

This file contains the relaxed structures of each candidate in Figure 5.

Ag1I1/icsd_001899

1.0000000000000000

4.6187383060000000	0.0000115320000000	-0.0000000020000000
-2.3093744219999999	3.9997196370000001	0.0000000210000000
0.0000001390000000	0.0000002580000000	15.1423606199999998

I Ag
4 4

Direct

0.0000162300000000	0.0000306399999985	0.0315701999999973
0.9999837499999984	0.9999693500000006	0.5315701999999973
0.6666112899999987	0.3332271100000028	0.2815061900000018
0.3333887000000004	0.6667728799999963	0.7815061900000018
0.0000524200000029	0.0001007099999981	0.7183438200000012
0.9999475999999987	0.9998993000000027	0.2183438200000012
0.6666344200000012	0.3332714599999989	0.4685798000000005
0.3333655800411727	0.6667285500426005	0.9679194009875249

Ag2Ge1S3/icsd_041711/

1.0000000000000000

0.0000000500000000	0.0000000350000000	6.4959046029999996
5.8617873109999996	3.5188509410000002	0.0000000130000000
-5.8617873810000001	3.5188510960000001	-0.0000000390000000

Ge S Ag
2 6 4

Direct

0.4582527499999998	0.6600615199999993	0.6600615300000001
0.9582527399999989	0.3399384900000015	0.3399384699999999
0.8761921500000014	0.3540623100000033	0.0352808900000028
0.8761920999999973	0.0352808499999995	0.3540622000000013
0.3761921500000014	0.6459376800000030	0.9647191199999980
0.3761921099999981	0.9647191299999989	0.6459377899999978
0.8218864999999980	0.6424133800000007	0.6424133399999974
0.3218864899999971	0.3575866500000018	0.3575866600000026
0.4922382999999968	0.2976021099999997	0.9938819999999993
0.4922382000000027	0.9938819300000006	0.2976021899999992
0.9922382999999968	0.7023978599999978	0.0061180000000007
0.9906987785256824	0.0061180800142218	0.7023978100010912

Al2Cd1Cl8/icsd_062037/

1.0000000000000000

12.8219399319999994	-0.00000000630000000	0.0075120640000000
0.0000000200000000	6.431125599999999	0.0000000400000000
-0.3496862020000000	0.0000000890000000	7.0388796219999996

Cl	Al	Cd
16	4	2

Direct

0.06051638999999965	0.38415231999999983	0.65730049999999981
0.56051638000000028	0.61584767000000008	0.65730050999999989
0.94218665999999973	0.05080510999999989	0.30294219000000031
0.44218664999999965	0.94919489000000011	0.30294218000000023
0.08534729000000014	0.57751532999999971	0.16389707999999981
0.58534728000000006	0.42248468999999974	0.16389708999999990
0.95318198999999974	0.92066332999999964	0.78404463999999976
0.45318198999999974	0.07933667999999973	0.78404462000000031
0.70121887999999990	0.88097562000000010	0.05193809000000002
0.20121886999999982	0.11902437999999990	0.05193812000000026
0.82846117999999979	0.55821312999999986	0.40775658999999982
0.32846117999999979	0.44178687000000014	0.40775659999999990
0.81505200000000014	0.41177855000000011	0.91548381999999986
0.31505201000000023	0.58822143999999981	0.91548382999999994
0.18873950999999978	0.91470143000000009	0.53588796999999974
0.68873950999999978	0.08529854999999974	0.53588794000000021
0.04437777999999978	0.06250958999999977	0.56184037999999996
0.54437777999999978	0.93749041000000023	0.56184036999999988
0.24037442000000020	0.43315868999999991	0.14952741999999983
0.74037441000000011	0.56684131000000009	0.14952739999999966
0.49954390999999999	0.75065063000000026	0.00078134000000032
0.9995051656321098	0.2493494000192804	-0.0006392992901723

Al2S4Zn1/icsd_609280

1.0000000000000000

3.6636340563899998	0.0000026308627393	0.0000275992274570
1.8318147557300000	-3.1728014900099999	0.0000275803985514
1.8317916685800000	-1.0575854156700000	-11.7707562237999994

S	Zn	Al
4	1	2

Direct

0.87357701999999990	0.87357701999999990	0.37927254000000023
0.12756774000000035	0.12756774999999972	0.61729349000000016
0.30028897999999977	0.30028897999999977	0.09911664999999991
0.70552070000000010	0.70552070000000010	0.88346235000000021
0.22837469000000025	0.22837470000000034	0.31487374000000030
0.99936280000000001	0.99936280000000001	0.00190515999999997
0.76902487655000000	0.7690248665499995	0.69292564176000015

As1K1Sn1/icsd_040815

1.0000000000000000

4.1450014599999996	-0.0000075610000000	0.0000000000000000
-2.0725072729999998	3.589639255999999	0.0000000030000000
0.0000000000000000	0.0000000090000000	12.6855507070000009

As	K	Sn
2	2	2

Direct

0.6666703499999996	0.3333576200000010	0.1720537300000018
0.3333296500000031	0.6666423799999990	0.6720537300000018
0.6666696899999991	0.3333320200000003	0.4949152299999966
0.3333303100000009	0.6666679799999997	0.9949152299999966
0.9999952300000032	0.9999724600000022	0.7781310399999981
0.0000047700009850	0.0000275400019743	0.2773427415468233

Au207Se2/icsd_037009/

1.0000000000000000

6.9673389160000001	-0.0000000050000000	-0.0000000030000000
0.0000000090000000	11.632966924999998	-0.0000000400000000
-0.0000000010000000	-0.0000000110000000	3.9518042539999998

Au	0	Se
4	14	4

Direct

0.6932117500000032	0.4348840700000025	0.5015570099999991
0.3067882400000030	0.5651159299999975	0.5015570099999991
0.8067882499999968	0.9348840700000025	0.5015570099999991
0.1932117599999970	0.0651159299999975	0.5015570099999991
0.8406813599999978	0.5827079000000026	0.5717221000000023
0.1593186300000013	0.4172921099999982	0.5717221199999969
0.6593186400000022	0.0827079000000026	0.5717221100000032
0.3406813599999978	0.9172920999999974	0.5717221100000032
0.5327427699999987	0.2888751300000010	0.4913288999999992
0.4672572200000005	0.7111248699999990	0.4913288899999984
0.9672572300000013	0.7888751300000010	0.4913288799999975
0.0327427799999995	0.2111248699999990	0.4913288999999992
0.8757936100000023	0.3727448799999991	0.1307393299999973
0.1242063899999977	0.6272551100000001	0.1307393200000035
0.6242063899999977	0.8727448799999991	0.1307393299999973
0.3757936100000023	0.1272551100000001	0.1307393299999973
0.5000000000000000	0.5000000000000000	0.8232645100000013
0.0000000000000000	0.0000000000000000	0.8232645100000013
0.6085521099999980	0.1738664100000022	0.2282204099999987
0.3914478900000020	0.8261335899999978	0.2282203999999979
0.8914478900000020	0.6738664100000022	0.2282203999999979
0.1085521099996348	0.3261335899976050	0.2256899202901711

