25.90700000	9.03800000
F	-10.57000000	-21.74600000	12.94100000
F	-10.74400000	-23.35400000	10.99300000
F	-7.85600000	-18.52000000	10.92900000
F	-9.10800000	-17.55200000	12.90500000
F	-7.78200000	-18.51300000	14.83600000
F	-10.67100000	-23.34700000	14.90000000
F	-6.12200000	-20.44400000	12.85400000
F	-10.84500000	-19.19300000	14.89500000
F	-8.19900000	-21.51900000	10.94200000
F	-8.12500000	-21.51200000	14.84800000
F	-10.91900000	-19.20100000	10.98800000
F	-13.03800000	-20.00900000	12.98400000
F	-10.64400000	-21.75400000	9.03400000
F	-10.49700000	-21.73900000	16.84700000
F	-9.03400000	-17.54500000	16.81200000
F	-9.18200000	-17.55900000	8.99900000
F	-6.11800000	-16.87900000	8.94000000
F	-10.77200000	-19.18600000	18.80200000
F	-10.99200000	-19.20800000	7.08200000
F	-5.97100000	-16.86400000	16.75300000
F	-8.27300000	-21.52600000	7.03500000
F	-8.05200000	-21.50400000	18.75500000
F	-6.04500000	-16.87100000	12.84600000
F	-12.96500000	-20.00100000	16.89100000
F	-13.11200000	-20.01600000	9.07700000
F	-13.11600000	-23.58200000	12.99200000
F	-3.40200000	-22.76300000	12.80800000
F	-6.04900000	-20.43700000	16.76100000
F	-6.19600000	-20.45200000	8.94800000
F	-13.04200000	-23.57500000	16.89900000
F	-10.69400000	-15.61300000	18.79400000
F	-3.32900000	-22.75500000	16.71400000
F	-13.18900000	-23.58900000	9.08500000
F	-10.91500000	-15.63500000	7.07400000
F	-3.47600000	-22.77000000	8.90100000
F	-5.21300000	-24.41100000	10.89100000
F	-13.21300000	-15.85500000	12.97900000
F	-13.13900000	-15.84800000	16.88600000
F	-13.28600000	-15.86200000	9.07300000
F	-5.14000000	-24.40400000	14.79700000
Pb	-5.02600000	-18.24600000	14.78400000
Pb	-5.78300000	-22.09800000	10.89700000
Pb	-5.70900000	-22.09100000	14.80400000

Pb	-12.02000000	-21.38300000	14.92100000
Pb	-8.61200000	-19.87300000	8.99200000
Pb	-8.35100000	-16.19900000	14.84300000
Pb	-12.09300000	-21.39100000	11.01500000
Pb	-9.14800000	-23.70300000	16.82600000
Pb	-8.53800000	-19.86500000	12.89900000
Pb	-5.10000000	-18.25300000	10.87700000
Pb	-11.93800000	-17.82600000	9.05100000
Pb	-9.29500000	-23.71800000	9.01200000
Pb	-8.46500000	-19.85800000	16.80500000
Pb	-8.42500000	-16.20700000	10.93600000
Pb	-11.86400000	-17.81900000	12.95800000
Pb	-9.22200000	-23.71000000	12.91900000
Pb	-11.79000000	-17.81200000	16.86400000
F	-10.81800000	-23.36200000	7.08600000
F	-3.50300000	-18.60200000	16.71000000
F	-10.59700000	-23.34000000	18.80600000
F	-3.65000000	-18.61600000	8.89600000
F	-7.70800000	-18.50500000	18.74300000
F	-7.92900000	-18.52700000	7.02300000
F	-13.46000000	-17.47000000	7.12500000
F	-13.24000000	-17.44800000	18.84500000
F	-13.38700000	-17.46300000	11.03200000
F	-3.57700000	-18.60900000	12.80300000
F	-13.31300000	-17.45600000	14.93800000
F	-6.39200000	-23.43600000	16.77300000
F	-6.53900000	-23.45100000	8.96000000

First co-ordination shell cluster of $PbCl_2$

Cl	25.78100000	-6.73900000	16.08200000
Cl	23.22700000	-5.63300000	13.94300000
Cl	25.31400000	-0.90500000	14.29900000
Cl	27.55500000	-3.02600000	16.36000000
Cl	23.97500000	-3.37300000	16.38100000
Cl	28.17500000	-5.44200000	13.89000000
Pb	25.63800000	-3.72700000	14.06500000
Cl	23.91300000	-3.00700000	11.88200000
Cl	25.71900000	-6.37300000	11.58400000
Cl	27.49300000	-2.66000000	11.86100000

Third co-ordination shell cluster of $PbCl_2$

Cl	31.44800000	-1.66400000	16.41700000
Cl	24.63200000	1.87700000	12.26900000
Cl	24.69400000	1.51100000	16.76800000
Cl	31.38600000	-1.29800000	11.91800000
Cl	19.64600000	-5.98100000	13.96400000
Cl	25.37600000	-1.27100000	18.79700000

Cl	25.25200000	-0.54000000	9.80000000
Cl	31.32400000	-0.93200000	7.42000000
Cl	31.51000000	-2.02900000	20.91600000
Cl	19.58500000	-5.61500000	9.46500000
Cl	19.70800000	-6.34600000	18.46300000
Cl	28.11300000	-5.07700000	9.39100000
Cl	23.16500000	-5.26700000	9.44400000
Cl	23.28900000	-5.99900000	18.44200000
Cl	28.23700000	-5.80800000	18.38900000
Cl	22.57000000	-10.88300000	18.05400000
Cl	29.64300000	1.70200000	16.71600000
Cl	22.50800000	-10.51800000	13.55500000
Cl	29.58100000	2.06800000	12.21700000
Cl	22.44600000	-10.15200000	9.05700000
Cl	30.00000000	-10.06000000	15.75400000
Cl	23.22700000	-5.63300000	13.94300000
Cl	29.93800000	-9.69400000	11.25500000
Cl	19.02700000	-3.56400000	16.43400000
Cl	23.97500000	-3.37300000	16.38100000
Cl	28.17500000	-5.44200000	13.89000000
Cl	18.96500000	-3.19800000	11.93500000
Cl	23.91300000	-3.00700000	11.88200000
Cl	25.71900000	-6.37300000	11.58400000
Cl	27.49300000	-2.66000000	11.86100000
Cl	25.78100000	-6.73900000	16.08200000
Cl	25.31400000	-0.90500000	14.29900000
Cl	27.55500000	-3.02600000	16.36000000
Cl	27.44600000	-8.95400000	13.61500000
Cl	30.71900000	-5.17500000	16.14200000
Cl	30.65700000	-4.80900000	11.64300000
Cl	21.42100000	-2.26700000	14.24100000
Cl	28.89400000	-0.55800000	14.27800000
Cl	28.83200000	-0.19200000	9.77900000
Cl	28.95600000	-0.92400000	18.77600000
Cl	27.38400000	-8.58800000	9.11600000
Cl	27.50800000	-9.32000000	18.11300000
Cl	27.08800000	2.80800000	14.57600000
Cl	31.33900000	-7.59200000	13.67200000
Cl	22.15000000	1.24400000	14.51700000
Cl	25.05100000	-10.25000000	15.80700000
Cl	24.99000000	-9.88500000	11.30800000
Cl	21.95000000	-8.46700000	20.52400000
Cl	27.02600000	3.17400000	10.07700000
Cl	27.15000000	2.44200000	19.07500000
Cl	31.27700000	-7.22600000	9.17300000
Cl	21.76400000	-7.36900000	7.02800000

Cl	31.40000000	-7.95800000	18.17100000
Cl	19.69400000	0.31400000	12.21000000
Cl	33.11300000	-3.87900000	13.94900000
Cl	33.05100000	-3.51300000	9.45100000
Cl	33.17500000	-4.24500000	18.44800000
Cl	19.75600000	-0.05200000	16.70900000
Pb	28.49800000	-6.99600000	11.49500000
Pb	27.23100000	-0.20400000	16.59400000
Pb	28.56000000	-7.36200000	15.99300000
Pb	21.56400000	-5.27900000	16.25900000
Pb	30.39600000	-3.62200000	18.53700000
Pb	24.60400000	-7.96500000	9.20500000
Pb	25.63800000	-3.72700000	14.06500000
Pb	24.66600000	-8.33100000	13.70400000
Pb	30.33400000	-3.25600000	14.03800000
Pb	27.16900000	0.16200000	12.09500000
Pb	24.72800000	-8.69700000	18.20200000
Pb	22.47400000	-0.31000000	12.12100000
Pb	22.53600000	-0.67500000	16.62000000
Pb	25.57600000	-3.36100000	9.56600000
Pb	30.27200000	-2.89000000	9.54000000
Pb	25.70000000	-4.09300000	18.56300000
Pb	21.50200000	-4.91300000	11.76000000
Cl	23.85100000	-2.64100000	7.38300000
Cl	22.08800000	1.61000000	10.01800000
Cl	30.78100000	-5.54100000	20.64000000
Cl	25.11300000	-10.61600000	20.30600000
Cl	24.92800000	-9.51900000	6.80900000
Cl	30.59500000	-4.44300000	7.14400000
Cl	22.21200000	0.87800000	19.01600000
Cl	24.03700000	-3.73900000	20.88000000
Cl	21.82600000	-7.73500000	11.52600000
Cl	21.88800000	-8.10100000	16.02500000
Cl	27.43100000	-2.29400000	7.36200000
Cl	21.35900000	-1.90200000	9.74300000
Cl	25.65700000	-6.00700000	7.08500000
Cl	25.84300000	-7.10500000	20.58100000
Cl	21.48300000	-2.63300000	18.74000000
Cl	27.61700000	-3.39200000	20.85900000

First co-ordination shell cluster of $PbBr_2$

Br	27.27900000	4.85700000	12.79700000
Br	26.95700000	-1.35600000	14.66300000
Br	29.30200000	0.55900000	17.13900000
Br	29.18600000	0.95100000	12.42500000
Br	27.39500000	4.46400000	17.51100000
Pb	27.24700000	1.57500000	14.89900000

Br	25.39400000	1.24100000	12.54200000
Br	24.71900000	3.66800000	15.13600000
Br	25.51000000	0.84900000	17.25600000
Br	29.91200000	3.46600000	14.99100000

