

Supporting information for

Spin-Orbit Effects on the ^{119}Sn Magnetic-Shielding Tensor in Solids:

A ZORA/DFT Investigation

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Table S1. Comparison of calculated principal components of ^{119}Sn magnetic-shielding tensors obtained with different linear threshold parameters (10^{-4} vs. 5×10^{-3}) at PBE/ZORA/SO level of theory.

Compounds	σ_{11} (ppm)	σ_{22} (ppm)	σ_{33} (ppm)
Tin(II)-containing solids			
<u>SnO</u>			
PBE/ 10^{-4}	2611	2614	3660
PBE/ 5×10^{-3}	2611	2614	3660
Difference	0	0	0
<u>SnHPO₄</u>			
PBE/ 10^{-4}	3536	3675	4296
PBE/ 5×10^{-3}	3536	3675	4296
Difference	0	0	0
<u>SnHPO₃</u>			
PBE/ 10^{-4}	3272	3297	4269
PBE/ 5×10^{-3}	3272	3297	4269
Difference	0	0	0
<u>SnC₂O₄</u>			
PBE/ 10^{-4}	3454	3518	4259
PBE/ 5×10^{-3}	3477	3531	4255
Difference	-23	-12	4
<u>SnSO₄</u>			
PBE/ 10^{-4}	3895	3942	4497
PBE/ 5×10^{-3}	3886	3920	4499
Difference	9	23	-2
<u>BaSnF₄</u>			

PBE/10 ⁻⁴	3386	3388	4345
PBE/5x10 ⁻³	3460	3461	4335
Difference	-73	-73	9
Tin(IV)-containing solids			
<u>SnO₂</u>			
PBE/10 ⁻⁴	3472	3497	3652
PBE/5x10 ⁻³	3467	3500	3610
Difference	5	-4	42
<u>Ca₂SnO₄</u>			
PBE/10 ⁻⁴	3341	3396	3514
PBE/5x10 ⁻³	3404	3423	3539
Difference	-63	-27	-25
<u>SnS₂</u>			
PBE/10 ⁻⁴	3608	3609	3686
PBE/5x10 ⁻³	3615	3616	3693
Difference	-7	-7	-8
<u>Pb₂SnO₄</u>			
PBE/10 ⁻⁴	3303	3335	3376
PBE/5x10 ⁻³	3303	3334	3373
Difference	0	1	3
<u>Na₆Sn₂S₇</u>			
PBE/10 ⁻⁴	2618	2826	3017
PBE/5x10 ⁻³	2607	2857	3011
Difference	11	-31	6
<u>Sr₂SnO₄</u>			
PBE/10 ⁻⁴	3403	3406	3668
PBE/5x10 ⁻³	3386	3389	3651
Difference	18	17	17

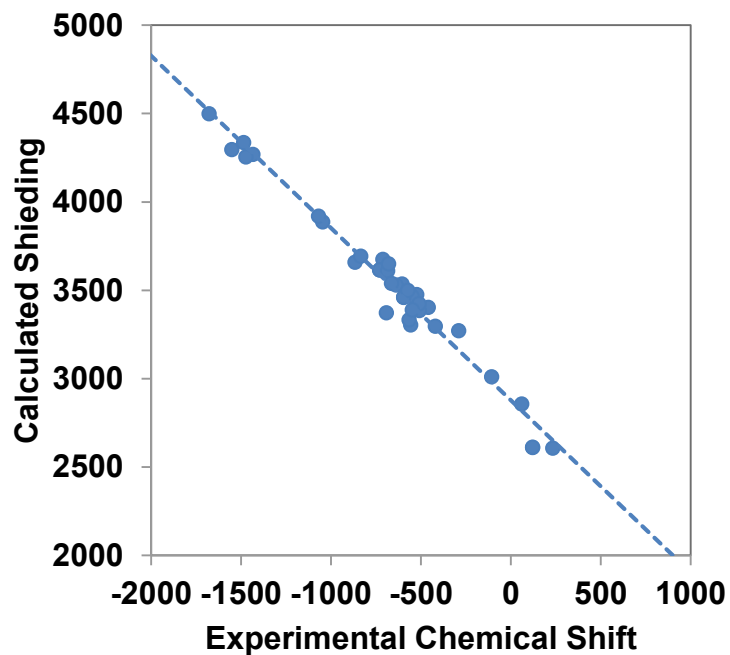


Figure S1. Correlations between calculated principal components of ^{119}Sn magnetic-shielding tensors and experimental ^{119}Sn chemical-shift tensors determined at PBE/ZORA/SO level of theory and 5×10^{-3} linear dependence threshold. The equation of the best-fit line is given as $\sigma_{\text{cal}} = -0.974\delta_{\text{exp}} + 2878$ with R^2 value of 0.973.