BiN1/icsd_162871/
 1.000000000000000
 2.5162508049999999 -0.0000045050000000 0.0000890240000000
 1.2581293050000000 -2.1791420360000000 0.0000714200000000
 1.2580174690000001 -0.7263445470000000 -3.2265456650000002

B N
 1 1

Direct
 0.9997923999999969 0.9997419199999982 0.0007238800000025
 0.3316746283105884 0.3316250540524259 0.0050753584116843

Bi1Cl1Te1/icsd_079362/
 1.000000000000000
 4.2567608750000003 0.0000005920000000 0.0000000200000000
 -2.1283799150000000 3.6864605859999999 0.0000000070000000
 0.0000000360000000 0.0000001020000000 12.5912648829999991

Te Bi Cl
 2 2 2

Direct
 0.3333345899999998 0.6666692299999966 0.7779750799999974
 0.6666653999999994 0.3333307600000026 0.2779750799999974
 0.3333317900000026 0.6666636499999967 0.1374216299999986
 0.6666682099999974 0.3333363500000033 0.6374216399999995
 0.9999986500000020 0.9999975300000017 0.0027032899999995
 0.0000013600177028 0.0000024800219737 0.5019090886157126

Bi1I1Te1/icsd_074501/
 1.000000000000000
 4.3648366259999998 0.0000017630000000 0.0000861650000000
 -2.1824167710000002 3.7800567350000001 -0.0000000440000000
 -0.0000280330000000 -0.0000161510000000 6.9254158840000004

I Te Bi
 1 1 1

Direct
 0.3333217200000007 0.6666608600000004 0.2265834499999997
 0.6666763400000022 0.3333381699999975 0.6718468500000014
 0.0000019176414637 0.0000009638304330 0.919425743396316

Bi1In103/icsd_171756/

1.000000000000000

6.0106130249999996	0.0000000050000000	0.0000000180000000
-0.0000000020000000	5.6706748690000000	0.0000000150000000
-0.0000000030000000	-0.0000000030000000	8.3119882890000003

Bi	0	In
4	12	4

Direct

0.5563852399999973	0.5011933899999974	0.7880689500000031
0.4436147700000035	0.4988066000000018	0.2880689500000031
0.9436147700000035	0.0011933899999974	0.2880689500000031
0.0563852299999965	0.9988066100000026	0.7880689500000031
0.4500743500000013	0.1173321400000020	0.7584580199999991
0.5499256499999987	0.8826678599999980	0.2584580199999991
0.0499256499999987	0.6173321400000020	0.2584580199999991
0.9500743500000013	0.3826678599999980	0.7584580199999991
0.7083489899999975	0.3045060099999972	0.4358639000000011
0.2916510000000017	0.6954939900000028	0.9358639000000011
0.7916510000000017	0.8045060099999972	0.9358639000000011
0.2083489999999983	0.1954939900000028	0.4358639000000011
0.8391917399999969	0.8421480700000004	0.5318806300000034
0.1608082600000031	0.1578519299999996	0.0318806300000034
0.6608082600000031	0.3421480700000004	0.0318806300000034
0.3391917399999969	0.6578519299999996	0.5318806300000034
0.4978712500000029	0.0007371599999999	0.0154285099999996
0.5021287400000034	0.9992628400000001	0.5154285099999996
0.0021287499999971	0.5007371599999999	0.5154285099999996
0.9978712499994025	0.4992628399993637	0.0142254284204413

Bi2Ge105/icsd_062488

1.0000000000000000

-0.0006154650000000	-0.0000001240000000	5.3649245880000000
-0.0000913400000000	-5.5246340810000003	0.0000002130000000
7.8681973500000000	2.7624485179999998	0.0006956300000000

Ge	Bi	O
2	4	10

Direct

0.7313356299999967	0.6880434400000013	0.0031349599999970
0.2313355699999988	0.3151070099999984	0.0031649200000032
0.7475566700000016	0.3945651299999966	0.3394694999999999
0.2475618499999968	0.9448980900000024	0.3394647100000014
0.7475796100000025	0.0582530599999984	0.6668408099999965
0.2475743899999969	0.6085880500000016	0.6668355099999985
0.4822460999999976	0.2584898899999999	0.5049600500000011
0.9822421900000009	0.2464619100000007	0.5049584300000021
0.4822356700000014	0.7566881500000022	0.5013405899999981
0.9822394899999978	0.7446583099999984	0.5013390000000015
0.6748503299999982	0.7277330599999985	0.8075067899999979
0.1747823400000001	0.0797217799999999	0.8075664500000030
0.6748341899999986	0.9233790999999982	0.1987572900000032
0.1749023599999973	0.2754901799999985	0.1988168099999967
0.0578618400000011	0.5990057200000010	0.0031409400000015
0.5559978209201446	0.4041170171367740	0.0031030941968169

Bi2Mo106/icsd_017070

1.0000000000000000

5.4842337399999996	0.0148160910000000	0.0090554410000000
0.0448694990000000	16.3518810439999989	-0.0525108740000000
0.0090491760000000	-0.0175211890000000	5.4821142839999997

Mo Bi O

4 8 24

Direct

0.5256916299999972	0.9996792499999998	0.5130936500000018
0.0151255800000030	0.5000309699999974	0.5286655800000020
0.4977385700000028	0.5001851099999968	0.0282753600000021
0.0264438199999972	0.0001356900000005	0.9959203100000025
0.5242462000000003	0.1717602200000030	0.0249031800000026
0.9985376099999996	0.3274821400000008	0.0236727500000029
0.4942964899999964	0.6723997100000005	0.5166572899999977
0.0159386899999987	0.8284414900000030	0.5205650300000002
0.5293352999999996	0.8280265400000033	0.9969272800000013
0.0194330400000027	0.6710988199999974	0.0310112100000026
0.5270204099999987	0.3293036199999975	0.5407713700000016
0.0400740700000028	0.1715681299999972	0.4983915899999971
0.7546739100000011	0.2505082599999966	0.2606447699999990
0.2647964000000016	0.2496827900000014	0.7593304199999977
0.2569570100000007	0.7523620799999975	0.2558635700000025
0.7477868300000026	0.7477821900000023	0.7485896399999987
0.2478097400000010	0.7498251000000025	0.7553219899999988
0.7547692999999995	0.7500428700000015	0.2520177800000027
0.7661060399999968	0.2475221500000018	0.7614011100000013
0.2544524400000014	0.2522054900000015	0.2562371499999969
0.6887090600000008	0.5172045199999999	0.2889263499999970
0.1714653100000021	0.0187230100000022	0.7051117600000012
0.2867043199999983	0.9806364599999995	0.1845848500000002
0.8241974100000036	0.5200028200000020	0.7893524200000002
0.3056751299999974	0.4824886099999972	0.6731513499999977
0.7857239200000024	0.9813220599999966	0.3192955800000021
0.6720751599999986	0.0196978500000000	0.8010008600000020
0.2091751900000034	0.4798860100000013	0.1743409799999966
0.4500317299999992	0.1086100699999974	0.4305943800000023
0.9347023899999982	0.3913178999999971	0.4616432099999983
0.4440618300000025	0.6093942700000028	0.9413831099999967
0.9321144999999973	0.8905363900000012	0.9407990600000034
0.4349232000000001	0.8910695699999991	0.5615261299999972
0.0616237999999996	0.6091969800000001	0.4316598699999972
0.5820937599999993	0.3916991700000025	0.9480130900000034
0.9554932259040743	0.1081697226784104	0.0785317925115255