Third co-ordination shell cluster of $PbBr_2$

Br	30.86500000	-2.03800000	19.26000000
Br	30.63400000	-1.25300000	9.83100000
Br	30.74900000	-1.64600000	14.54500000
Br	25.27900000	1.63400000	7.82800000
Br	23.47200000	-3.27100000	9.83900000
Br	26.41000000	8.96400000	8.41000000
Br	32.78700000	2.47400000	21.96300000
Br	23.70300000	-4.05500000	19.26800000
Br	25.62600000	0.45700000	21.97100000
Br	32.44000000	3.65100000	7.82000000
Br	26.75700000	7.78700000	22.55300000
Br	21.07000000	-2.66500000	17.07300000
Br	35.30400000	1.47600000	19.44300000
Br	35.07300000	2.26000000	10.01500000
Br	20.95500000	-2.27200000	12.35900000
Br	35.18900000	1.86800000	14.72900000
Br	25.39400000	1.24100000	12.54200000
Br	24.71900000	3.66800000	15.13600000
Br	25.51000000	0.84900000	17.25600000
Br	29.91200000	3.46600000	14.99100000
Br	27.27900000	4.85700000	12.79700000
Br	26.95700000	-1.35600000	14.66300000
Br	29.30200000	0.55900000	17.13900000
Br	29.18600000	0.95100000	12.42500000
Br	27.39500000	4.46400000	17.51100000
Br	20.81100000	4.35000000	10.53800000
Br	33.19400000	-0.06400000	7.49300000
Br	21.04200000	3.56600000	19.96700000
Br	33.54100000	-1.24100000	21.63500000
Br	26.34700000	-4.26300000	16.81100000
Br	26.23200000	-3.87100000	12.09600000
Br	33.16600000	6.16600000	10.38700000
Br	23.38700000	5.48000000	22.44400000
Br	33.39700000	5.38100000	19.81500000
Br	28.74900000	-4.86900000	9.57700000
Br	28.98000000	-5.65400000	19.00500000
Br	23.04000000	6.65700000	8.30100000
Br	29.27400000	6.78900000	20.03300000
Br	29.04300000	7.57400000	10.60500000
Br	23.15600000	6.26500000	13.01500000
Br	23.27100000	5.87200000	17.72900000

Br	29.15800000	7.18100000	15.31900000
Br	27.07300000	-1.74800000	19.37700000
Br	26.84200000	-0.96300000	9.94800000
Br	33.28200000	5.77400000	15.10100000
Br	28.86500000	-5.26100000	14.29100000
Br	26.52500000	8.57200000	13.12500000
Br	26.64100000	8.18000000	17.83900000
Br	23.58800000	-3.66300000	14.55300000
Br	20.31700000	1.05000000	17.40100000
Br	31.71900000	8.37000000	12.98000000
Br	20.20100000	1.44300000	12.68600000
Br	31.83400000	7.97800000	17.69500000
Br	24.60300000	4.06000000	10.42100000
Br	24.83400000	3.27500000	19.85000000
Br	30.02800000	3.07400000	19.70600000
Br	29.79600000	3.85900000	10.27700000
Br	23.99700000	8.38700000	20.29600000
Br	23.88200000	8.78000000	15.58200000
Br	23.76600000	9.17200000	10.86700000
Br	31.42500000	-4.07200000	11.95200000
Br	31.54100000	-4.46500000	16.66600000
Br	33.31000000	-0.45700000	12.20700000
Br	20.92700000	3.95800000	15.25300000
Br	33.42500000	-0.84900000	16.92100000
Pb	29.01200000	-2.37200000	16.90300000
Pb	32.30600000	1.22200000	14.74600000
Pb	22.98200000	2.94200000	17.49300000
Pb	23.95300000	-2.01900000	17.05600000
Pb	30.27700000	5.11000000	17.49400000
Pb	32.42200000	0.83000000	19.46000000
Pb	26.39100000	6.14300000	20.05000000
Pb	27.36200000	1.18200000	19.61400000
Pb	27.24700000	1.57500000	14.89900000
Pb	22.86600000	3.33400000	12.77800000
Pb	28.89700000	-1.97900000	12.18800000
Pb	23.83800000	-1.62700000	12.34200000
Pb	26.16000000	6.92800000	10.62200000
Pb	27.13100000	1.96700000	10.18500000
Pb	32.19100000	1.61500000	10.03200000
Pb	30.16200000	5.50200000	12.78000000
Pb	26.27600000	6.53600000	15.33600000
Br	29.41800000	0.16600000	21.85400000
Br	22.95000000	-0.34000000	19.59500000
Br	27.51000000	4.07200000	22.22500000
Br	22.71800000	0.44400000	10.16700000
Br	27.16300000	5.24900000	8.08300000

Br	29.07100000	1.34300000	7.71100000
Br	32.67100000	2.86600000	17.24900000
Br	32.55600000	3.25800000	12.53400000
Br	22.83400000	0.05200000	14.88100000

First co-ordination shell cluster of PbClOH

H	0.92000000	-22.18400000	-16.20100000
Cl	-3.24800000	-25.41000000	-18.70500000
Cl	-4.53500000	-22.36300000	-16.27200000
Cl	-3.28300000	-25.95300000	-14.72300000
Cl	0.43500000	-25.12900000	-14.57900000
Cl	0.46900000	-24.58600000	-18.56100000
O	-1.90700000	-21.95800000	-18.22300000
Pb	-1.66900000	-23.56700000	-16.41200000
H	-2.78700000	-21.68500000	-18.19300000
O	0.04000000	-21.91100000	-16.17200000
O	-1.94100000	-22.50100000	-14.24100000
H	-2.82100000	-22.22800000	-14.21100000

Third co-ordination shell cluster of PbClOH

O	-6.10300000	-19.72200000	-11.86900000
O	4.23600000	-24.14700000	-22.52600000
O	-5.84300000	-25.27100000	-20.73700000
O	-1.97500000	-23.04400000	-10.25800000
O	-6.03400000	-18.63600000	-19.83400000
O	-1.87300000	-21.41500000	-22.20600000
O	4.13300000	-25.77600000	-10.57800000
O	-1.78300000	-29.67900000	-11.16100000
O	-5.91100000	-26.35700000	-12.77200000
O	-1.68100000	-28.05000000	-23.10900000
Cl	3.05400000	-27.29700000	-16.88000000
Cl	0.85500000	-30.37700000	-17.31900000
Cl	-8.25300000	-23.18600000	-16.41700000
Cl	2.60000000	-22.59200000	-10.15700000
Cl	2.70200000	-20.96300000	-22.10500000
Cl	0.88900000	-29.83400000	-21.30100000
Cl	-8.28700000	-23.72900000	-12.43400000
Cl	-8.21900000	-22.64400000	-20.39900000
Cl	0.82100000	-30.92000000	-13.33600000
Cl	-2.30200000	-18.74000000	-19.81600000
Cl	0.40100000	-25.67200000	-10.59600000
Cl	-3.31700000	-26.49600000	-10.74000000
Cl	-2.37000000	-19.82600000	-11.85100000
Cl	-3.21400000	-24.86700000	-22.68800000
Cl	0.50300000	-24.04300000	-22.54400000
Cl	-3.24800000	-25.41000000	-18.70500000
Cl	-4.53500000	-22.36300000	-16.27200000

Cl	-3.28300000	-25.95300000	-14.72300000
Cl	0.43500000	-25.12900000	-14.57900000
Cl	0.46900000	-24.58600000	-18.56100000
Cl	-5.51600000	-29.57600000	-11.17900000
Cl	1.41500000	-17.91700000	-19.67200000
Cl	1.34700000	-19.00200000	-11.70700000
Cl	-5.41400000	-27.94700000	-23.12700000
H	4.15100000	-25.05600000	-22.65000000
H	-0.56000000	-25.74100000	-20.75600000
H	-1.83400000	-30.04600000	-15.26800000
H	5.35700000	-21.83700000	-20.17300000
H	0.95400000	-21.64100000	-20.18400000
H	-2.85500000	-22.77100000	-10.22800000
H	-6.01800000	-18.81300000	-11.74400000
H	-7.22400000	-22.03200000	-14.22200000
H	-2.82100000	-22.22800000	-14.21100000
H	-4.99700000	-26.08800000	-16.78400000
H	-5.98400000	-18.27000000	-15.72700000
H	-7.19000000	-21.48900000	-18.20500000
H	-2.78700000	-21.68500000	-18.19300000
H	-8.70400000	-25.58900000	-18.77600000
H	-5.95000000	-17.72700000	-19.70900000
H	-2.75300000	-21.14200000	-22.17600000
H	4.04900000	-26.68500000	-10.70300000
H	-1.86800000	-30.58900000	-11.28600000
H	5.28900000	-22.92300000	-12.20800000
H	-5.03100000	-26.63100000	-12.80200000
H	5.32300000	-22.38000000	-16.19000000
H	-0.62800000	-26.82600000	-12.79100000
H	4.11700000	-25.59900000	-18.66800000
H	4.08300000	-26.14200000	-14.68500000
H	-1.80000000	-29.50300000	-19.25100000
H	0.92000000	-22.18400000	-16.20100000
H	-0.59400000	-26.28400000	-16.77300000
H	-8.73800000	-26.13200000	-14.79400000
H	0.88600000	-22.72700000	-12.21900000
H	-4.96300000	-25.54500000	-20.76700000
H	-1.76500000	-28.96000000	-23.23300000
O	-7.10500000	-20.58000000	-18.08000000
O	5.20400000	-23.83200000	-12.33200000
O	5.27200000	-22.74700000	-20.29700000
O	5.23800000	-23.29000000	-16.31500000
O	-7.85800000	-26.40500000	-14.82400000
O	-7.14000000	-21.12300000	-14.09700000
O	-7.82400000	-25.86200000	-18.80600000
Cl	-2.89700000	-31.74300000	-13.48000000