The positions of atoms (in Angström units) in clusters discussed in the text of the article.

Third co-ordination shell cluster of SnO

Sn	-25.13000000	8.62100000	14.12200000
Sn	-25.84600000	3.36900000	15.03100000
O	-24.68000000	1.68400000	14.16700000
Sn	-20.13300000	4.90400000	12.48500000
O	-18.27600000	8.86700000	12.98500000
O	-26.98700000	4.65800000	13.62300000
O	-27.34500000	2.03200000	14.07700000
Sn	-22.44000000	7.87700000	11.94100000
O	-18.63400000	6.24100000	13.43900000
O	-18.99200000	3.61500000	13.89300000
O	-20.94100000	9.21500000	12.89500000
O	-21.29900000	6.58900000	13.34900000
Sn	-20.51600000	2.67400000	15.21100000
O	-23.60600000	9.56200000	12.80500000
Sn	-22.82300000	5.64800000	14.66700000
Sn	-23.15600000	2.62500000	12.85000000
O	-19.35000000	0.98900000	14.34800000
Sn	-25.46300000	5.59900000	12.30500000
O	-21.65700000	3.96300000	13.80300000
O	-22.01500000	1.33600000	14.25800000
O	-23.96400000	6.93600000	13.25900000
O	-24.32200000	4.31000000	13.71300000
O	-26.27100000	9.91000000	12.71400000
O	-26.62900000	7.28400000	13.16900000
Sn	-19.80000000	7.92600000	14.30300000

Third co-ordination shell cluster of SnHPO₄

O	15.05000000	-22.26800000	-4.00700000
O	7.66100000	-20.67400000	2.56100000
O	10.00100000	-20.52500000	3.87900000
O	16.93100000	-21.56000000	-1.42900000
O	10.20600000	-17.64600000	0.10800000
O	14.95200000	-17.72000000	-3.26700000
O	11.68500000	-22.05700000	-2.74200000
O	16.86000000	-19.15400000	0.66200000
O	13.59300000	-23.49100000	1.18600000
O	8.09300000	-19.09100000	-0.04900000
O	10.27700000	-20.05200000	-1.98200000
O	12.84000000	-19.16400000	-3.42400000
O	14.31500000	-22.18100000	3.11500000
O	16.85800000	-21.38600000	1.64800000
O	8.77400000	-18.03700000	2.15000000
O	12.21200000	-23.62900000	3.29500000
O	15.42800000	-19.54400000	2.70400000

O	10.30400000	-22.19500000	-0.63200000
O	14.95000000	-19.95200000	-2.28000000
O	12.18500000	-21.48600000	1.94600000
O	14.74700000	-20.59800000	0.50400000
O	13.52000000	-18.11000000	-1.22400000
O	10.20400000	-19.87800000	1.09500000
O	12.40700000	-20.74700000	-0.81400000
P	9.28700000	-18.67400000	0.87200000
P	14.03300000	-18.74700000	-2.50300000
P	11.13800000	-21.26400000	-1.49500000
P	15.94100000	-20.18200000	1.42400000
P	13.04600000	-22.69800000	2.43300000
Sn	14.66100000	-21.90700000	-1.43300000
Sn	9.91500000	-21.83400000	1.94200000
Sn	12.77500000	-19.48600000	0.88900000