Bi2O3/icsd_041764

1.0000000000000000

7.8006164519999999	-0.0000002430000000	-0.0000003370000000
0.0000000020000000	7.8006165320000003	0.0000003216000000

-0.0000002050000000	0.0000023930000000	5.5805121570000003
Bi 0		
8 12		
Direct		
0.7561726699999980	0.5199998300000033	0.2303332800000035
0.2561727300000030	0.9800000899999972	0.2696667100000028
0.2438272699999970	0.4800009200000019	0.2303329399999967
0.7438273400000028	0.0199991499999967	0.26966671300000020
0.5199995400000006	0.2438269499999990	0.7696667100000028
0.9800003400000037	0.7438276700000017	0.7303328899999997
0.4800005199999973	0.7561723299999983	0.76966671599999974
0.0199995400000006	0.2561730199999985	0.7303332899999972
0.8115805500000022	0.7899478200000019	0.0323821699999982
0.3115807900000007	0.7100522100000006	0.4676176199999986
0.1884194699999995	0.2100524100000030	0.0323822499999977
0.6884193100000005	0.2899475600000017	0.4676176299999995
0.7899477699999977	0.1884194100000016	0.9676177699999968
0.7100522599999977	0.6884191700000031	0.5323823499999989
0.2100522300000023	0.8115807200000020	0.9676177500000023
0.2899476999999990	0.3115807000000004	0.5323823599999997
0.9999999599999967	0.4999999799999983	0.9026785599999982
0.5000000300000025	0.0000000200000017	0.5973214300000009
0.4999999799999983	0.9999998899999980	0.0973214400000018
0.9999999899529067	0.5000001405497151	0.4008865897777473

Bi206W1/icsd_023584

1.0000000000000000

5.5084358379999996	-0.0000000170000000	-0.0000000180000000
-0.0000000170000000	-0.0000346940000000	-5.4976013789999998
0.0000000010000000	8.2685481000000003	2.7488606610000001

0	Bi	W
12	4	2

Direct

0.2589922599999994	0.9916806600000001	0.4969291100000035
0.7410056599999990	0.4947479200000018	0.5030843099999984
0.2410077400000006	0.4916806600000001	0.4969291100000035
0.7589943300000002	0.9947479200000018	0.5030843099999984
0.2452517899999975	0.7986853499999995	0.0420532699999967
0.7546560400000004	0.7567179500000023	0.9579342400000002
0.2547482100000025	0.2986853499999995	0.0420532699999967
0.7453439599999996	0.2567179500000023	0.9579342400000002
0.4218989000000022	0.4520040199999968	0.7823176799999985
0.5781057700000005	0.6697200999999993	0.2176681799999969
0.0781010999999978	0.9520040299999977	0.7823176799999985
0.9218942299999995	0.1697200999999993	0.2176681799999969
0.0215659500000029	0.2946354799999966	0.6545508199999972
0.9784390200000033	0.6400864100000021	0.3454666700000004
0.4784340499999971	0.7946354799999966	0.6545508199999972
0.5215609799999967	0.1400864100000021	0.3454666599999996
0.5000070099999974	0.4917221099999978	0.9999957200000011

0.9999929900056163 0.9935410889129104 0.9999957276322544

Br103Tl1/icsd_076966/

1.000000000000000

4.4349828909999998	0.0068168340000000	0.0065270690000000
0.2079941490000000	4.4301099270000002	0.0065270380000000
0.2079939460000000	0.1987631270000000	4.4256535699999997

Tl	0	Br
1	3	1

Direct

0.0165408499999984	0.0165408299999967	0.0165408200000030
0.1189589800000022	0.5590771700000019	0.5590771700000019
0.5590771899999964	0.1189590999999979	0.5590771399999994
0.5590771600000011	0.5590771199999978	0.1189590999999979
0.5004470658097658	0.5004470056636733	0.4980859281196089

Br7Nb3S1/icsd_081078

1.000000000000000

7.1280903799999997	0.0000035740000000	-0.0000257030000000
-3.5640421000000000	6.1730998460000004	-0.0000000580000000
-0.0000230340000000	-0.0000133460000000	6.3123794630000001

Nb	S	Br
3	1	7

Direct

0.6041028200000014	0.8020514000000034	0.2231915799999982
0.1979573500000029	0.3959057499999972	0.2231912900000026
0.1979573500000029	0.8020515999999986	0.2231913000000034
0.3333421000000030	0.6666710800000004	0.4988291000000018
0.0000037200000023	0.0000018400000030	0.9992626100000024
0.8313453000000024	0.1686673600000006	0.4526470200000006
0.3373352600000032	0.1686676699999978	0.4526464799999985
0.8313452399999974	0.6626779099999993	0.4526469500000019
0.9944119000000029	0.4972059199999990	0.9530973800000027
0.5027995100000027	0.0055936199999991	0.9530981699999970
0.5027994431683129	0.4972058565750513	0.9515139413340962

Br7S1Ta3/icsd_051101

1.000000000000000

-0.0000006000000000	7.0910250350000004	0.0000057660000000
-6.1458193300000001	3.5455130349999999	-0.0010341510000000
-0.0542906850000000	3.5455176700000002	6.3201224470000001

S	Br	Ta
1	7	3

Direct

0.3500193400000029	0.4092597499999968	0.8907008099999985
0.2630136800000002	0.0813085300000012	0.3926649100000006
0.8724569000000031	0.4162192499999975	0.8388664100000014

0.7902882599999970	0.0786411599999965	0.3407836100000026
0.3801102799999967	0.9092691199999976	0.8393268399999982
0.8712927300000004	0.9092692199999988	0.8393267800000004
0.7888397299999994	0.5861571800000007	0.3436524899999966
0.2813514500000025	0.5861568999999989	0.3436523800000018
0.3517446800000030	0.6822657199999966	0.6142446100000001
0.3525486599999965	0.2788265000000010	0.6126905799999989
0.7567184357231669	0.2788406571050672	0.6111083337459512

Cl1K103/icsd_009483

1.0000000000000000

4.3085742319999998	0.0411920130000000	0.0381250420000000
0.4015798160000000	4.2900121369999997	0.0381283800000000
0.4015796860000000	0.3692743890000000	4.2742619460000002

K O Cl
1 3 1

Direct

0.0367725600000028	0.0367726300000015	0.0367726099999999
0.1592120899999969	0.5828666100000035	0.5828665700000002
0.5828666000000027	0.1592113399999988	0.5828671299999968
0.5828664900000007	0.5828670900000006	0.1592115099999987
0.5134820327271568	0.5134821047135628	0.5109390208069109

Cl2Mg1/icsd_051245

1.0000000000000000

3.8735546809999999	-0.0000000020000000	-0.0000000080000000
0.0000000020000000	3.8735546820000000	-0.0000000020000000
-0.0000000020000000	-0.0000000010000000	5.2360543479999997

Mg Cl
1 2

Direct

0.5000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.7421571699999987
-0.00000000000098609	0.4999999999995069	0.2559329949724448