Cl	-4.92100000	-16.57200000	-17.51500000
Cl	-4.95500000	-17.11500000	-13.53200000
Cl	-2.86200000	-31.20000000	-17.46300000
Cl	-2.82800000	-30.65700000	-21.44500000
O	4.16700000	-25.23300000	-14.56100000
O	-5.87700000	-25.81400000	-16.75500000
O	4.20200000	-24.69000000	-18.54300000
O	-6.06900000	-19.17900000	-15.85200000
Cl	1.38100000	-18.45900000	-15.69000000
Cl	-5.48200000	-29.03300000	-15.16200000
Cl	-5.44800000	-28.49000000	-19.14400000
O	-1.71500000	-28.59300000	-19.12600000
O	-1.74900000	-29.13600000	-15.14400000
O	0.04000000	-21.91100000	-16.17200000
O	-1.94100000	-22.50100000	-14.24100000
O	-1.90700000	-21.95800000	-18.22300000
O	-0.67800000	-27.19300000	-16.89800000
Cl	3.02000000	-27.84000000	-12.89800000
Cl	3.08800000	-26.75400000	-20.86300000
Pb	-2.88000000	-28.11700000	-17.04300000
Pb	-1.70300000	-24.11000000	-12.43000000
Pb	0.45300000	-28.21200000	-14.99900000
Pb	3.03700000	-24.21300000	-16.46000000
Pb	3.07100000	-23.67000000	-20.44200000
Pb	-6.11400000	-24.20600000	-18.56600000
Pb	-1.63500000	-23.02400000	-20.39500000
Pb	0.48700000	-27.67000000	-18.98100000
Pb	-2.84600000	-27.57400000	-21.02500000
Pb	-0.23200000	-20.84500000	-14.00000000
Pb	-6.14900000	-24.74900000	-14.58300000
Pb	-4.93800000	-20.19900000	-13.95200000
Pb	-0.19800000	-20.30200000	-17.98300000
Pb	-1.66900000	-23.56700000	-16.41200000
Pb	-4.90400000	-19.65600000	-17.93500000
Pb	3.00200000	-24.75600000	-12.47700000
Pb	-2.91400000	-28.66000000	-13.06000000
Cl	-2.33600000	-19.28300000	-15.83400000
Cl	2.63400000	-22.04900000	-14.14000000
Cl	2.66800000	-21.50600000	-18.12200000
Cl	-4.57000000	-22.90600000	-12.29000000
Cl	-4.50100000	-21.82000000	-20.25500000
O	-0.71300000	-27.73600000	-12.91500000
O	0.07400000	-21.36800000	-20.15400000
O	-0.64400000	-26.65000000	-20.88000000
O	0.00600000	-22.45400000	-12.18900000

First co-ordination shell cluster of PbBrOH

Br	-27.60000000	5.66000000	-14.48900000
Br	-28.11500000	9.48100000	-13.65500000
Br	-28.10800000	10.35300000	-17.64600000
H	-24.92300000	5.42500000	-16.62700000
O	-24.52900000	6.26100000	-16.44400000
O	-24.65700000	8.64000000	-18.01500000
H	-24.26200000	9.47600000	-17.83200000
O	-24.66300000	7.76800000	-14.02300000
H	-24.26800000	8.60300000	-13.84000000
Pb	-26.01700000	8.08300000	-16.04800000
Br	-27.59400000	6.53200000	-18.48000000
Br	-24.55500000	10.91400000	-15.42700000

Third co-ordination shell cluster of PbBrOH

Br	-24.54900000	11.78600000	-19.41800000
Br	-24.56100000	10.04100000	-11.43500000
Br	-21.59200000	8.36900000	-15.97800000
Br	-31.07800000	12.02600000	-13.10300000
Br	-31.07100000	12.89800000	-17.09400000
Br	-21.07700000	4.54800000	-16.81300000
O	-29.95300000	8.39200000	-20.16800000
O	-24.52200000	7.13300000	-20.43500000
O	-29.96600000	6.64700000	-12.18600000
O	-24.53500000	5.38800000	-12.45200000
Br	-27.59400000	6.53200000	-18.48000000
Br	-24.55500000	10.91400000	-15.42700000
Br	-27.60000000	5.66000000	-14.48900000
Br	-28.11500000	9.48100000	-13.65500000
Br	-28.10800000	10.35300000	-17.64600000
Br	-18.76700000	10.26300000	-13.46900000
Br	-33.89600000	11.00400000	-19.60400000
Br	-33.90200000	10.13100000	-15.61200000
Br	-18.76100000	11.13600000	-17.46000000
Br	-33.90800000	9.25900000	-11.62100000
Br	-21.59800000	7.49600000	-11.98700000
Br	-21.58600000	9.24100000	-19.97000000
Br	-31.08400000	11.15400000	-9.11200000
Br	-21.08300000	3.67500000	-12.82100000
Br	-31.06500000	13.77100000	-21.08600000
Br	-21.07100000	5.42000000	-20.80400000
O	-26.48200000	1.15300000	-17.56300000
O	-28.14100000	14.13400000	-12.63800000
O	-26.48800000	0.28100000	-13.57200000
O	-22.70400000	13.74800000	-16.89600000
O	-28.13400000	15.00600000	-16.62900000
O	-26.47600000	2.02600000	-21.55400000

O	-22.71000000	12.87500000	-12.90400000
O	-28.01300000	11.75400000	-11.06700000
O	-28.00000000	13.49900000	-19.04900000
O	-28.07100000	1.03400000	-11.31900000
O	-31.53000000	10.01600000	-21.90700000
O	-24.66900000	6.89600000	-10.03200000
O	-21.12100000	12.99500000	-19.14900000
O	-31.54900000	7.40000000	-9.93300000
O	-28.05200000	3.65000000	-23.29300000
O	-21.13300000	11.25100000	-11.16600000
O	-24.65100000	9.51300000	-22.00600000
H	-24.92300000	5.42500000	-16.62700000
H	-20.19700000	11.97800000	-15.18700000
H	-23.63400000	13.89300000	-16.86500000
H	-24.26200000	9.47600000	-17.83200000
H	-27.74000000	15.84200000	-16.44600000
H	-20.19000000	12.85000000	-19.17900000
H	-32.46600000	9.28900000	-17.88500000
H	-29.00100000	1.17900000	-11.28800000
H	-24.93000000	4.55300000	-12.63600000
H	-27.74600000	14.97000000	-12.45400000
H	-28.40700000	10.91900000	-11.25000000
H	-25.55200000	1.00800000	-17.59300000
H	-25.55800000	0.13600000	-13.60200000
H	-28.99500000	2.05100000	-15.28000000
H	-32.47900000	7.54500000	-9.90300000
H	-28.98900000	2.92300000	-19.27100000
H	-29.03600000	6.50200000	-12.21600000
H	-32.47300000	8.41700000	-13.89400000
H	-29.02900000	7.37500000	-16.20700000
H	-24.91700000	6.29700000	-20.61800000
H	-32.46000000	10.16100000	-21.87700000
H	-29.02300000	8.24700000	-20.19900000
H	-28.40100000	11.79100000	-15.24100000
H	-28.98300000	3.79500000	-23.26200000
H	-25.54500000	1.88100000	-21.58400000
H	-24.25600000	10.34800000	-21.82300000
H	-28.39500000	12.66400000	-19.23200000
H	-23.64000000	13.02000000	-12.87400000
H	-20.20300000	11.10600000	-11.19600000
H	-24.27500000	7.73100000	-9.84900000
H	-24.26800000	8.60300000	-13.84000000
O	-21.12700000	12.12300000	-15.15700000
O	-28.06500000	1.90600000	-15.31000000
O	-28.00600000	12.62700000	-15.05800000
O	-28.05900000	2.77800000	-19.30100000

Br	-33.39400000	5.43800000	-12.45500000
Br	-25.07600000	13.86300000	-10.60100000
Br	-24.62400000	4.85900000	-23.02300000
Br	-33.38100000	7.18300000	-20.43800000
Br	-24.64300000	2.24300000	-11.04900000
Br	-25.06300000	15.60700000	-18.58400000
O	-24.65700000	8.64000000	-18.01500000
O	-24.66300000	7.76800000	-14.02300000
O	-29.96000000	7.51900000	-16.17700000
O	-24.52900000	6.26100000	-16.44400000
O	-31.53600000	9.14400000	-17.91500000
O	-31.54200000	8.27200000	-13.92400000
Br	-33.38700000	6.31000000	-16.44700000
Br	-25.06900000	14.73500000	-14.59300000
Pb	-30.68700000	8.87000000	-11.70100000
Pb	-30.67500000	10.61400000	-19.68400000
Pb	-26.65300000	12.31100000	-13.03400000
Pb	-30.68100000	9.74200000	-15.69300000
Pb	-30.81500000	6.92200000	-18.40000000
Pb	-27.19700000	4.24800000	-21.07000000
Pb	-26.01100000	8.95600000	-20.03900000
Pb	-26.01700000	8.08300000	-16.04800000
Pb	-30.82100000	6.05000000	-14.40900000
Pb	-23.17500000	5.94500000	-14.41900000
Pb	-27.20300000	3.37600000	-17.07800000
Pb	-21.98800000	10.65300000	-13.38900000
Pb	-23.16900000	6.81800000	-18.41100000
Pb	-26.64600000	13.18400000	-17.02500000
Pb	-21.98200000	11.52500000	-17.38000000
Pb	-27.21000000	2.50300000	-13.08700000
Pb	-26.02300000	7.21100000	-12.05600000
Br	-27.60600000	4.78800000	-10.49700000
Br	-28.12100000	8.60900000	-9.66300000
Br	-28.10200000	11.22600000	-21.63700000
Br	-30.43100000	2.89300000	-13.00700000
Br	-27.58700000	7.40400000	-22.47100000
Br	-30.41800000	4.63800000	-20.99000000
Br	-24.63700000	3.11500000	-15.04000000
Br	-24.63100000	3.98700000	-19.03200000
Br	-30.42400000	3.76500000	-16.99800000

First co-ordination shell of PbIOH

H	-6.88700000	-19.43700000	9.33000000
Pb	-8.93800000	-19.92100000	11.31600000
O	-8.84000000	-17.56600000	11.56700000
I	-11.66300000	-19.48300000	13.37300000
O	-7.89600000	-19.43400000	13.52200000

I	-11.50400000	-19.04400000	9.19500000
H	-7.04600000	-19.87600000	13.50800000
I	-9.57000000	-23.08500000	13.07500000
I	-9.41100000	-22.64700000	8.89600000
H	-9.69100000	-17.12400000	11.58100000
I	-5.91400000	-21.58200000	11.25600000
O	-7.73800000	-18.99600000	9.34400000

Third co-ordination shell of PbIOH

O	-7.42900000	-24.79500000	6.63100000
O	-2.16200000	-20.03100000	7.33200000
O	-2.68800000	-22.13100000	9.20600000
O	-7.74700000	-25.67200000	14.98700000
O	-6.48600000	-26.66300000	8.58600000
O	-13.32200000	-24.63700000	16.99900000
O	-2.84700000	-22.57000000	13.38400000
O	-14.57400000	-16.97000000	17.75700000
O	-6.64500000	-27.10200000	12.76400000
O	-2.48000000	-20.90800000	15.68800000
O	-8.05500000	-19.87300000	17.70000000
O	-14.09700000	-15.65300000	5.22300000
O	-12.84500000	-23.32100000	4.46500000
O	-13.73000000	-13.99100000	7.52600000
O	-14.25600000	-16.09200000	9.40100000
O	-14.04800000	-14.86900000	15.88200000
O	-14.41500000	-16.53100000	13.57900000
O	-13.88900000	-14.43000000	11.70400000
O	-7.57900000	-18.55700000	5.16600000
H	-13.22200000	-13.74900000	11.80100000
H	-15.08300000	-17.21200000	13.48200000
H	-9.69100000	-17.12400000	11.58100000
H	-11.97000000	-21.41700000	11.04300000
H	-13.83100000	-24.88000000	12.72400000
H	-8.43900000	-24.79200000	10.82300000
H	-8.28000000	-24.35300000	6.64500000
H	-15.24100000	-17.65100000	17.66000000
H	-9.85000000	-17.56300000	15.75900000
H	-12.12800000	-21.85600000	15.22100000
H	-13.98900000	-25.31800000	16.90200000
H	-8.59800000	-25.23100000	15.00100000
H	-13.67200000	-24.44100000	8.54600000
H	-11.81100000	-20.97800000	6.86500000
H	-9.53200000	-16.68600000	7.40300000
H	-14.92400000	-16.77300000	9.30400000
H	-13.06300000	-13.31000000	7.62300000
H	-13.51300000	-24.00200000	4.36800000
H	-14.76500000	-16.33400000	5.12600000