Third co-ordination shell cluster of SnHPO_3

O	-14.07100000	3.58400000	19.26300000
O	-4.44700000	0.77200000	19.08000000
O	-4.89500000	3.29700000	17.46800000
O	-11.87100000	2.37600000	20.93400000
O	-6.49300000	2.07100000	22.42100000
O	-9.49400000	0.52800000	22.09600000
O	-12.02500000	2.28500000	15.92200000
O	-9.11000000	6.30300000	17.64300000
O	-7.27200000	5.14400000	16.30600000
O	-10.29100000	4.12300000	16.27600000
O	-10.53500000	0.14400000	19.81500000
O	-5.78200000	3.00400000	20.19800000
O	-10.98300000	2.66900000	18.20400000
O	-7.98200000	4.21200000	18.52900000
O	-8.80200000	1.98300000	20.16700000
O	-7.62000000	4.16300000	21.53500000
P	-7.83800000	5.46800000	17.66600000
P	-6.34800000	3.32700000	21.55800000
P	-10.79800000	2.76400000	16.68600000
P	-9.30900000	0.62400000	20.57900000
Sn	-9.36400000	4.05100000	20.16700000
Sn	-6.23400000	1.90600000	18.41500000
Sn	-12.32300000	1.27800000	19.14900000
H	-8.21402064	-0.34062383	20.24058447
H	-9.70322053	1.80019217	16.34462574
H	-6.80751667	6.31517494	18.34747100
H	-5.31501319	4.17218704	22.23814787

Third co-ordination shell cluster of SnC_2O_4

O	6.38300000	9.96900000	14.34400000
O	11.41900000	12.21200000	16.36700000
O	13.07300000	10.73200000	20.21600000
O	3.36600000	17.04800000	18.26100000
O	16.45500000	14.45500000	18.38900000
O	-1.95400000	11.34300000	19.68300000
O	8.11800000	15.82900000	23.72800000
O	-0.25600000	11.17200000	23.78500000
O	4.59700000	8.01400000	24.76300000
O	-5.10900000	14.33000000	22.80700000
O	4.18300000	12.17800000	24.05300000
O	12.47900000	14.50800000	23.54600000
O	-4.33300000	15.95400000	20.52200000
O	-1.07300000	16.04100000	17.99300000
O	-0.67100000	15.33600000	23.07600000
O	8.63400000	9.72500000	19.94800000
O	9.03600000	9.02100000	25.03100000
O	12.29600000	9.10700000	22.50100000
O	-1.25600000	10.64000000	16.94800000
O	2.02300000	11.29000000	14.52700000
O	7.05900000	13.53300000	16.54900000
O	2.40600000	10.02200000	19.50100000
O	15.75700000	15.15800000	21.12500000
O	12.09500000	15.77600000	18.57200000
O	4.58400000	12.08000000	14.73200000
O	9.62000000	14.32300000	16.75500000
O	14.65700000	16.56600000	18.77800000
O	-0.15500000	9.23200000	19.29500000
O	6.53500000	9.99500000	25.16600000
O	11.13600000	8.75100000	19.81200000
O	-3.17200000	16.31100000	23.21100000
O	1.42900000	15.06600000	17.85700000
O	9.91700000	13.71800000	23.34000000
O	1.68100000	13.15300000	24.18900000
O	13.25500000	16.13300000	21.26100000
O	1.24600000	9.66600000	16.81200000
O	9.73500000	8.31700000	22.29500000
O	-1.77100000	16.74400000	20.72800000
C	4.01500000	12.05700000	18.07100000
C	7.14300000	11.18000000	22.05300000
C	5.67400000	10.72300000	21.94800000
C	2.28900000	14.33800000	21.07500000
C	0.82100000	13.88100000	20.97100000
C	9.05200000	14.29900000	20.09300000
C	5.45000000	11.49900000	17.97900000
C	10.48600000	13.74100000	20.00200000

O	8.21900000	13.89000000	19.23800000
O	6.28200000	11.90800000	18.83400000
O	4.88100000	11.47500000	21.31800000
O	7.93600000	10.42800000	22.68300000
O	11.31800000	14.15100000	20.85700000
O	3.08200000	13.58600000	21.70600000
O	0.02800000	14.63300000	20.34000000
O	3.18300000	11.64700000	17.21600000
O	7.44200000	12.26500000	21.52300000
O	5.68500000	10.67200000	17.08000000
O	0.52100000	12.79600000	21.50000000
O	3.78000000	12.88300000	18.97000000
O	10.72100000	12.91500000	19.10200000
O	5.37400000	9.63800000	22.47700000
O	2.58900000	15.42300000	20.54600000
O	8.81700000	15.12600000	20.99300000
Sn	3.82700000	10.19100000	15.65100000
Sn	8.86300000	12.43400000	17.67300000
Sn	13.89900000	14.67700000	19.69600000
Sn	0.60200000	11.12100000	18.37700000
Sn	10.49200000	10.20600000	21.37700000
Sn	2.32500000	11.69800000	22.62400000
Sn	7.17900000	8.54000000	23.60100000
Sn	0.78500000	16.52200000	19.42200000
Sn	-2.52800000	14.85600000	21.64600000
Sn	5.63800000	13.36400000	20.39900000
Sn	10.67400000	15.60700000	22.42200000