Cl2Zr1/icsd_030052

1.0000000000000000

3.3866709730000002	0.0000008050000000	0.0000334000000000
1.6933347880000000	-2.9329435230000001	0.0000333960000000
1.6932713760000000	-0.9776107040000001	-6.4658617539999996

Zr Cl
1 2

Direct

0.0000688499999981	0.0000688399999973	0.9997933799999998
0.2444487699999982	0.2444487599999974	0.2666721300000034
0.4218668831394491	0.4218668831306521	0.7343810689320395

Co1F3/icsd_029133

1.0000000000000000

4.7066184719999997	0.0000009750000000	-0.0001073400000000
-2.3533083800000001	4.0760432220000000	-0.0000017290000000
0.0001591270000000	0.0000892020000000	6.7034476930000002

Co F
3 9

Direct

0.9999996999999975	0.9999994300000026	0.0000001200000028
0.6666677799999974	0.3333343500000012	0.3385472499999977
0.3333321799999993	0.6666665600000030	0.6614525900000032
0.9999998699999963	0.3570133400000017	0.4999999899999992
0.3570136599999998	0.0000010799999970	0.5000000900000003
0.6429862299999982	0.6429876500000020	0.5000001200000028
0.2924003700000029	0.3326796300000012	0.8216557399999971
0.0402758099999971	0.7075945099999998	0.8216571000000030
0.6673135699999975	0.9597194600000023	0.8216601700000012
0.7075995800000001	0.0402792100000013	0.1783441600000018
0.3326869300000013	0.2924059799999981	0.1783397600000001
0.9597241267588089	0.6673188226465590	0.1768511303240405

Cs2Te3/icsd_053245

1.0000000000000000

-4.2403791080000000	-6.0684056269999997	0.0000005940000000
-4.2403791210000001	6.0684055920000004	0.0000005540000000
0.0000010780000000	-0.0000000480000000	-8.4713441910000000

Cs Te
4 6

Direct

0.0870122199999983	0.9129877700000009	0.3691614800000025
0.9129877700000009	0.0870122199999983	0.8691614800000025
0.5810522299999974	0.4189477700000026	0.6536390300000008
0.4189477700000026	0.5810522299999974	0.1536390300000008
0.7763474899999991	0.2236525400000033	0.3002700600000026
0.2236525400000033	0.7763474899999991	0.8002700600000026
0.5762342800000013	0.9142265799999976	0.5079647199999968
0.0857734000000008	0.4237657099999979	0.5079647199999968
0.4237657099999979	0.0857734000000008	0.0079647199999968
0.9142265801453774	0.5762342801547182	0.0091451702065442

Cu103V1/icsd_009414/

1.0000000000000000

5.3827720560000003	-0.0864282090000000	-0.5648428450000000
2.5805694280000000	4.8429372559999999	-0.9976085380000000
-3.2475272479999999	0.4766001270000000	2.8957599009999999

O Cu V

3 1 1
Direct

0.2334105600000029	0.1850873699999980	0.2325753399999968
0.8923794800000024	0.8674652099999989	0.3303437799999998
0.5096774499999981	0.6328536500000013	0.2984062199999968
0.0566791700000024	0.5388485699999990	0.0567542000000003
0.3746898353766033	0.8981771084221384	0.0331009553841335

Cu2S4W1/icsd_098909

1.000000000000000

-5.4132132280000000	-0.0000033210000000	0.0000055920000000
-0.0000033270000000	-5.4132146329999999	0.0000055910000000
2.7066031960000001	2.7066038930000000	5.0507596399999999

S Cu W

4 2 1

Direct

0.3683652100000003	0.3683651300000008	0.2588179800000034
0.8904518699999997	0.8904519499999992	0.2588180600000030
0.6316345400000003	0.1095484200000030	0.7411821099999969
0.1095485100000033	0.6316346199999998	0.7411821099999969
0.9999998899999980	0.4999999500000030	0.9999998400000010
0.4999999500000030	0.9999998899999980	0.9999998400000010
-0.0009899171433763	-0.0009899171424624	-0.0019798380039034

F2N1P1/icsd_009684

1.000000000000000

0.0000000910000000	-0.0000003430000000	4.9949402909999998
4.1995415960000004	2.5770768010000000	-0.0000000890000000
-4.1995424210000003	2.5770780860000002	-0.0000002810000000

P F N

2 4 2

Direct

0.5047587099999973	0.8555101000000036	0.8555101399999998
0.0047586800000019	0.1444896300000025	0.1444895899999992
0.5685395200000016	0.8084527500000007	0.5261633499999974
0.5685395300000025	0.5261631699999967	0.8084527099999974
0.0685395100000008	0.1915472499999993	0.4738366899999988
0.0685395000000000	0.4738368599999987	0.1915473000000034
0.6971624500000004	0.0930865999999995	0.0930865999999995
0.1951600640662720	0.9069136298884581	0.9069136198450752

F3Rh1/icsd_029134

1.000000000000000

4.9727899139999998	-0.0000056420000000	-0.0000367410000000
-2.4863998359999999	4.3065593260000004	-0.0000027030000000
0.0000648970000000	0.0000321000000000	7.3085444749999997

Rh F

3 9

Direct

0.9999998199999993	0.9999996600000003	0.9999999200000005
0.6666669399999989	0.3333336099999968	0.3397950800000018
0.3333331299999998	0.6666670299999993	0.6602057099999996
0.9999996600000003	0.3456518300000013	0.4999999200000005
0.3456518400000022	0.0000001900000015	0.5000002399999985
0.6543482200000028	0.6543484800000030	0.4999998400000010
0.2991337599999966	0.3331362799999980	0.8218496300000027
0.0340007000000000	0.7008651599999993	0.8218495099999998
0.6668627600000008	0.9659981699999989	0.8218507799999983
0.7008662900000004	0.0340010899999967	0.1781505900000013
0.3331375100000002	0.2991345499999980	0.1781492100000008
0.9659993929557489	0.6668639601987039	0.1767813085037035

F5K1Sn2/icsd_036452

1.000000000000000

7.2338439470000004	-0.0000051240000000	-0.0000019190000000
-3.6169264090000000	6.2646881600000004	-0.0000008820000000
-0.0000023210000000	-0.0000028060000000	9.5876383529999991

K Sn F

3 6 15

Direct

0.0000055399999965	0.0000030699999982	0.3225689799999998
0.3333391899999967	0.6666700500000005	0.3411501900000005
0.6666720899999987	0.3333362899999983	0.3848031300000017
0.6679468499999999	0.6821588299999988	0.6742141499999974
0.0142203500000022	0.3320621599999996	0.6742140799999987
0.3178498300000001	0.9857880100000003	0.6742141000000004
0.3368094100000008	0.3432365099999970	0.0033400399999977
0.0064357600000022	0.6631990099999996	0.0033400299999968
0.6567719199999971	0.9935715100000024	0.0033392699999979
0.3333384600000002	0.6666687499999995	0.0346999799999992
0.3333389599999990	0.6666695400000009	0.6294032799999982
0.0000057000000027	0.0000030100000004	0.6322746700000010
0.4366044399999964	0.3340399900000008	0.6311190500000023
0.8974442499999995	0.5634046699999971	0.6311189999999982
0.6659683900000033	0.1025641000000022	0.6311188299999984
0.7646948000000009	0.7772511800000004	0.0548370899999995
0.0125651999999974	0.2353123800000034	0.0548355800000024
0.2227564100000023	0.9874430200000006	0.0548366499999986
0.3850361800000002	0.3622473799999995	0.2139063099999987