H	-7.20400000	-20.31500000	17.68600000
H	-1.81300000	-20.22700000	15.78500000
H	-5.79400000	-27.54400000	12.75000000
H	-7.04600000	-19.87600000	13.50800000
H	-3.51500000	-23.25100000	13.28700000
H	-1.65400000	-19.78800000	11.60700000
H	-6.72800000	-18.99800000	5.15200000
H	-5.63500000	-27.10500000	8.57200000
H	-6.88700000	-19.43700000	9.33000000
H	-3.35600000	-22.81200000	9.10900000
H	-1.49500000	-19.34900000	7.42900000
H	-13.38000000	-14.18800000	15.97900000
I	-10.66300000	-14.97900000	9.65400000
I	-11.50400000	-19.04400000	9.19500000
I	-6.07300000	-22.02100000	15.43400000
I	-9.41100000	-22.64700000	8.89600000
I	-5.91400000	-21.58200000	11.25600000
I	-5.07300000	-17.51700000	11.71500000
I	-15.38900000	-19.14600000	11.15200000
I	-10.82200000	-15.41800000	13.83200000
I	-11.66300000	-19.48300000	13.37300000
I	-5.75500000	-21.14400000	7.07800000
I	-9.57000000	-23.08500000	13.07500000
O	-7.58800000	-25.23400000	10.80900000
O	-12.47800000	-21.65900000	6.76800000
O	-8.84000000	-17.56600000	11.56700000
O	-12.63700000	-22.09800000	10.94700000
O	-13.16300000	-24.19900000	12.82100000
O	-8.68100000	-17.12700000	7.38900000
O	-7.89600000	-19.43400000	13.52200000
O	-8.99900000	-18.00500000	15.74500000
O	-12.79600000	-22.53700000	15.12500000
O	-2.32100000	-20.46900000	11.51000000
O	-13.00400000	-23.76000000	8.64300000
O	-7.73800000	-18.99600000	9.34400000
Pb	-11.79400000	-24.30500000	10.74700000
Pb	-11.95300000	-24.74400000	14.92500000
Pb	-8.93800000	-19.92100000	11.31600000
Pb	-13.20500000	-17.07600000	15.68300000
Pb	-13.04600000	-16.63700000	11.50500000
Pb	-13.84700000	-21.55300000	8.84300000
Pb	-11.63500000	-23.86600000	6.56900000
Pb	-8.77900000	-19.48200000	7.13800000
Pb	-12.88700000	-16.19800000	7.32600000
Pb	-3.69000000	-20.36300000	13.58400000
Pb	-6.54700000	-24.74700000	13.01500000

Pb	-7.64000000	-16.64000000	9.59500000
Pb	-6.38800000	-24.30800000	8.83700000
Pb	-3.53100000	-19.92400000	9.40600000
Pb	-7.79900000	-17.07900000	13.77300000
Pb	-14.00600000	-21.99200000	13.02100000
Pb	-9.09700000	-20.36000000	15.49400000
I	-7.32500000	-14.35400000	16.19200000
I	-3.98000000	-25.62400000	15.13600000
I	-10.50400000	-14.54000000	5.47600000
I	-11.34500000	-18.60600000	5.01700000
I	-9.25200000	-22.20800000	4.71800000
I	-5.23200000	-17.95600000	15.89300000
I	-4.91400000	-17.07800000	7.53700000
I	-3.82100000	-25.18500000	10.95800000
I	-1.34700000	-17.85400000	13.93700000
I	-9.72900000	-23.52400000	17.25300000
I	-7.16600000	-13.91500000	12.01400000
I	-11.82200000	-19.92200000	17.55100000
I	-10.98100000	-15.85600000	18.01000000
I	-7.00700000	-13.47600000	7.83600000
I	-1.18800000	-17.41600000	9.75900000
I	-3.66200000	-24.74600000	6.78000000
I	-10.09300000	-26.27300000	4.25900000
I	-15.23000000	-18.70700000	6.97400000
I	-10.57000000	-27.59000000	16.79400000
I	-16.38900000	-23.65000000	14.87100000
I	-14.29600000	-27.25200000	14.57200000
I	-15.54800000	-19.58400000	15.33000000
I	-10.41100000	-27.15100000	12.61600000
I	-16.23000000	-23.21100000	10.69300000
I	-10.25200000	-26.71200000	8.43700000
I	-16.07100000	-22.77200000	6.51500000
I	-13.97800000	-26.37500000	6.21600000
I	-14.13700000	-26.81300000	10.39400000

First co-ordination shell cluster of $PbSiO_3$ (site 1)

O	12.95400000	23.91100000	-3.44200000
Pb	13.10400000	21.78400000	-2.57300000
O	11.40900000	19.44000000	-3.16700000
O	13.87900000	21.32500000	-4.68800000
O	10.71900000	21.87600000	-3.34900000
O	15.91200000	21.18400000	-2.46500000
O	11.95600000	23.53700000	-0.62800000

Third co-ordination shell cluster of $PbSiO_3$ (site 1)

O	12.21600000	-25.61600000	0.43600000
O	19.92400000	-20.27700000	-6.70300000
O	13.29900000	-25.89000000	-4.87300000
O	20.53400000	-22.42800000	-2.25800000
O	14.35500000	-25.96400000	-1.06200000
O	17.58200000	-15.80500000	-5.71600000
O	13.92500000	-19.51700000	-8.14800000
O	19.43300000	-17.24300000	-4.20100000
O	20.33500000	-19.63700000	-3.27500000
O	11.46900000	-23.34900000	-5.45700000
O	13.97700000	-23.32200000	1.86800000
O	10.85800000	-20.92100000	-4.68600000
O	17.72600000	-19.29500000	-5.68800000
O	13.94200000	-16.65600000	-4.28600000
O	15.30000000	-21.35100000	0.83600000
O	11.87100000	-18.21700000	-0.76100000
O	12.47700000	-18.09300000	-5.93400000
O	18.94000000	-20.50000000	-0.59400000
O	10.30200000	-17.50700000	-2.85600000
O	16.62300000	-19.38100000	-0.19600000
O	17.25500000	-24.13900000	-4.72500000
O	16.04600000	-23.85500000	0.36400000
O	10.69600000	-20.04400000	-2.22200000
O	18.54700000	-17.96300000	-1.22700000
O	14.82600000	-23.80900000	-5.60000000
O	12.99700000	-21.26800000	-6.18400000
O	15.28300000	-24.21200000	-3.02600000
O	12.61900000	-18.62600000	-3.25400000
O	13.02700000	-22.09800000	-3.59300000
O	14.68700000	-19.16000000	-4.75800000
O	13.83600000	-22.78800000	-0.81200000
O	17.37200000	-19.79000000	-2.68900000
O	15.97400000	-21.88800000	-4.24100000
Pb	18.70600000	-21.05200000	-4.03300000
Pb	14.68600000	-20.78500000	-2.72300000
Pb	13.13900000	-24.23700000	-2.35500000
Pb	17.16700000	-17.67000000	-4.15300000
Pb	15.21800000	-20.68500000	-6.40100000
Si	12.14700000	-21.90600000	-4.95600000
Si	14.78900000	-22.86200000	0.49700000
Si	13.43100000	-18.16600000	-4.62500000
Si	17.88800000	-19.42200000	-1.19000000
Si	15.81800000	-23.50200000	-4.38100000
Si	11.35400000	-18.58500000	-2.26000000

Fifth co-ordination shell cluster of $PbSiO_3$ (site 1)

O	-11.71900000	16.89800000	-5.39700000
O	-11.59800000	15.02300000	-16.46900000
O	-20.78800000	22.54800000	-21.08500000
O	-8.84300000	26.59200000	-13.49000000
O	-8.91400000	19.01800000	-8.94100000
O	-23.59300000	20.42800000	-17.54100000
O	-22.00700000	27.52600000	-13.76700000
O	-7.61300000	18.32700000	-11.08700000
O	-19.27800000	16.05700000	-7.58900000
O	-16.39600000	29.04500000	-6.80000000
O	-11.43000000	25.96000000	-15.74500000
O	-25.57300000	24.31400000	-12.38000000
O	-6.83300000	19.58100000	-13.24200000
O	-9.49400000	16.75500000	-10.12300000
O	-9.24400000	21.35400000	-7.56200000
O	-9.12300000	19.47900000	-18.63400000
O	-20.75300000	29.46300000	-12.30300000
O	-23.01300000	22.69100000	-16.35900000
O	-11.60400000	16.32900000	-18.75700000
O	-9.69500000	25.50300000	-11.24800000
O	-12.29500000	15.74800000	-9.41200000
O	-16.06400000	29.70700000	-9.89300000
O	-16.65200000	16.16700000	-14.91400000
O	-13.65200000	27.93400000	-15.57300000
O	-13.47400000	28.17600000	-18.58300000
O	-18.65400000	22.51600000	-6.18700000
O	-13.85400000	16.93000000	-20.29600000
O	-11.79800000	20.78800000	-5.81900000
O	-17.89200000	30.15600000	-11.85800000
O	-11.03600000	28.42900000	-11.49000000
O	-14.18500000	14.39100000	-18.72500000
O	-11.46600000	23.32800000	-7.39000000
O	-18.32200000	25.05500000	-7.75800000
O	-18.58100000	19.93200000	-8.05300000
O	-16.91400000	15.94500000	-11.90900000
O	-14.30600000	16.26600000	-7.65300000
O	-19.15200000	17.47600000	-9.78000000
O	-22.45000000	25.22800000	-14.94100000
O	-15.64900000	18.87000000	-20.38100000
O	-21.45800000	26.94400000	-10.47200000
O	-20.78200000	21.24200000	-18.79700000
O	-20.08600000	25.11600000	-19.26100000
O	-16.52800000	18.24000000	-7.48100000
O	-8.99900000	21.55200000	-11.20000000
O	-18.45400000	16.75100000	-16.83700000