Third co-ordination shell cluster of SnSO₄

O	-3.97100000	-13.44800000	8.86200000
O	-5.56400000	-17.77200000	6.05600000
O	-3.95900000	-13.63000000	14.17700000
O	-5.54100000	-18.13600000	16.68800000
O	-10.16300000	-16.95100000	8.75500000
O	-7.75200000	-24.25000000	11.16100000
O	-10.15200000	-17.13300000	14.07000000
O	-8.14900000	-19.39400000	18.09700000
O	-12.52900000	-18.79700000	15.46500000
O	-5.36800000	-22.68400000	12.65500000
O	-9.70100000	-15.03100000	12.92700000
O	-5.37400000	-22.58600000	9.76700000
O	-12.54700000	-18.51600000	7.26100000
O	-9.70800000	-14.93300000	10.03800000
O	-8.17800000	-18.93100000	4.57600000
O	-6.35400000	-15.01300000	7.36800000
O	-3.56200000	-18.48600000	7.24300000

O	-6.34800000	-15.11200000	10.25600000
O	-6.34300000	-15.19500000	12.68300000
O	-3.54500000	-18.76700000	15.44700000
O	-6.33700000	-15.29400000	15.57200000
O	-1.25500000	-19.26600000	8.65700000
O	-9.14500000	-12.63100000	11.56200000
O	-1.24300000	-19.44800000	13.97300000
O	-10.47900000	-18.25100000	6.05000000
O	-10.45600000	-18.61500000	16.68200000
O	-13.10300000	-20.91600000	8.62600000
O	-13.09200000	-21.09800000	13.94100000
O	-6.15800000	-19.92600000	13.96600000
O	-6.16900000	-19.74400000	8.65100000
O	-12.08500000	-16.59700000	11.43300000
O	-5.55300000	-17.95400000	11.37200000
O	-4.81100000	-20.28400000	11.29000000
O	-6.90000000	-17.59600000	14.04800000
O	-10.46800000	-18.43300000	11.36600000
O	-6.91100000	-17.41400000	8.73300000
O	-12.54000000	-18.61500000	10.15000000
O	-12.53600000	-18.69800000	12.57600000
O	-8.17100000	-19.03000000	7.46500000
O	-8.16700000	-19.11300000	9.89100000
O	-8.15500000	-19.29500000	15.20800000
O	-8.16000000	-19.21200000	12.78000000
O	-3.55600000	-18.58500000	10.13100000
O	-3.55100000	-18.66800000	12.55800000
S	-11.89800000	-18.04000000	11.38300000
S	-7.30000000	-19.02200000	14.00000000
S	-4.41100000	-18.85800000	11.33800000
S	-7.31100000	-18.84000000	8.68400000
Sn	-3.26600000	-20.26500000	8.62700000
Sn	-5.01900000	-16.20300000	8.77000000
Sn	-3.25500000	-20.44700000	13.94200000
Sn	-5.00700000	-16.38500000	14.08500000
Sn	-8.46700000	-17.25100000	6.08000000
Sn	-11.21100000	-19.70600000	8.66300000
Sn	-11.03700000	-13.84200000	11.52500000
Sn	-8.45600000	-17.43300000	11.39600000
Sn	-6.70400000	-21.49500000	11.25300000
Sn	-11.20000000	-19.88800000	13.97800000
Sn	-8.44500000	-17.61600000	16.71200000