0.9772187100000025	0.6149707599999985	0.2139061000000027
0.6377613800000006	0.0227908299999982	0.2139052400000026
0.0243228100000010	0.3272919200000004	0.4602513900000034
0.3029769400000006	0.9756854199999978	0.4602513900000034
0.6727164294317620	0.6970316095328312	0.4592084602793793

Ga1In1S3/icsd_062340

1.0000000000000000

-0.0000768580000000	0.0000000110000000	-3.7833525849999998
0.0000000220000000	6.1877539890000000	-0.0000000070000000
9.6133891919999996	-0.0000000050000000	1.8918660089999999

S	Ga	In
6	2	2

Direct

0.7795912599999966	0.7430321699999993	0.5590705099999980
0.2204087499999972	0.2430321800000002	0.4409294900000020
0.4366817399999974	0.7083713199999977	0.8733567499999992
0.5633182600000026	0.2083713299999985	0.1266432500000008
0.1006963499999998	0.6953240699999981	0.2014350399999998
0.8993036399999994	0.1953240500000035	0.7985649499999994
0.8857641199999975	0.5566474199999973	0.7715377000000032
0.1142358800000025	0.0566474399999990	0.2284623099999976
0.3341976800000026	0.0025249999999986	0.6683504399999975
0.6684454889233148	0.5025250199953015	0.3316495811318502

Ga1Se1/icsd_073387

1.0000000000000000

3.7859205349999998	-0.0000021200000000	0.0000000400000000
-1.8929621000000001	3.2786969419999998	0.0000000430000000
0.0000001830000000	0.0000003110000000	16.0361514679999999

Se	Ga
4	4

Direct

0.6666820200000032	0.3333635500000014	0.8500308400000023
0.6666817899999984	0.3333633199999966	0.1499691599999977
0.3333347700000004	0.6666693600000002	0.3499677599999984
0.3333345300000019	0.6666691300000025	0.6500322400000016
0.0000156899999979	0.0000313000000034	0.9236530399999978
0.0000154499999994	0.0000310699999986	0.0763469600000022
0.6666680100000022	0.3333362600000029	0.4236602800000000
0.6666677500597199	0.3333360000591533	0.5757161289831682

Ga2Se2Te1/icsd_064617

1.0000000000000000

-7.3138207739999999	-0.0000062240000000	-0.0000073530000000
-0.0000062260000000	-7.3138207760000000	-0.0000073390000000
3.6569183879999998	3.6569183949999999	5.3543720730000004

Te	Se	Ga
2	4	4

Direct

0.2725380400000006	0.7725378499999991	0.5450762700000027
0.0225378499999991	0.0225380400000006	0.0450762700000027
0.6556980699999997	0.4032571799999971	0.8065149000000034
0.1508167100000009	0.4032575800000018	0.8065143800000030
0.6532575800000018	0.9008167100000009	0.3065143800000030
0.6532571799999971	0.4056980699999997	0.3065149000000034
0.4501195200000012	0.1759737900000005	0.3519474499999973
0.9018277999999995	0.1759734700000024	0.3519470000000027
0.4259734700000024	0.6518277999999995	0.8519470000000027
0.4250399711553431	0.1991857011535564	0.8500798148070503

Ge1Hf1Te4/icsd_241122

1.0000000000000000

3.9907710229700002	0.0000294052914565	0.0000000000000000
-1.9954445134200001	-7.9916886574900001	0.0000000000000000
0.0000000000000000	0.0000000000000000	-11.0110803399999995

Ge	Te	Hf
2	8	2

Direct

0.2284411300000002	0.4568920000000034	0.9603063799999987
0.7715588699999998	0.5431079999999966	0.4603063799999987
0.0164016000000018	0.0328335999999965	0.2409680600000002
0.9835984099999990	0.9671664000000035	0.7409680600000002
0.1018489100000011	0.2036730299999974	0.4613893000000004
0.8981510899999989	0.7963269700000026	0.9613893000000004
0.2783833499999986	0.5567524900000009	0.1981534999999965
0.7216166500000014	0.4432475099999991	0.6981535000000036
0.3822096000000030	0.7643947500000010	0.4997565899999969
0.6177903999999970	0.2356052499999990	0.9997565899999969
0.6516651999999965	0.3033243599999977	0.2715861699999991
0.3483348000000036	0.6966756400000024	0.7724943461000020

Ge103Zn1/icsd_183725

1.0000000000000000

5.0650474159999996	-0.0000017180000000	-0.0000023070000000
2.5325251980000001	-4.3864588790000001	-0.0000023140000000
2.5325261299999999	-1.4621546510000001	-4.3789303989999997

Ge	Zn	
2	2	6

Direct

0.4990056299999992	0.4990056400000000	0.5029830300000029
0.9990056400000000	0.9990056299999992	0.0029830300000029
0.7235180400000019	0.7235176000000010	0.8294465199999976
0.2235176000000010	0.2235180400000019	0.3294465199999976
0.8730023199999977	0.2726848499999974	0.2199233099999987
0.6343893299999976	0.8730023999999972	0.2199235000000002
0.2726847599999971	0.6343894399999996	0.2199236299999967
0.3730023999999972	0.1343893199999968	0.7199235000000002
0.7726848499999974	0.3730023199999977	0.7199233099999987
0.1336282182567380	0.7719235282512169	0.7222072934991673

Ge1Te1/icsd_655497

1.0000000000000000

-4.2049041459999996	-0.0000030380000000	0.0000057920000000
-2.1024547020000002	-3.6415522810000001	0.0000057940000000
-2.1024579200000000	-1.2138546480000001	3.5788789890000001

Ge Te
1 1

Direct

0.7641221299999970	0.7641221299999970	0.7076295800000025
0.2368092635492828	0.2368092635552496	0.2895762459522407

Ge1Te4Zr1/icsd_240906

1.0000000000000000

3.9999928643499998	0.0000364673992896	0.0000000000000000
-2.0000694470800000	-8.0113241096699994	0.0000000000000000
0.0000000000000000	0.0000000000000000	-11.0530160900999999

Ge Te Zr
2 8 2

Direct

0.2285612000000015	0.4571372199999999	0.5368348299999965
0.7714387999999985	0.5428627800000001	0.0368348299999965
0.9848042100000001	0.9695803999999981	0.7576049600000019
0.0151957799999991	0.0304196000000019	0.2576049600000019
0.8996159900000009	0.7992547500000029	0.5380728000000019
0.1003840099999991	0.2007452499999971	0.0380728000000019
0.7202712699999978	0.4405625300000011	0.8011315299999993
0.2797287300000022	0.5594374699999989	0.3011315299999993
0.3821313600000025	0.7642330099999981	0.0003249100000033
0.6178686399999975	0.2357669900000019	0.5003249000000025
0.3486735999999979	0.6973567499999973	0.7270309800000021
0.6513263900000013	0.3026432500000027	0.2279357104300027