O	-18.96000000	27.80200000	-10.32700000
O	-22.95600000	24.80900000	-8.29800000
O	-11.38800000	23.70600000	-17.10400000
O	-23.20700000	20.21000000	-10.85900000
O	-18.28600000	27.68700000	-16.11300000
O	-20.64700000	18.58700000	-14.83700000
O	-11.98300000	24.19900000	-21.03100000
O	-11.72500000	18.20400000	-7.68500000
O	-13.93200000	20.82000000	-20.71700000
O	-15.69900000	28.31900000	-13.85700000
O	-13.35100000	25.26400000	-7.82200000
O	-9.54500000	24.02300000	-15.31400000
O	-9.88100000	16.97300000	-16.80600000
O	-14.48000000	23.34100000	-21.17600000
O	-8.29500000	24.07100000	-13.03200000
O	-18.46000000	18.05600000	-19.12400000
O	-12.82600000	18.85900000	-13.05700000
O	-19.68200000	20.58700000	-13.42500000
O	-20.90900000	24.42300000	-10.01300000
O	-14.05300000	22.69600000	-9.64600000
O	-16.40100000	25.75100000	-15.68100000
O	-14.46900000	20.05500000	-11.45500000
O	-21.32500000	21.78200000	-11.82200000
O	-13.23000000	23.38900000	-18.89300000
O	-18.03900000	19.39100000	-15.02800000
O	-16.73700000	18.70000000	-17.17300000
O	-14.60100000	25.21600000	-10.10400000
O	-15.77000000	20.74600000	-9.30900000
O	-15.15100000	25.79900000	-13.39900000
O	-20.05700000	25.51300000	-12.25500000
O	-13.20100000	23.78500000	-11.88700000
O	-16.55100000	27.23000000	-11.61600000
O	-13.92600000	19.51500000	-18.43000000
O	-15.85500000	23.28000000	-11.56800000
O	-15.97900000	21.20600000	-19.00200000
O	-13.35600000	21.97100000	-16.70300000
O	-20.54500000	23.03600000	-13.97800000
O	-13.68900000	21.30800000	-13.61000000
O	-18.20100000	23.18000000	-18.82900000
O	-11.86000000	20.85900000	-11.64500000
O	-18.71600000	22.58600000	-12.01300000
O	-10.79200000	23.21300000	-13.17700000
O	-13.97500000	18.80600000	-9.22400000
O	-17.64800000	24.94100000	-13.54400000
O	-11.67700000	18.91300000	-16.89100000
O	-18.53300000	20.64000000	-17.25900000

O	-16.15700000	20.96400000	-15.99200000
O	-16.35100000	18.48200000	-10.49100000
O	-15.59400000	23.50100000	-14.57400000
O	-14.03700000	25.63900000	-20.00100000
O	-9.30100000	19.23600000	-15.62400000
O	-13.79100000	16.86000000	-14.47000000
Pb	-9.37000000	20.03900000	-12.87500000
Pb	-16.28100000	17.68000000	-13.24000000
Pb	-16.75000000	16.68900000	-9.14700000
Pb	-16.22700000	21.76600000	-13.24300000
Pb	-15.75700000	22.75700000	-17.33500000
Pb	-23.08300000	23.49400000	-13.61000000
Pb	-13.87400000	26.38300000	-17.24000000
Pb	-14.10300000	18.39300000	-7.01900000
Pb	-11.09700000	22.84500000	-10.98100000
Pb	-13.98200000	16.51700000	-18.09100000
Pb	-11.67000000	21.20100000	-8.02400000
Pb	-11.54900000	19.32600000	-19.09600000
Pb	-17.95300000	24.57200000	-11.34900000
Pb	-18.52600000	22.92900000	-8.39200000
Pb	-18.40500000	21.05300000	-19.46400000
Pb	-11.79900000	26.44300000	-12.15500000
Pb	-18.65500000	28.17000000	-12.52200000
Pb	-13.85700000	19.79300000	-16.14100000
Pb	-11.79400000	17.92600000	-9.97400000
Pb	-19.89800000	25.17700000	-14.53200000
Pb	-20.71400000	21.52000000	-16.50900000
Pb	-18.65000000	19.65300000	-10.34100000
Pb	-16.71000000	27.56600000	-9.33900000
Pb	-13.04200000	23.44900000	-14.16400000
O	-11.96300000	16.41000000	-12.50500000
O	-14.15800000	27.51400000	-8.93000000
O	-16.27500000	27.16900000	-17.87200000
O	-16.40700000	16.36500000	-18.55300000
O	-16.10000000	23.08100000	-7.93000000
O	-13.89700000	27.73500000	-11.93500000
O	-20.90300000	23.11800000	-7.72600000
O	-20.83100000	20.53300000	-9.59200000
O	-18.81900000	18.13800000	-12.87300000
O	-14.04700000	21.39000000	-7.35800000
O	-22.71100000	25.00700000	-11.93600000
Si	-14.45500000	23.73200000	-10.85800000
Si	-15.01600000	22.00300000	-8.50700000
Si	-14.89500000	20.12800000	-19.57900000
Si	-21.31100000	25.45900000	-11.22500000
Si	-21.87200000	23.73100000	-8.87500000

Si	-17.49100000	17.44300000	-17.97500000
Si	-15.29800000	27.28300000	-12.64600000
Si	-13.16800000	20.33100000	-12.44500000
Si	-12.32100000	22.55600000	-17.78500000
Si	-19.34000000	19.11500000	-14.03800000
Si	-20.02400000	22.05900000	-12.81200000
Si	-19.17700000	24.28300000	-18.15200000
Si	-17.31000000	26.58400000	-16.79000000
Si	-12.48400000	17.38700000	-13.67000000
Si	-9.35100000	23.25300000	-13.91500000
Si	-15.14400000	19.50300000	-10.10200000
Si	-10.50800000	18.21500000	-16.01300000
Si	-16.20700000	24.98000000	-14.28200000
Si	-22.00000000	21.23100000	-10.47000000
Si	-17.36400000	19.94300000	-16.38000000
Si	-13.54500000	26.03500000	-9.22100000
Si	-13.42400000	24.15900000	-20.29200000
O	-8.73800000	21.77300000	-14.20600000
O	-12.10400000	26.07400000	-9.95900000
O	-11.34500000	21.45200000	-18.46200000
O	-20.21200000	23.69800000	-17.07000000
O	-22.62700000	22.47300000	-9.67700000
O	-11.18300000	17.66400000	-14.66000000
O	-18.24400000	25.43400000	-17.47100000

First co-ordination shell cluster of $PbSiO_3$ (site 2)

O	-18.06200000	7.05500000	20.60600000
O	-20.28100000	5.64800000	20.77900000
O	-22.61800000	6.52500000	17.76900000
O	-19.65800000	4.25900000	16.27200000
O	-18.26600000	3.98500000	18.93400000
O	-21.25500000	3.83200000	18.93800000
Pb	-19.83200000	5.51500000	18.38900000

Third co-ordination shell cluster of $PbSiO_3$ (site 2)

O	2.53700000	-24.88300000	-21.19100000
O	4.57300000	-15.65400000	-15.83700000
O	-0.24100000	-17.66000000	-14.69700000
O	6.69300000	-23.95700000	-17.92600000
O	-1.41900000	-17.24200000	-24.06900000
O	7.79400000	-19.35300000	-16.29000000
O	6.70000000	-16.22500000	-17.24200000
O	1.62600000	-15.91900000	-23.14200000
O	3.64800000	-25.28000000	-18.85400000
O	0.37900000	-16.16100000	-18.36600000
O	1.55900000	-23.57400000	-23.38100000
O	1.41700000	-18.48900000	-24.78900000

O	-2.22600000	-17.46300000	-17.18400000
O	-0.95900000	-18.44800000	-19.72400000
O	2.32800000	-21.05300000	-24.76600000
O	-0.10500000	-22.80000000	-20.76800000
O	-0.82900000	-22.45700000	-16.14800000
O	1.73100000	-22.13800000	-15.80100000
O	2.84500000	-15.07300000	-18.50000000
O	2.73700000	-16.31500000	-20.80400000
O	0.75600000	-20.76500000	-22.22200000
O	0.87300000	-24.10900000	-18.57800000
O	-2.46400000	-22.64500000	-18.33000000
O	4.40100000	-17.09000000	-23.41700000
O	4.01000000	-21.16800000	-15.05000000
O	5.09800000	-15.58400000	-19.76500000
O	5.27200000	-19.64200000	-23.53100000
O	6.88100000	-20.49400000	-20.86600000
O	-1.89500000	-20.23400000	-17.20400000
O	6.49100000	-18.79600000	-18.89000000
O	3.85700000	-22.71000000	-17.20600000
O	5.37900000	-18.39900000	-21.22700000
O	0.00200000	-21.55700000	-18.46400000
O	3.01800000	-19.13100000	-22.26700000
O	2.25600000	-22.06800000	-19.72900000
O	3.71500000	-17.62500000	-18.61400000
O	2.94600000	-20.14500000	-17.22900000
O	4.51800000	-20.43400000	-19.77300000
Pb	5.21800000	-18.35900000	-17.05400000
Pb	2.46400000	-19.63100000	-19.34400000
Pb	-0.24600000	-18.43300000	-17.61300000
Pb	2.81000000	-21.56800000	-22.65200000
Pb	0.87700000	-18.32200000	-22.55500000
Pb	4.39700000	-22.87600000	-19.44000000
Si	-1.35700000	-21.72500000	-17.55500000
Si	4.47800000	-18.51900000	-22.62900000
Si	3.63900000	-16.19500000	-19.40200000
Si	0.79600000	-22.67900000	-19.36600000
Si	3.15100000	-21.51800000	-16.39100000
Si	5.80000000	-19.52600000	-20.17000000

Fifth co-ordination shell cluster of $PbSiO_3$ (site 2)

O	-25.97000000	-14.80400000	14.95800000
O	-28.29300000	1.56900000	11.03700000
O	-29.51700000	-0.33600000	22.03600000
O	-30.97500000	-12.14600000	6.63200000
O	-26.97300000	-10.88100000	21.46300000
O	-37.51300000	-5.98400000	12.93500000
O	-19.09300000	-7.08400000	12.61600000