Third co-ordination shell cluster of BaSnF₄

F	-9.64100000	17.46500000	12.25800000
F	-18.33000000	17.46800000	12.35100000

F	-9.55100000	16.33100000	20.87400000
F	-18.24000000	16.33600000	20.96600000
F	-11.81700000	15.42800000	12.01400000
F	-9.62200000	15.14500000	14.14500000
F	-16.16200000	15.43000000	12.06000000
F	-18.31100000	15.14800000	14.23600000
F	-9.57700000	14.57800000	18.45300000
F	-18.26600000	14.58100000	18.54400000
F	-11.72700000	14.29600000	20.62900000
F	-16.07200000	14.29700000	20.67500000
F	-7.42100000	18.28900000	16.72700000
F	-20.45500000	18.29400000	16.86400000
F	-14.00600000	19.14100000	10.33300000
F	-13.87100000	17.44100000	23.25700000
Ba	-11.74700000	16.05700000	18.67000000
Ba	-16.09200000	16.05800000	18.71500000
Ba	-11.79200000	16.62400000	14.36200000
Ba	-16.13700000	16.62600000	14.40800000
F	-18.30500000	18.57600000	14.68700000
F	-9.57100000	18.00700000	18.90400000
F	-16.15600000	18.85900000	12.51000000
F	-11.81100000	18.85700000	12.46400000
F	-9.61600000	18.57300000	14.59500000
F	-18.26000000	18.01000000	18.99500000
F	-11.72100000	17.72500000	21.08000000
F	-16.06600000	17.72600000	21.12600000
F	-13.96700000	15.14600000	14.19100000
F	-11.77200000	14.86200000	16.32200000
F	-16.11600000	14.86400000	16.36700000
F	-13.92200000	14.58000000	18.49800000
F	-13.98600000	17.46600000	12.30500000
F	-9.59600000	16.89900000	16.56700000
F	-18.28600000	16.90200000	16.65800000
F	-13.89600000	16.33400000	20.92000000
F	-11.76600000	18.29100000	16.77300000
F	-16.11000000	18.29200000	16.81800000
F	-13.91600000	18.00900000	18.94900000
F	-13.96100000	18.57500000	14.64200000
F	-13.94100000	16.90000000	16.61200000
Sn	-13.93700000	18.98300000	16.88600000
Sn	-18.28200000	18.98500000	16.93200000
Sn	-13.89200000	18.41600000	21.19400000
Sn	-13.98200000	19.54900000	12.57800000
Sn	-9.59200000	18.98200000	16.84100000

Third co-ordination shell cluster of SnO₂

O	12.71300000	-15.70700000	0.81500000
O	13.54600000	-14.69600000	-3.08500000
O	12.50000000	-19.76300000	3.25100000
O	14.68800000	-17.10800000	-6.99900000
O	13.64200000	-22.17400000	-0.66300000
O	14.47400000	-21.16400000	-4.56200000
O	15.80100000	-15.43000000	1.54500000
O	16.63300000	-14.42000000	-2.35400000
O	15.58800000	-19.48600000	3.98200000
O	17.77500000	-16.83100000	-6.26800000
O	16.72900000	-21.89800000	0.06800000
O	17.56200000	-20.88800000	-3.83100000
O	10.24500000	-19.03000000	-1.37900000
O	10.76800000	-18.39400000	-3.83100000
O	11.40600000	-14.09100000	-1.21600000
O	11.19300000	-18.14800000	1.22100000
O	11.55100000	-20.64500000	0.65100000
O	18.86900000	-22.50300000	-1.80100000
O	12.54900000	-16.50300000	-5.12900000
O	12.90700000	-19.00000000	-5.70000000
O	12.69400000	-23.05600000	-3.26300000
O	20.03000000	-17.56400000	-1.63800000
O	19.08300000	-18.44600000	-4.23900000
O	18.72400000	-15.94900000	-3.66800000
O	19.50800000	-18.20000000	0.81400000
O	17.58100000	-13.53800000	0.24600000
O	17.36800000	-17.59500000	2.68200000
O	17.72700000	-20.09100000	2.11200000
O	11.76500000	-16.58800000	-1.78600000
O	18.51100000	-20.00600000	-1.23200000
O	12.33600000	-20.55900000	-2.69300000
O	17.94100000	-16.03500000	-0.32500000
O	14.49400000	-13.81500000	-0.48500000
O	14.28100000	-17.87100000	1.95200000
O	14.63900000	-20.36900000	1.38100000
O	15.63600000	-16.22700000	-4.39900000
O	15.99500000	-18.72300000	-4.96900000
O	15.78200000	-22.77900000	-2.53300000
O	16.42000000	-18.47700000	0.08200000
O	14.85300000	-16.31200000	-1.05500000
O	13.85500000	-18.11700000	-3.10000000
O	13.33200000	-18.75300000	-0.64800000
O	15.42300000	-20.28200000	-1.96200000
O	16.94300000	-17.84100000	-2.36900000
Sn	13.12900000	-15.20200000	-1.13500000
Sn	12.91600000	-19.25900000	1.30100000