Hg2P2S7/icsd_002490

1.0000000000000000
0.0000005200000000 -5.8623403170000001 -0.0000000240000000
5.4914718630000001 2.9311696750000000 0.0401622740000000
-1.9031576130000001 0.0000002050000000 7.8731816300000004

P S Hg
2 7 2

Direct

0.0856147100000015	0.1765925099999990	0.7055846399999979
0.9090221900000017	0.8234075000000018	0.2944153600000021
0.3710962600000016	0.4869799499999985	0.6414278900000028
0.8841163100000031	0.5130199899999965	0.3585720900000027
0.7766741200000027	0.0000000300000025	0.5000000100000008
0.8744044700000018	0.2489180099999970	0.8933789299999972
0.6254864300000023	0.7510820500000008	0.1066210899999973
0.2161308700000006	0.9493949399999977	0.7611403300000035
0.2667358500000034	0.0506049800000028	0.2388596799999974
0.7922394300000022	0.5813601600000027	0.8028355800000000
0.2106596656688176	0.4182004813538280	0.1958965069392324

Hg306S1/icsd_024147

1.0000000000000000
7.1607207040000000 -0.0000095820000000 0.0000085710000000
-3.5803686500000000 6.2013625990000003 -0.0000066320000000
0.0000117480000000 -0.0000039030000000 10.0419000109999992

S Hg 0
3 9 18

Direct

0.2293644299999968	0.0000020199999966	0.3333397899999966
0.7706386300000005	0.7706358200000025	0.0000062499999984
0.9999966800000024	0.2293617400000016	0.6666725600000021
0.5070434000000006	0.1914213800000013	0.6877637699999966
0.6843784100000008	0.4929574100000025	0.3544305100000003
0.8085786299999995	0.3156214700000035	0.0210972599999977
0.4929582999999980	0.6843785699999998	0.6455837199999976
0.1914206800000002	0.5070424199999977	0.3122502800000007
0.3156211700000000	0.8085795200000021	0.9789169200000032
0.7052497500000001	0.9999997500000006	0.3333391800000030
0.2947497700000028	0.2947505300000017	0.0000066899999993
0.0000010500000016	0.7052503500000000	0.6666738899999984
0.3269475199999974	0.8464027799999982	0.7193277000000009
0.5194556800000001	0.6730534599999984	0.3859934600000017
0.1535976699999964	0.4805441600000009	0.0526599700000006
0.6730543199999985	0.5194553899999974	0.6140200500000006
0.8464015899999993	0.3269466699999981	0.2806860499999999
0.4805444699999981	0.1535991399999972	0.9473538000000019
0.8393571699999995	0.0311350799999985	0.5936673300000024
0.1917706999999993	0.1606382800000006	0.2603373199999979
0.9688665600000022	0.8082268200000016	0.9270013900000009
0.1606210799999985	0.1917450799999969	0.7396740200000025

0.0311264899999983	0.8393741300000030	0.4063440700000029
0.8082532800000024	0.9688753599999984	0.0730097499999971
0.1133880800000000	0.4101776899999976	0.5667349599999980
0.2967887000000005	0.8866132499999964	0.2333999100000028
0.5898234900000006	0.7032115499999989	0.9000681799999981
0.8866222699999966	0.2967997299999965	0.7666146999999981
0.4101798000000016	0.1133787999999996	0.4332797300000024
0.7032002313203963	0.5898216093732517	0.0989509725182403

I2Pb1/icsd_024263

1.000000000000000

4.5532946379999997	-0.0000004450000000	0.0000000020000000
-2.2766477020000000	3.9432304189999998	-0.0000000020000000
-0.0000000040000000	0.0000000070000000	14.1180142180000008

Pb I
2 4

Direct

0.6666676700000025	0.3333353399999979	0.4999891499999976
0.3333323299999975	0.6666646600000021	0.9999891499999976
0.0000033600000009	0.0000068200000030	0.6348742300000012
0.9999966399999991	0.9999931799999970	0.1348742400000020
0.3333336999999972	0.6666673400000036	0.3651366100000004
0.6666663000000091	0.3333326600012609	0.8644282950878898

I3Na108/icsd_418336

1.000000000000000

7.9445366420000001	-0.0000006930000000	-0.0000001390000000
-0.0000005710000000	7.9445378289999997	-0.0000001050000000
-0.0000001290000000	-0.0000001520000000	5.6860469309999999

I Na 0
6 2 16

Direct

0.7352495000000019	0.2469455000000025	0.0979823400000015
0.2647504899999973	0.7530545099999983	0.0979823400000015
0.7530539799999971	0.7352497500000013	0.9020181100000002
0.2469460399999974	0.2647502499999987	0.9020180999999994
0.0000000200000017	0.5000000100000008	0.4200418900000003
0.4999999899999992	0.0000000000000000	0.5799578199999971
0.4999999699999975	0.4999999799999983	0.4999999799999983
0.0000000100000008	0.9999999799999983	0.4999999899999992
0.7634545499999987	0.4008424700000006	0.3721975599999965
0.2365454600000021	0.5991575500000010	0.3721975400000019
0.5991575700000027	0.7634544900000009	0.6278025000000014
0.4008424299999973	0.2365454799999966	0.6278025000000014
0.7662690299999966	0.0529374300000001	0.2689726899999982
0.2337309600000026	0.9470625800000008	0.2689726500000020
0.9470629599999967	0.7662690499999982	0.7310269199999979
0.0529370300000025	0.2337309500000018	0.7310269000000034
0.5082682999999975	0.2696499899999978	0.1484517499999995

0.4917317199999971	0.7303500299999968	0.1484517499999995
0.7303500100000022	0.5082680599999989	0.8515482000000034
0.2696499899999978	0.4917319300000003	0.8515481800000018
0.9411870699999980	0.6750626700000026	0.2142574699999997
0.0588129300000020	0.3249373399999982	0.2142574599999989
0.3249372300000033	0.9411870100000002	0.7857426500000031
0.6750627699714399	0.0588129799663506	0.7839839889231660

I7Nb3Te1/icsd_086724

1.000000000000000

7.6556141489999998	0.0000270730000000	0.0000125350000000
-3.8277835450000000	6.6299392690000003	0.0000023310000000
0.0000115970000000	0.0000091380000000	6.9015375340000000

I	Nb	Te
7	3	1

Direct

0.6666592899999984	0.3333295400000011	0.7133524799999975
0.6606796599999996	0.8303399699999972	0.7660565300000002
0.1696482300000000	0.3393090100000009	0.7660558600000016
0.1696483999999998	0.8303394400000030	0.7660559500000019
0.0030446499999996	0.5015220599999992	0.2745674100000031
0.4984719500000026	0.9969493899999975	0.2745669500000005
0.4984716599999999	0.5015222600000016	0.2745670300000000
0.2653136899999993	0.1326570100000026	0.4990108300000031
0.8673332600000023	0.7346768600000004	0.4990114900000009
0.8673333799999980	0.1326566500000013	0.4990119200000009
0.9999958431934503	0.9999978119970648	0.1958945975092275