O	-36.37200000	-10.37500000	15.75000000
O	-27.95800000	-1.37800000	6.56600000
O	-29.02700000	2.73700000	18.36700000
O	-35.17600000	-2.88900000	8.76200000
O	-34.52200000	2.32100000	13.71000000
O	-27.35400000	-12.84400000	17.49300000
O	-26.13000000	-10.93900000	6.49300000
O	-34.36300000	-1.54400000	22.17400000
O	-34.74600000	-5.91700000	8.86100000
O	-29.51400000	-11.49200000	21.79700000
O	-30.97800000	-0.99000000	6.87100000
O	-25.95200000	-5.96600000	6.56900000
O	-24.09300000	-7.68800000	8.90700000
O	-36.37100000	-0.97500000	12.69500000
O	-33.46900000	-7.79200000	7.37400000
O	-35.55000000	0.55200000	15.37000000
O	-32.86500000	3.46700000	12.01300000
O	-31.18600000	4.14400000	14.63700000
O	-21.33600000	-11.80000000	14.54800000
O	-20.37100000	-10.62400000	11.22800000
O	-26.56100000	2.03000000	13.10000000
O	-21.99600000	-9.66700000	20.99100000
O	-35.09500000	-6.83500000	17.13800000
O	-24.94300000	-13.03400000	13.29900000
O	-24.03700000	-8.39200000	22.40600000
O	-29.06300000	-3.41600000	22.70900000
O	-31.42900000	-9.06800000	5.95900000
O	-22.83900000	-0.90600000	15.42000000
O	-27.86700000	4.07000000	15.72300000
O	-26.62200000	-7.55300000	22.52900000
O	-31.64900000	-2.57700000	22.83200000
O	-28.84400000	-9.90600000	5.83600000
O	-30.94300000	-12.79900000	19.55700000
O	-34.69300000	-9.69700000	18.37300000
O	-30.82600000	2.19200000	10.59800000
O	-20.77300000	-7.76200000	9.99200000
O	-23.08500000	-9.59200000	10.57000000
O	-23.84700000	0.99800000	13.75700000
O	-29.14600000	2.86900000	13.22200000
O	-28.09100000	-13.29300000	12.63300000
O	-32.40200000	0.81000000	16.03400000
O	-33.13800000	0.36200000	11.17600000
O	-36.33700000	-4.22300000	11.40600000
O	-29.54900000	0.31700000	9.11100000
O	-31.79900000	-12.27200000	14.77300000
O	-36.02400000	-4.85000000	15.56300000

O	-25.31600000	-9.59400000	19.90600000
O	-24.12100000	-11.50800000	15.97500000
O	-21.53400000	-2.94700000	12.79700000
O	-21.56400000	-7.73800000	17.51100000
O	-33.90100000	-9.72100000	10.85400000
O	-21.13300000	-5.80900000	14.03100000
O	-31.15700000	-5.96200000	6.79600000
O	-25.80800000	-1.35700000	19.89700000
O	-22.46300000	-0.96100000	11.22200000
O	-29.71900000	-10.89400000	8.55800000
O	-30.77400000	-1.58800000	20.11000000
O	-32.00000000	-5.90400000	21.76600000
O	-28.49300000	-6.57900000	6.90300000
O	-32.48600000	-10.96100000	12.63200000
O	-23.95300000	-2.09600000	8.59200000
O	-34.74300000	-3.50800000	18.20500000
O	-24.49100000	-5.31300000	21.73300000
O	-25.74800000	-8.97600000	10.46300000
O	-29.33600000	-6.52100000	21.87200000
O	-24.00000000	-2.24000000	18.06400000
O	-22.40900000	-3.93500000	15.51900000
O	-27.43600000	1.04200000	15.82100000
O	-31.37400000	-9.77200000	19.45900000
O	-26.59100000	-2.76100000	17.81400000
O	-29.49600000	-2.65600000	13.40700000
O	-30.99700000	-9.82700000	15.26100000
O	-24.46900000	-7.63200000	13.10500000
O	-22.97900000	-6.49800000	15.73400000
O	-28.00500000	-1.52100000	16.03700000
O	-29.71700000	-8.48400000	17.90200000
O	-31.96000000	-3.45700000	13.02100000
O	-28.69300000	-0.21000000	13.89600000
O	-28.53300000	-9.02500000	15.64800000
O	-33.56000000	-4.04800000	15.95000000
O	-26.93300000	-8.43400000	12.71800000
O	-25.49700000	-9.40200000	14.76400000
O	-24.12000000	-2.10700000	12.91900000
O	-30.52300000	-4.42500000	15.06700000
O	-27.83900000	-1.50900000	11.71100000
O	-29.97000000	-8.05700000	13.60100000
O	-26.36200000	-6.82400000	14.85000000
O	-34.13100000	-5.65900000	13.81900000
O	-25.39800000	-5.64800000	11.53000000
O	-31.38900000	-1.84700000	15.15300000
O	-30.42400000	-0.67200000	11.83300000
O	-29.10400000	-10.63600000	13.51600000

O	-30.14900000	-7.86500000	8.46000000
O	-30.34400000	-4.61700000	20.20900000
O	-29.18300000	-3.28300000	17.56500000
O	-24.15600000	-8.26000000	17.26200000
O	-31.30900000	-9.19900000	11.10400000
O	-28.11100000	-4.61500000	10.87300000
O	-27.37500000	-4.16700000	15.73200000
O	-33.11700000	-8.31600000	12.93600000
O	-29.14700000	-6.53100000	16.27700000
O	-25.79900000	-2.78500000	10.29500000
O	-31.34500000	-5.95200000	12.39200000
O	-27.17600000	-7.87300000	17.56800000
O	-28.29000000	-9.58700000	10.79700000
O	-25.74700000	-6.56500000	19.80700000
O	-32.20300000	-2.89600000	17.87100000
O	-22.81200000	-6.48600000	11.40800000
O	-32.65300000	-10.97300000	16.95800000
O	-27.02300000	-4.69000000	21.29400000
Pb	-26.13100000	-6.14900000	9.42300000
Pb	-25.73900000	-6.21300000	16.96400000
Pb	-27.35400000	-8.05500000	20.42100000
Pb	-31.15700000	-1.17300000	9.72500000
Pb	-30.76600000	-1.23700000	17.26700000
Pb	-32.38100000	-3.07900000	20.72400000
Pb	-29.72700000	-11.24600000	11.40100000
Pb	-28.11100000	-9.40400000	7.94400000
Pb	-29.33600000	-11.31000000	18.94300000
Pb	-34.75300000	-6.27000000	11.70400000
Pb	-23.41500000	-10.54900000	14.06900000
Pb	-21.60800000	-8.59200000	11.90600000
Pb	-25.32400000	-0.00200000	12.42100000
Pb	-28.44200000	-5.57200000	14.37100000
Pb	-26.63500000	-3.61600000	12.20900000
Pb	-33.46900000	-0.59600000	14.67300000
Pb	-31.66100000	1.36100000	12.51200000
Pb	-27.02400000	-11.88700000	13.99400000
Pb	-32.05000000	-6.91000000	14.29700000
Pb	-33.85700000	-8.86700000	16.45900000
Pb	-25.72000000	-9.93100000	16.99800000
Pb	-23.64500000	-8.02800000	20.16300000
Pb	-27.44800000	-1.14600000	9.46700000
Pb	-30.74700000	-4.95400000	17.30000000
Pb	-28.67200000	-3.05100000	20.46600000
Pb	-24.51100000	-2.47200000	15.16300000
Pb	-29.53800000	2.50500000	15.46500000
Pb	-29.74600000	-7.52900000	11.36700000

Pb	-31.82000000	-9.43100000	8.20200000
Pb	-34.77300000	-2.55200000	11.67000000
O	-30.06800000	-11.81200000	16.83600000
O	-24.52200000	-4.66000000	8.80800000
O	-26.31800000	-10.92800000	12.08900000
O	-34.17400000	-1.55400000	16.58000000
O	-32.38100000	-7.86800000	17.79600000
O	-22.34800000	-9.14400000	15.42900000
O	-34.99600000	-3.08100000	13.90400000
O	-33.31700000	-4.61000000	11.10000000
O	-29.11900000	-2.71200000	9.20900000
O	-23.26700000	-3.40700000	10.73400000
O	-25.17800000	-4.00200000	19.59200000
Si	-25.83300000	-8.05700000	13.91800000
Si	-24.10500000	-6.21600000	12.35200000
Si	-22.82700000	-2.37700000	11.97400000
Si	-30.86000000	-3.08100000	14.22100000
Si	-29.13200000	-1.24100000	12.65400000
Si	-29.63300000	-9.40100000	14.44700000
Si	-31.36100000	-11.24200000	16.01300000
Si	-34.65900000	-4.42500000	14.75000000
Si	-25.36600000	-2.52500000	18.86300000
Si	-27.81700000	-2.99900000	16.76600000
Si	-29.34300000	-4.12500000	9.94000000
Si	-30.56800000	-6.03100000	20.93900000
Si	-29.92500000	-6.45200000	7.72900000
Si	-32.67500000	-9.48400000	11.90300000
Si	-31.14900000	-8.35700000	18.72800000
Si	-22.79000000	-7.97500000	16.46200000
Si	-22.52800000	-5.34200000	14.70900000
Si	-24.40400000	-3.25200000	9.61700000
Si	-28.62800000	-7.95900000	16.83900000
Si	-27.55500000	-0.36500000	15.01200000
Si	-25.62800000	-5.15800000	20.61600000
Si	-33.65500000	-2.98200000	17.14200000
Si	-26.83700000	-9.50000000	11.52600000
Si	-31.86300000	-4.52400000	11.82900000
O	-29.63400000	-5.28800000	8.83400000
O	-30.85800000	-7.19400000	19.83400000
O	-26.15900000	-0.83200000	14.33400000
O	-23.66600000	-5.18700000	13.59300000
O	-30.77500000	-3.99900000	10.76600000

First co-ordination shell cluster of $PbSiO_3$ (site 3)

O	-7.03500000	-12.91600000	18.68000000
O	-10.22700000	-11.52600000	18.92000000
O	-5.80200000	-10.91900000	16.77100000

Pb	-8.20400000	-11.24200000	17.58600000
O	-6.59200000	-8.48000000	17.25000000
O	-7.90100000	-10.19900000	19.60200000
O	-7.81900000	-13.39600000	15.55100000

Third co-ordination shell cluster of $PbSiO_3$ (site 3)