Sn	14.27100000	-17.61300000	-5.04900000
Sn	12.05000000	-18.57400000	-2.23900000
Sn	14.05800000	-21.66900000	-2.61300000
Sn	16.21700000	-14.92500000	-0.40500000
Sn	16.00400000	-18.98100000	2.03200000
Sn	17.35900000	-17.33700000	-4.31900000
Sn	15.13800000	-18.29800000	-1.50900000
Sn	17.14600000	-21.39300000	-1.88200000
Sn	18.22600000	-18.02000000	-0.77800000

Third co-ordination shell cluster of Ca_2SnO_4

O	13.38200000	8.84200000	12.38400000
O	24.85700000	12.58700000	12.85400000
O	13.33600000	8.57700000	15.64000000
O	24.81000000	12.32200000	16.10900000
O	15.21600000	6.76500000	12.24100000
O	23.02400000	14.66400000	12.99700000
O	15.16900000	6.50000000	15.49600000
O	22.97700000	14.39900000	16.25200000
O	17.23000000	14.68000000	17.83200000
O	20.96200000	6.48400000	10.66200000
O	17.32400000	15.21100000	11.32100000
O	20.86900000	5.95300000	17.17200000
O	13.89300000	11.55900000	10.97400000
O	24.39300000	10.13600000	11.00900000
O	13.80000000	11.02800000	17.48500000
O	24.30000000	9.60500000	17.51900000
Ca	17.30500000	8.20000000	12.38800000
Ca	15.38500000	10.70700000	12.56500000
Ca	20.46100000	8.00200000	12.41700000
Ca	17.77800000	13.42700000	12.82100000
Ca	20.93400000	13.22900000	12.85000000
Ca	22.85500000	10.72300000	12.67300000
Ca	17.25800000	7.93500000	15.64300000
Ca	15.33800000	10.44100000	15.82000000
Ca	20.41400000	7.73700000	15.67200000
Ca	17.73200000	13.16200000	16.07600000
Ca	20.88800000	12.96400000	16.10500000
Ca	22.80800000	10.45700000	15.92800000
O	18.45900000	6.13800000	12.23600000
O	19.78100000	15.29200000	13.00200000
O	18.41200000	5.87200000	15.49200000
O	19.73400000	15.02600000	16.25700000
O	22.82100000	8.19300000	12.46600000
O	15.41800000	13.23700000	12.77200000
O	22.77500000	7.92700000	15.72200000

O	15.37200000	12.97200000	16.02700000
O	17.79100000	11.16300000	9.35900000
O	20.54100000	10.79800000	9.36900000
O	17.65200000	10.36600000	19.12500000
O	20.40100000	10.00100000	19.13400000
O	20.91600000	6.21900000	13.91700000
O	17.27700000	14.94500000	14.57700000
O	22.30700000	11.97500000	17.68400000
O	15.88600000	9.18900000	10.81000000
O	22.40000000	12.50600000	11.17300000
O	15.79300000	8.65800000	17.32000000
O	13.84600000	11.29400000	14.23000000
O	24.34700000	9.87000000	14.26400000
O	15.83900000	8.92300000	14.06500000
O	22.35300000	12.24100000	14.42900000
O	19.22400000	12.30900000	17.66700000
O	18.87600000	8.32400000	17.33700000
O	18.96900000	8.85500000	10.82600000
O	19.31700000	12.84000000	11.15600000
O	17.69800000	10.63200000	15.87000000
O	20.49500000	10.53200000	12.62400000
O	17.74500000	10.89700000	12.61400000
O	20.44800000	10.26700000	15.87900000
O	18.92300000	8.58900000	14.08200000
O	19.27000000	12.57500000	14.41200000
Sn	19.05000000	10.31700000	17.50200000
Sn	19.14300000	10.84800000	10.99100000
Sn	19.09600000	10.58200000	14.24700000