In1Se1/icsd_041477

1.000000000000000

4.0450470420000002	0.0008499600000000	-0.0060852550000000
2.0217874409999999	-3.5035385200000002	-0.0060853120000000
2.0348583840000001	-1.1748261550000001	-8.4118099950000005

Se	In
2	2

Direct

0.8307037000000008	0.8307037200000025	0.5112558300000032
0.6146324899999982	0.6146324600000028	0.1523372999999992
0.0000649300000006	0.0000649199999998	0.9982545299999970
0.1118999530511016	0.1118999729969088	0.6662417219728998

In2S4Zn1/icsd_016200

1.000000000000000

3.8945872680000000	-0.0000009420000000	-0.0000000570000000
-1.9472944470000000	3.3728189359999998	-0.0000000680000000
-0.0000004500000000	-0.0000007260000000	24.5824776249999992

Zn	S	In
2	8	4

Direct

0.9999877699999971	0.9999747000000028	0.9128168399999979
0.0000123800000011	0.0000254500000025	0.4128168200000033
0.0000134599999981	0.0000272799999976	0.5498962400000025
0.9999863700000020	0.9999725400000017	0.0498962300000017
0.6666667699999991	0.3333335999999998	0.6940991299999979
0.3333331299999998	0.6666663399999990	0.1940991199999971
0.9999969899999996	0.9999936600000012	0.8081220500000015
0.0000030899999999	0.0000064199999983	0.3081220299999998
0.3333209600000018	0.6666412499999979	0.9350313899999989
0.6666792099999981	0.3333589200000020	0.4350313699999973
0.3333304200000029	0.6666607200000030	0.7565220099999976
0.6666695899999979	0.3333392799999970	0.2565219900000031
0.6666808800000013	0.3333619100000007	0.5940123999999969
0.3333189899092179	0.6666379599124402	0.0936055861791130

In2Te5/icsd_000501

1.0000000000000000

-4.3385048810000004	0.0002627450000000	-0.0613908440000000
-2.1687533790000000	-8.2532564229999998	-0.0306856860000000
-0.1927795880000000	0.0000180000000000	13.5336418359999993

Te	In
10	4

Direct

0.9876171299999967	0.0165546699999979	0.8559852799999987
0.0043114400000022	0.9834452099999993	0.3559854599999994
0.3919994299999985	0.2082484700000009	0.5982079099999993
0.6001405800000015	0.7917516400000011	0.0982078099999981
0.6897607200000024	0.6123589899999970	0.7323430100000010
0.3021719700000034	0.3876411500000003	0.2323427800000033
0.2226549100000028	0.5466318599999980	0.8859965299999999
0.7693297499999971	0.4533684299999976	0.3859963199999967
0.1594158500000020	0.6733447200000029	0.5764364999999998
0.8327286999999970	0.3266547899999992	0.0764362500000004
0.9999488999999997	0.9922386200000020	0.6411540799999997
0.9921803499999982	0.0077613699999972	0.1411543500000008
0.3798540599999995	0.2321848799999984	0.8125769800000029
0.6121190463423234	0.7678152194338561	0.3118379894920653

Li706Sb1/icsd_015631

1.0000000000000000

5.5902495569999999	0.0000036160000000	0.0000030400000000
2.7951216390000000	-4.8412962979999996	0.0000026160000000
2.7951208740000002	-1.6137629540000000	-4.8765070140000004

Sb	0	Li
1	6	7

Direct

0.0012519300000022	0.0012517999999986	0.9962448100000003
0.7981185399999973	0.3769033900000025	0.7495767799999982
0.0754025499999997	0.7981184100000007	0.7495761999999999
0.3769039800000016	0.0754008099999979	0.7495773099999994

0.6425400600000017	0.8828403600000030	0.2409383600000012
0.2336820700000004	0.6425401899999983	0.2409389700000020
0.8828401299999982	0.2336824300000018	0.2409381699999997
0.9362700399999966	0.4865092799999999	0.3410825300000013
0.2361393799999973	0.9362718699999988	0.3410821599999991
0.4865104100000011	0.2361384700000002	0.3410826799999995
0.1218866999999975	0.4983916400000012	0.6555076599999978
0.7242142899999990	0.1218854800000031	0.6555064300000026
0.4983904799999976	0.7242136599999967	0.6555067800000032
0.6551658916655744	0.6551686614262154	0.0344918273394045

Mo108V2/icsd_025378

1.0000000000000000

0.0001423020000000	3.7159048100000001	0.0143135040000000
0.0000217350000000	-0.0156619740000000	-4.0133604380000003
-9.6361186320000005	-1.8583296800000000	-0.0071054060000000

Mo 0 V
1 8 2

Direct

0.9454916500000010	0.0121230199999971	0.9999971900000020
0.4739297899999997	0.9257851400000021	0.0000022199999989
0.9612918400000012	0.4459291599999986	0.9999918199999982
0.8315033100000022	0.4418152300000031	0.6246041400000024
0.2067694300000014	0.4418261499999971	0.3754048300000008
0.9101178199999964	0.9453481700000026	0.8046374700000030
0.1054757799999990	0.9454009000000028	0.1953597400000007
0.3068930299999977	0.9589442400000010	0.5823266100000026
0.7245139400000014	0.9589345799999975	0.4176708299999987
0.8287765099999973	0.0354404699999975	0.6233051600000010
0.2052473950882112	0.0379446549800193	0.376699957753863

Mo1S2/icsd_038401

1.0000000000000000

3.1756176090000001	-0.0000047110000000	0.0000205440000000
1.5878128860000000	-2.7501631600000001	0.0000205450000000
1.5877704950000000	-0.9166997160000000	-6.1521195559999997

Mo S
1 2

Direct

0.9999902400000025	0.9999902400000025	0.0000331199999977
0.2482565199999982	0.2482565199999982	0.2552410500000022
0.4179114360558881	0.4179114360595954	0.7462512824390778

Mo1Se2/icsd_016948

1.0000000000000000

3.3106495560000000	-0.0000151930000000	0.0001036390000000
1.6553379380000000	-2.8671062759999999	0.0000435970000000
1.6551311110000000	-0.9557219860000000	-6.5057366200000004