O	-8.64200000	-0.60600000	-22.15100000
O	1.35300000	-6.77700000	-21.75700000
O	0.48400000	-5.02400000	-17.16000000
O	-4.04000000	-9.82300000	-19.05700000
O	-7.36400000	-4.07600000	-26.27300000
O	-0.70900000	-3.40700000	-24.93800000
O	-9.37900000	-2.99600000	-22.97700000
O	0.85000000	-3.76200000	-22.65100000
O	0.99500000	-4.16000000	-19.96200000
O	-9.84100000	-5.22100000	-21.35500000
O	-10.43600000	-2.63300000	-19.94900000
O	-8.38300000	-7.17200000	-20.32400000
O	-7.02800000	-4.40200000	-16.39800000
O	-3.42700000	-1.22600000	-21.62800000
O	-3.12200000	-6.58500000	-25.25000000
O	-5.35700000	-1.95200000	-25.48800000
O	-7.76400000	-6.79300000	-17.22300000
O	-4.63600000	-7.23500000	-17.64900000
O	-1.13100000	-1.22800000	-22.91400000
O	-1.03100000	-6.23700000	-20.81800000
O	-7.44900000	-8.05300000	-22.60700000
O	-4.43900000	-8.23900000	-23.75800000
O	-3.95000000	-4.74700000	-17.30700000
O	-5.56500000	-0.95000000	-23.06000000
O	-1.29800000	-1.50800000	-20.19900000
O	-7.70900000	-1.48700000	-24.43400000
O	-8.72800000	-4.58300000	-18.48500000
O	-5.74900000	-7.87200000	-20.52000000
O	-5.65500000	-6.02500000	-24.81000000
O	-6.09400000	-5.28500000	-18.68100000
O	-6.71200000	-5.66300000	-21.78200000
O	-2.04500000	-3.49200000	-21.71200000
O	-3.83600000	-5.88800000	-22.79000000
O	-6.25100000	-3.43800000	-23.40300000
O	-3.74200000	-5.74800000	-19.73400000
Pb	-1.21200000	-4.44000000	-19.43300000
Pb	-3.50600000	-7.67500000	-20.92300000
Pb	-8.53400000	-3.51200000	-20.70600000
Pb	-7.55800000	-5.14700000	-24.05200000
Pb	-1.02900000	-5.02100000	-23.10300000
Pb	-4.88900000	-4.27400000	-21.52600000

Si	-7.46100000	-5.27700000	-17.72000000
Si	-7.01500000	-7.17800000	-21.28500000
Si	-4.31100000	-6.63000000	-24.13500000
Si	-1.93700000	-1.88900000	-21.67200000
Si	-6.22000000	-1.98000000	-24.10800000
Si	-4.60500000	-5.77600000	-18.35500000

Fifth co-ordination shell cluster of $PbSiO_3$ (site 3)

O	8.86200000	-24.95100000	-16.31700000
O	2.44300000	-25.15000000	-25.52900000
O	16.24500000	-30.26500000	-25.24100000
O	2.47900000	-21.87600000	-21.76000000
O	5.77000000	-17.04200000	-26.83400000
O	19.23200000	-22.17000000	-26.30900000
O	15.52800000	-26.96500000	-31.90100000
O	4.92900000	-15.41000000	-22.16600000
O	10.73200000	-15.17100000	-26.21500000
O	10.56600000	-28.83500000	-32.52100000
O	2.82300000	-20.08000000	-30.64700000
O	8.62700000	-19.84100000	-34.69600000
O	18.18200000	-19.78700000	-29.91100000
O	18.41800000	-20.08200000	-24.92400000
O	5.07000000	-18.21600000	-31.56600000
O	3.49600000	-23.96400000	-20.55000000
O	11.99900000	-20.28100000	-34.13600000
O	18.27400000	-22.64800000	-32.43300000
O	8.12200000	-26.58000000	-18.24900000
O	2.07400000	-19.95200000	-23.65700000
O	4.07500000	-19.06000000	-20.73600000
O	11.42000000	-25.18500000	-33.95100000
O	18.47500000	-23.92600000	-28.08800000
O	16.98500000	-28.63500000	-23.30800000
O	17.29200000	-17.77700000	-26.40200000
O	11.48900000	-18.01600000	-22.35400000
O	8.69100000	-26.74400000	-34.02900000
O	15.80000000	-28.43300000	-20.79000000
O	12.60700000	-17.26300000	-24.70600000
O	6.80400000	-17.50200000	-20.65800000
O	15.57100000	-31.19700000	-21.94500000
O	8.92000000	-23.98000000	-32.87300000
O	3.87700000	-18.56900000	-25.58100000
O	4.45900000	-18.82100000	-28.22800000
O	16.83900000	-25.18600000	-30.50800000
O	8.13300000	-16.95200000	-25.74600000
O	13.93600000	-16.71300000	-29.79500000
O	13.78100000	-27.09400000	-19.72800000

O	11.57400000	-16.80300000	-30.88300000
O	7.62600000	-22.64800000	-18.21100000
O	3.92200000	-27.44300000	-23.80400000
O	17.83900000	-24.98500000	-24.73800000
O	10.44200000	-30.50400000	-21.19200000
O	14.04900000	-24.67200000	-33.62600000
O	13.01600000	-22.36900000	-32.92600000
O	3.02500000	-21.35800000	-26.30200000
O	13.68000000	-19.47400000	-31.75500000
O	5.61700000	-25.42400000	-29.90200000
O	9.05300000	-16.41800000	-31.32600000
O	6.44200000	-27.82700000	-23.36000000
O	8.26300000	-29.38600000	-27.64900000
O	9.38100000	-28.63200000	-30.00200000
O	15.24700000	-20.92000000	-21.13900000
O	12.87300000	-29.50000000	-25.71300000
O	3.91000000	-23.49100000	-24.10400000
O	14.66500000	-24.71200000	-20.36500000
O	8.96300000	-28.21200000	-22.91700000
O	7.01000000	-22.60900000	-31.47200000
O	13.45500000	-29.75200000	-28.35900000
O	13.63200000	-22.40800000	-19.66500000
O	17.12900000	-27.88300000	-25.87800000
O	11.18200000	-28.87400000	-19.26000000
O	12.61500000	-20.32100000	-20.87500000
O	6.86900000	-24.40500000	-19.99100000
O	9.24200000	-19.88000000	-21.43500000
O	15.04600000	-19.64100000	-25.48300000
O	13.07200000	-29.99100000	-20.86800000
O	7.98900000	-17.70400000	-23.17700000
O	13.79200000	-17.46500000	-27.22500000
O	7.50600000	-26.54100000	-31.51000000
O	15.68200000	-18.58200000	-28.83300000
O	12.24600000	-27.58800000	-27.40900000
O	13.85900000	-21.90300000	-24.76100000
O	13.05200000	-19.09500000	-29.15800000
O	7.24900000	-19.33400000	-25.10900000
O	8.24600000	-24.91100000	-29.57800000
O	8.48500000	-21.63600000	-23.21400000
O	13.42900000	-22.40900000	-22.26000000
O	9.72500000	-27.20400000	-27.85200000
O	14.28800000	-21.39700000	-27.26300000
O	8.28200000	-21.63700000	-25.80900000
O	11.32600000	-28.12200000	-21.82900000
O	7.21300000	-22.60800000	-28.87700000
O	14.08500000	-21.39800000	-29.85800000

O	13.92500000	-26.34100000	-22.29800000
O	9.71300000	-23.25200000	-28.15200000
O	5.78200000	-20.99400000	-26.53400000
O	11.58500000	-20.75500000	-30.58300000
O	12.03600000	-25.22400000	-20.68900000
O	7.61800000	-24.53300000	-26.98100000
O	13.42100000	-24.29400000	-31.02900000
O	7.87700000	-19.71300000	-27.70600000
O	11.03600000	-25.42500000	-26.45900000
O	12.67200000	-24.16600000	-24.04000000
O	15.33900000	-23.78000000	-23.66100000
O	11.61800000	-25.67600000	-29.10500000
O	5.81500000	-25.91500000	-25.05700000
O	9.68000000	-18.33000000	-29.63000000
O	9.53600000	-24.01900000	-19.61200000
O	6.66700000	-23.12600000	-24.33500000
O	12.47000000	-22.88700000	-28.38400000
O	8.82800000	-21.11900000	-30.35100000
O	15.11000000	-26.54400000	-24.81600000
O	15.10200000	-23.48600000	-28.64800000
O	10.42500000	-26.02900000	-23.12100000
O	9.29900000	-23.72500000	-24.59900000
O	15.51600000	-23.01300000	-32.20100000
O	10.26300000	-18.58200000	-32.27600000
Pb	11.07600000	-20.05500000	-23.27700000
Pb	6.80700000	-18.47300000	-29.30200000
Pb	16.87900000	-19.81600000	-27.32500000
Pb	8.68900000	-25.77200000	-25.38400000
Pb	10.83800000	-23.99000000	-22.19800000
Pb	14.49200000	-25.53300000	-29.43300000
Pb	16.64200000	-23.75100000	-26.24600000
Pb	4.27400000	-20.54100000	-24.62300000
Pb	5.70400000	-18.31300000	-22.44200000
Pb	10.07700000	-20.30200000	-28.67200000
Pb	11.50800000	-18.07400000	-26.49000000
Pb	10.40700000	-25.97200000	-18.98400000
Pb	5.41800000	-23.94300000	-26.01500000
Pb	16.21000000	-25.73300000	-23.03300000
Pb	11.22100000	-23.70400000	-30.06400000
Pb	9.79100000	-25.93300000	-32.24500000
Pb	14.70000000	-29.24400000	-22.57300000
Pb	10.17600000	-20.88100000	-32.40500000
Pb	5.31900000	-23.36500000	-22.28200000
Pb	11.12200000	-23.12600000	-26.33100000
Pb	12.70800000	-26.45900000	-24.25400000
Pb	16.92500000	-22.88700000	-30.37900000

Pb	4.37300000	-21.12000000	-28.35600000
O	5.23300000	-25.66400000	-22.41000000
O	9.30700000	-26.78300000	-20.76800000
O	6.57500000	-20.26600000	-21.81400000
O	16.22800000	-25.79000000	-27.16900000
O	12.37800000	-20.02600000	-25.86200000
O	6.19600000	-20.52000000	-30.08800000
O	9.87900000	-18.82100000	-24.78500000
O	7.36200000	-27.29400000	-28.94000000
O	14.76600000	-27.97300000	-26.96600000
Si	7.28600000	-20.41000000	-26.35100000
Si	8.36700000	-18.21000000	-24.67200000
Si	13.08900000	-20.17100000	-30.40000000
Si	14.17000000	-17.97100000	-28.72100000
Si	11.56000000	-29.38000000	-20.75500000
Si	13.54700000	-25.83500000	-20.80200000
Si	8.20900000	-23.83500000	-28.33500000
Si	7.12800000	-26.03500000	-30.01400000
Si	14.01200000	-23.59600000	-32.38400000
Si	8.06100000	-20.91300000	-21.78400000
Si	10.12700000	-17.60300000	-31.00800000
Si	13.86400000	-20.67400000	-25.83200000
Si	8.05000000	-23.37200000	-19.64200000
Si	5.36900000	-26.64200000	-23.67800000
Si	13.85300000	-23.13300000	-23.69100000
Si	11.17200000	-26.40300000	-27.72700000
Si	13.31900000	-28.77300000	-27.09100000
Si	7.32100000	-21.69200000	-30.18700000
Si	8.17400000	-22.55300000	-24.50000000
Si	10.01000000	-27.26500000	-22.14500000
Si	13.97700000	-22.31400000	-28.54800000
Si	15.81400000	-27.02600000	-26.19400000
Si	8.67800000	-28.15000000	-28.62400000
Si	13.74000000	-21.49300000	-20.97500000
O	8.05600000	-22.14200000	-20.71300000