Third co-ordination shell cluster of SnS₂

S	4.76300000	-12.59000000	2.91500000
S	8.30200000	-13.00100000	2.17400000
S	9.49900000	-18.99100000	11.20800000
S	2.24100000	-14.10700000	9.56900000
S	5.96100000	-18.58000000	11.94900000
S	12.85500000	-15.33600000	7.34500000
S	4.51700000	-15.27500000	12.15500000
S	11.59400000	-16.09400000	10.67200000
S	2.66900000	-15.48600000	3.45000000
S	9.74500000	-16.30600000	1.96800000
S	1.40800000	-16.24500000	6.77800000
S	12.02200000	-17.47400000	4.55400000
S	10.76100000	-18.23200000	7.88100000
S	8.05600000	-15.68500000	11.41400000
S	6.20700000	-15.89600000	2.70900000
S	3.68500000	-17.41300000	9.36300000

S	3.50200000	-13.34900000	6.24200000
S	10.57800000	-14.16900000	4.76000000
S	7.22300000	-17.82200000	8.62200000
S	9.31700000	-14.92600000	8.08700000
S	5.77900000	-14.51700000	8.82800000
S	7.04000000	-13.75800000	5.50100000
S	8.48400000	-17.06400000	5.29500000
S	4.94600000	-16.65400000	6.03600000
Sn	4.85500000	-14.62300000	4.47500000
Sn	8.39300000	-15.03200000	3.73500000
Sn	3.59300000	-15.38100000	7.80200000
Sn	7.13100000	-15.79000000	7.06200000
Sn	10.67000000	-16.20000000	6.32000000
Sn	5.87000000	-16.54800000	10.38800000
Sn	9.40900000	-16.95800000	9.64800000

Third co-ordination shell cluster of Pb₂SnO₄

O	30.01900000	2.78800000	-10.06600000
O	17.68200000	3.02900000	-9.09400000
O	18.33700000	6.30800000	-11.57500000
O	29.52400000	4.84800000	-6.48300000
O	23.24800000	-0.74900000	-8.79700000
O	23.95800000	8.62700000	-6.77900000
O	24.18400000	9.24900000	-9.87500000
O	24.17100000	-0.15400000	-11.76600000
O	20.42100000	5.04900000	-13.06400000
O	28.51000000	4.65600000	-11.61000000
O	21.67600000	3.26100000	-5.02600000
O	24.37900000	3.39800000	-4.48600000
O	23.42500000	5.43500000	-14.04900000
O	26.08100000	4.88000000	-13.65700000
O	19.27100000	3.83100000	-6.99900000
O	27.36000000	3.43700000	-5.54500000
O	19.84600000	4.44100000	-10.03200000
O	24.48500000	2.84000000	-12.73700000
O	27.93500000	4.04600000	-8.57700000
O	24.44700000	6.86500000	-11.93500000
O	23.33500000	1.62100000	-6.67300000
O	23.29700000	5.64600000	-5.87200000
O	23.90900000	2.23100000	-9.70500000
O	23.87200000	6.25600000	-8.90400000
O	22.27500000	4.21500000	-7.98400000
O	24.93100000	3.66100000	-7.59200000
O	25.52900000	4.61500000	-10.55000000
O	22.82600000	4.48000000	-11.09000000
Pb	24.71200000	0.95100000	-8.17800000

Pb	20.41600000	2.95300000	-8.59000000
Pb	22.49400000	6.92600000	-7.39800000
Pb	26.78900000	4.92400000	-6.98600000
Pb	22.88300000	1.73100000	-11.63200000
Pb	27.27600000	3.13900000	-10.51700000
Pb	25.47300000	7.36500000	-10.00900000
Pb	21.08000000	5.95700000	-11.12500000
Sn	24.46600000	4.85200000	-12.33600000
Sn	23.31600000	3.63400000	-6.27200000
Sn	23.89000000	4.24300000	-9.30400000