Mo	Se	
1	2	
Direct		
0.3332166499999971	0.3331830799999977	0.0004235299999991
0.7525174499999991	0.7525222200000030	0.7424111500000024
0.5801536314754501	0.5800823275952354	0.2597024133616314
N1Na1Sn1/icsd_172471		
1.000000000000000		
3.3458590060000000	0.0000001510000000	0.0000000080000000
-1.6729293740000000	2.8975984659999998	0.0000000070000000
0.0000000080000000	0.0000000280000000	10.8627084840000006
Na	Sn	N
2	2	2
Direct		
0.66667489000000030	0.3333496999999994	0.74460641000000029
0.33332510999999970	0.66665030000000006	0.24460641000000029
0.99999430999999982	0.99998870999999967	0.49981138999999979
0.00000569000000018	0.00001129999999970	0.99981139999999987
0.33332887000000026	0.66665781999999975	0.60022218999999967
0.6666711300066465	0.3333421800088981	0.0993016192797536
N3Na1/icsd_029380		
1.000000000000000		
4.0820471539999996	2.6178398380000001	-1.1627026250000001
3.7207790369999998	-1.7848883510000000	-0.9543061819999999
4.0491721880000000	0.5682048380000000	-4.4395880329999997
Na	N	
1	3	
Direct		
0.87490714999999985	0.09144420999999988	0.01695784999999972
0.65816136000000011	0.24812084999999994	0.48424845000000026
0.87566666000000003	0.91383545000000005	0.60452175000000035
0.0896209713555245	0.2451423115628418	0.3972681643894688
Na1P1Sn1/icsd_409010		
1.000000000000000		
3.9040004790000000	0.0000016340000000	0.0000000130000000
-1.9519988180000001	3.3809382580000000	0.0000000150000000
0.0000000063000000	0.0000000920000000	11.5633507800000004
Na	Sn	P
2	2	2
Direct		
0.66667678999999968	0.33335318999999969	0.7779896199999996
0.33332321999999969	0.66664681999999969	0.2779896199999996
0.99999342000000027	0.99998732000000025	0.49860573000000013
0.00000658999999981	0.00001267999999975	0.99860573000000013
0.66667237000000006	0.33334451999999971	0.11420464999999978
0.3333276200257203	0.6666554600235335	0.6133398487680490

01Sn1/icsd_020624

1.000000000000000

3.3591187560000000	-0.0000000020000000	0.0000001080000000
0.0000000030000000	3.8151272719999998	0.0000002360000000
-0.0000000170000000	-0.0000004650000000	5.8342209350000003

Sn 0

2 2

Direct

0.4999999899999992	0.96712981999999967	0.7316585000000018
0.0000000100000008	0.4671298000000021	0.2683414999999982
0.5000000100000008	0.7828701899999970	0.3833475200000009
0.9999999899913250	0.2828701997910871	0.6149384550922331

03Pb1Rb2/icsd_001413

1.000000000000000

-0.0000000030000000	-0.0000008190000000	6.0890835630000000
5.4737957960000001	3.6848377260000000	-0.0000004970000000
-5.4737962070000004	3.6848381710000000	-0.0000004960000000

Pb 0 Rb

2 6 4

Direct

0.7410959500000018	0.9047972199999990	0.9047972099999981
0.2410958099999974	0.0952030799999974	0.0952030899999983
0.5021017199999989	0.1545632300000008	0.8922370599999994
0.5021017199999989	0.8922370000000015	0.1545631700000030
0.0021016199999977	0.8454367499999975	0.1077628399999995
0.0021016199999977	0.1077628999999973	0.8454368000000017
0.6603425200000004	0.6341421999999994	0.6341421300000007
0.1603428199999968	0.3658574800000025	0.3658575500000012
0.7671790899999991	0.1931407800000002	0.5183895799999974
0.7671791100000007	0.5183895799999974	0.1931407800000002
0.2671789899999979	0.8068593400000026	0.4816104499999980
0.2655367367406993	0.4816104498170394	0.8068593398179442

05Sb2V1/icsd_203130

1.000000000000000

17.8645877810000009	-0.0000000350000000	-0.0000000680000000
0.0000000070000000	4.7131958159999998	-0.0000295390000000
0.0000000270000000	0.0000380100000000	5.4102689670000004

Sb 0 V

8 20 4

Direct

0.9105037499999966	0.0221154400000003	0.6782160200000007
0.5849421699999979	0.4935728100000034	0.1748804899999996
0.4150575600000010	0.9935711700000027	0.3251196100000016
0.0894964000000016	0.5221165999999968	0.8217846200000025
0.0849424399999990	0.9935711800000036	0.3251196100000016
0.4105035899999976	0.5221165900000031	0.8217846200000025
0.5894962500000034	0.0221154299999995	0.6782160200000007
0.9150578300000021	0.4935728100000034	0.1748804899999996

0.7500000000000000	0.6986134400000026	0.8354410800000025
0.7500000000000000	0.7858895000000032	0.3103834599999971
0.2500000000000000	0.2858902600000022	0.1896169199999989
0.2500000000000000	0.1986136900000020	0.6645593800000000
0.8204351700000032	0.2571933999999985	0.5540100500000023
0.6710683100000026	0.2281947700000018	0.0542354999999972
0.3289313200000024	0.7281959499999999	0.4457642100000001
0.1795653200000018	0.7571938500000002	0.9459900000000019
0.1710686799999976	0.7281959600000008	0.4457642100000001
0.3204346799999982	0.7571938500000002	0.9459900000000019
0.6795648299999968	0.2571933999999985	0.5540100500000023
0.8289316899999974	0.2281947800000026	0.0542354999999972
0.9590136999999999	0.3579512600000001	0.8487444599999989
0.5396474300000023	0.1570583000000028	0.3554277799999994
0.4603527299999968	0.6570576100000025	0.1445712900000018
0.0409860299999991	0.8579516499999968	0.6512553600000004
0.0396472700000032	0.6570576200000033	0.1445712900000018
0.4590139700000009	0.8579516400000031	0.6512553600000004
0.5409863000000001	0.3579512499999993	0.8487444599999989
0.9603525599999969	0.1570583099999965	0.3554277799999994
0.7500000000000000	0.3518143200000026	0.8255397000000002
0.7500000000000000	0.1315087099999985	0.2874696599999993
0.2500000000000000	0.6315096299999965	0.2125303999999986
0.25000000000027935	0.8518148249060832	0.6726122730576832

Pb1S1/icsd_183255

1.0000000000000000

4.0972295689999996	-0.0000008220000000	-0.0000000210000000
-2.0486154870000002	3.5482742439999999	0.0000001000000000
-0.0000000240000000	0.0000001280000000	7.4002836150000002

Pb S
2 2

Direct

0.0000006499999969	0.0000013300000035	0.4754708800000031
0.9999993500000031	0.9999986699999965	0.9754708800000031
0.3333317100000031	0.6666636200000013	0.7037291199999984
0.6666682900164549	0.3333363900487462	0.2023778204390289

S2Sn1/icsd_043003

1.0000000000000000

3.6808035380000002	0.0000001180000000	0.0000000210000000
-1.8404016620000001	3.1876702140000002	0.0000000240000000
0.0000000690000000	0.0000001250000000	11.7993693529999994

S Sn
4 2

Direct

0.0000005400000020	0.0000010500000016	0.4992126799999994
0.9999994799999996	0.9999989700000000	0.9992126799999994
0.6666655900000009	0.3333311800000018	0.7507134800000017
0.3333343899999974	0.6666687999999965	0.2507134800000017

0.3333311299999977	0.6666622300000000	0.6250738399999989
0.6666688700325062	0.3333377700332336	0.1242263370783739

S2W1/icsd_202367

1.0000000000000000

3.1759339980000001	0.0000006090000000	0.0000343460000000
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1.5879664689999999	-2.7504398200000000	0.0000343590000000
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1.5878998120000001	-0.9167743450000000	-6.2027772719999996
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S W

2 1

Direct

0.2492236499999976	0.2492236599999984	0.2523484700000012
--------------------	--------------------	--------------------

0.4188153200000002	0.4188153099999994	0.7435321299999984
--------------------	--------------------	--------------------

0.0001236609658800	0.0001236609983231	0.9996315751018182
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