First co-ordination shell cluster of $Pb_3(PO_4)_2$ (site 1)

O	-6.37600000	25.98400000	2.99700000
O	-4.63900000	25.11400000	6.71600000
O	-8.62700000	24.11900000	3.52100000
O	-5.27900000	27.34600000	5.89900000
O	-9.38200000	23.92800000	6.79900000
O	-8.27200000	21.97100000	4.66800000
O	-7.59100000	26.38700000	7.72700000
Pb	-6.85300000	24.68100000	5.37200000
O	-8.45600000	26.72800000	5.32400000
O	-7.01800000	23.14900000	7.46700000

O	-4.98100000	22.69200000	5.03100000

Third co-ordination shell cluster of $Pb_3(PO_4)_2$ (site 1)

O	0.07900000	23.14300000	5.46200000
O	-7.78100000	24.46800000	-1.66400000
O	-4.59900000	31.76200000	8.95800000
O	-12.37400000	18.55400000	5.56800000
O	-6.97900000	21.68300000	-0.23100000
O	-0.75900000	25.93800000	4.07200000
O	-6.56000000	17.94300000	7.21600000
O	-2.17200000	21.27800000	5.98600000
O	-7.43800000	26.88800000	0.02100000
O	-7.04300000	31.38800000	3.41000000
O	-3.48900000	29.80400000	6.82700000
O	-10.06200000	19.51200000	3.74000000
O	-5.65600000	24.95300000	12.02000000
O	-13.47400000	25.99100000	5.00300000
O	-11.27700000	19.91400000	8.47100000
O	-7.88900000	31.03900000	8.59500000
O	-6.21700000	20.36500000	8.90100000
O	-9.29400000	29.52300000	3.93300000
O	-13.01400000	20.78500000	4.75100000
O	-4.24300000	29.61300000	10.10600000
O	-4.18000000	19.90800000	6.46400000
O	-7.21400000	28.78000000	1.60600000
O	-7.62200000	18.84900000	4.24000000
O	-4.23300000	29.97300000	4.36400000
O	-2.00000000	23.88600000	7.78900000
O	-9.81700000	24.92400000	0.77200000
O	-8.29500000	26.18000000	10.94700000
O	-12.28300000	25.18600000	7.75200000
O	-12.67200000	23.20700000	6.43500000
O	-6.49400000	27.74800000	10.62900000
O	-9.19800000	19.17100000	6.14300000
O	-5.85200000	30.58200000	6.15900000
O	-3.57700000	24.20900000	9.69200000
O	-11.43700000	25.53300000	2.56700000
O	-10.39000000	28.16100000	1.03100000
O	-2.92700000	21.08600000	9.26400000
O	-5.82700000	22.34400000	10.21700000
O	-11.09500000	27.95500000	4.25100000
O	-9.01700000	22.14000000	2.20500000
O	-2.83800000	26.68200000	6.39900000
O	-3.36300000	22.08300000	3.23700000
O	-4.80000000	25.66100000	1.09300000
O	-8.63600000	23.75900000	9.26200000
O	-10.03200000	27.05000000	7.22700000

O	-10.63500000	22.74900000	3.99900000
O	-4.41400000	27.00400000	8.30200000
O	-9.02700000	21.77900000	7.94700000
O	-5.72600000	22.86200000	2.56900000
O	-3.93500000	25.32000000	3.49600000
O	-8.23100000	28.61800000	6.91000000
O	-5.37100000	20.71300000	3.71600000
O	-4.57500000	27.55200000	2.67900000
O	-8.45600000	26.72800000	5.32400000
O	-7.01800000	23.14900000	7.46700000
O	-4.98100000	22.69200000	5.03100000
O	-6.37600000	25.98400000	2.99700000
O	-4.63900000	25.11400000	6.71600000
O	-8.62700000	24.11900000	3.52100000
O	-5.27900000	27.34600000	5.89900000
O	-9.38200000	23.92800000	6.79900000
O	-8.27200000	21.97100000	4.66800000
O	-7.59100000	26.38700000	7.72700000
P	-9.13100000	22.73500000	3.64500000
P	-4.86700000	22.09700000	3.59100000
P	-4.87800000	26.10900000	2.57100000
P	-8.52200000	23.16400000	7.82200000
P	-4.33600000	26.55700000	6.82400000
P	-8.53400000	27.17600000	6.80200000
Pb	-6.85300000	24.68100000	5.37200000
Pb	-6.01800000	29.05100000	8.25300000
Pb	-10.80100000	21.21800000	6.09400000
Pb	-6.72100000	20.61800000	5.76400000
Pb	-2.94300000	24.13100000	5.23900000
Pb	-7.27800000	24.21400000	1.47300000
Pb	-6.59800000	25.19800000	9.46900000
Pb	-4.47800000	22.43900000	8.16900000
Pb	-9.39800000	26.97200000	2.77500000
Pb	-10.93300000	25.28100000	5.70300000
Pb	-6.27100000	28.53500000	4.15700000

First co-ordination shell cluster of $Pb_3(PO_4)_2$ (site 2)

O	21.09800000	5.52000000	20.16200000
O	23.76300000	1.29000000	21.07500000
O	25.63100000	4.76000000	19.06300000
O	21.40000000	4.53000000	22.42900000
O	23.40800000	2.59100000	18.16300000
O	25.98500000	3.45900000	21.97400000
O	23.99600000	3.40500000	23.33200000
O	21.02800000	2.42800000	19.93000000
O	24.01600000	6.18300000	21.54700000
Pb	23.40100000	3.99500000	21.02400000

Third co-ordination shell cluster of $Pb_3(PO_4)_2$ (site 2)

O	28.40500000	-0.94800000	22.82100000
O	30.15200000	5.26700000	20.61100000
O	30.21200000	3.71300000	18.55700000
O	30.62300000	1.24500000	23.67000000
O	16.28400000	4.45200000	18.41200000
O	16.69500000	1.98300000	23.52400000
O	24.42700000	3.71500000	26.66000000
O	21.44900000	4.60600000	27.32900000
O	16.51700000	6.56600000	20.66900000
O	16.92800000	4.09900000	25.78100000
O	30.10300000	5.19100000	15.71100000
O	30.51400000	2.72300000	20.82400000
O	27.88500000	2.99800000	14.86200000
O	20.96500000	-0.46100000	16.88700000
O	23.43400000	10.04900000	18.59300000
O	28.42900000	6.51100000	23.25100000
O	19.29100000	0.85900000	24.42700000
O	21.05200000	9.88600000	20.36000000
O	23.56000000	-1.58600000	17.78800000
O	21.46300000	7.41900000	25.47300000
O	28.32100000	7.98900000	20.40600000
O	21.07300000	-1.93900000	19.73200000
O	24.19900000	6.28100000	26.61700000
O	18.77100000	4.80400000	16.46800000
O	16.45900000	7.73300000	18.46700000
O	16.87100000	5.26500000	23.58000000
O	28.29600000	0.53000000	19.97500000
O	18.84100000	7.89700000	16.70000000
O	27.95500000	6.09000000	15.09500000
O	21.43900000	-0.04000000	25.04300000
O	27.99400000	1.52000000	17.70800000
O	20.98900000	6.99800000	17.31700000
O	28.79200000	3.96700000	23.46400000
O	20.60200000	2.08300000	16.67400000
O	25.37800000	-0.13300000	18.59100000
O	19.26700000	8.24100000	19.95700000
O	19.67800000	5.77300000	25.06900000
O	21.50900000	3.05200000	25.27400000
O	21.01300000	-0.38400000	21.78700000
O	28.38100000	6.43400000	18.35100000
O	28.36600000	3.62300000	20.20800000
O	23.58000000	1.19100000	16.00400000
O	25.81300000	4.85800000	24.13300000
O	19.24200000	0.78200000	19.52600000
O	23.99100000	-1.27600000	21.11600000

O	23.35200000	3.75800000	15.96200000
O	26.04200000	2.29200000	24.17600000
O	23.84500000	7.58200000	23.70600000
O	21.03800000	7.07400000	22.21600000
O	18.88000000	3.32600000	19.31400000
O	25.40200000	7.32500000	19.02100000
O	23.78800000	8.74900000	21.50400000
O	23.82100000	0.12300000	23.27600000
O	25.57400000	5.92700000	16.86200000
O	19.18200000	2.33700000	21.58100000
O	25.80900000	0.17700000	21.91900000
O	25.83400000	7.63500000	22.34800000
O	19.25200000	5.42900000	21.81300000
O	23.58500000	5.87300000	18.21900000
O	25.39800000	2.64500000	16.80600000
O	21.09800000	5.52000000	20.16200000
O	23.76300000	1.29000000	21.07500000
O	25.63100000	4.76000000	19.06300000
O	21.40000000	4.53000000	22.42900000
O	23.40800000	2.59100000	18.16300000
O	25.98500000	3.45900000	21.97400000
O	23.99600000	3.40500000	23.33200000
O	21.02800000	2.42800000	19.93000000
O	24.01600000	6.18300000	21.54700000
P	19.58100000	2.17100000	20.09700000
P	25.05300000	5.99400000	18.33300000
P	23.93000000	2.52400000	16.69100000
P	20.69900000	5.68600000	21.64600000
P	25.46500000	3.52600000	23.44600000
P	24.36500000	7.51400000	22.23400000
P	24.34100000	0.05600000	21.80400000
Pb	22.31900000	0.27200000	19.16700000
Pb	22.75400000	5.26400000	24.70900000
Pb	27.07500000	5.77800000	20.97100000
Pb	22.34300000	7.73100000	19.59700000
Pb	18.58900000	6.43100000	18.65300000
Pb	19.00000000	3.96300000	23.76500000
Pb	27.70300000	4.62400000	17.04800000
Pb	21.28000000	3.89400000	17.97700000
Pb	23.40100000	3.99500000	21.02400000
Pb	28.11400000	2.15600000	22.16100000
Pb	21.69100000	1.42500000	23.09000000
Pb	25.99200000	2.05400000	19.11300000