Third co-ordination shell cluster of Na₆Sn₂S₇

S	-25.19200000	31.08100000	-0.15400000
S	-22.12000000	25.70600000	-4.65800000
S	-18.57700000	36.66800000	3.73500000
S	-24.67500000	28.26700000	-3.32300000
S	-19.95300000	34.21100000	-2.81200000
S	-16.88100000	28.83600000	-7.31600000
S	-21.76900000	24.66500000	6.67700000
S	-16.08200000	22.62400000	1.41300000
S	-26.04200000	27.29000000	1.72400000
S	-14.26500000	25.54200000	0.49400000
S	-10.85800000	28.29700000	3.60300000
S	-16.02200000	34.10700000	2.40100000
S	-25.25000000	26.71000000	5.59200000
S	-17.87700000	35.99100000	0.00400000
S	-16.34100000	23.76300000	-2.32200000
S	-18.18700000	27.12600000	6.87600000
S	-21.98400000	33.91400000	0.62700000
S	-15.50500000	31.29300000	-0.76900000
S	-17.39800000	31.65000000	-4.14600000
S	-12.60400000	28.61600000	-0.18200000
S	-18.19600000	25.64700000	-4.71800000
S	-20.23800000	33.59500000	4.41200000
S	-18.77100000	24.09000000	4.19700000
S	-20.45900000	28.78000000	-5.33400000
S	-15.13500000	28.51700000	-3.53000000
S	-13.75900000	30.97400000	3.01600000
S	-23.29900000	30.72400000	3.22400000
S	-21.44400000	28.84000000	5.62000000
S	-14.96500000	26.21900000	4.22500000
S	-21.61400000	31.13800000	-2.13500000
S	-17.33700000	30.91700000	4.99800000
S	-22.82000000	26.38300000	-0.92700000
S	-22.56100000	25.24400000	2.80900000
S	-19.56300000	24.66900000	0.32900000

Na	-17.79700000	28.64800000	-4.43200000
Na	-16.42100000	31.10500000	2.11500000
Na	-16.94300000	28.20700000	4.66300000
Na	-18.31900000	25.75100000	-1.88400000
Na	-20.06100000	30.74900000	3.94700000
Na	-21.43700000	28.29200000	-2.60000000
Na	-19.25900000	34.08200000	1.67800000
Na	-13.58200000	28.12900000	2.55200000
Na	-17.25600000	25.25300000	2.03000000
Na	-23.73500000	27.87300000	3.42500000
Na	-18.77200000	31.43200000	-1.65200000
Na	-21.92500000	30.94200000	0.73000000
Na	-15.44600000	28.32100000	-0.66500000
Na	-20.53400000	26.34900000	4.55900000
S	-20.74400000	28.16300000	1.88900000
S	-16.82000000	28.10400000	1.82900000
S	-18.71300000	28.46100000	-1.54900000
S	-19.08300000	31.23600000	1.21300000
Sn	-18.74400000	28.93900000	0.74700000
Sn	-21.38100000	26.03100000	0.91100000

Third co-ordination shell cluster of Sr_2SnO_4

O	11.86900000	-15.77300000	-12.51900000
O	14.61200000	-3.62800000	-12.12800000
O	10.93700000	-9.95700000	-18.08700000
O	15.54400000	-9.44400000	-6.56000000
O	6.69600000	-9.05500000	-10.55700000
O	19.78500000	-10.34600000	-14.09000000
O	19.75500000	-10.42600000	-11.22200000
O	6.72600000	-8.97500000	-13.42500000
O	19.21600000	-7.52600000	-14.00300000
O	7.26500000	-11.87500000	-10.64400000
O	11.49400000	-10.19800000	-6.64600000
O	14.98700000	-9.20300000	-18.00100000
O	10.56100000	-4.38200000	-12.21400000
O	15.92000000	-15.01900000	-12.43300000
O	7.29600000	-11.79500000	-13.51200000
O	19.18600000	-7.60600000	-11.13500000
O	9.38100000	-13.18300000	-12.07500000
O	17.61300000	-9.41900000	-9.52800000
O	17.10000000	-6.21800000	-12.57200000
O	8.86900000	-9.98200000	-15.11800000
O	13.16500000	-5.49500000	-7.92800000
O	13.31600000	-13.90600000	-16.71800000
O	13.90400000	-14.06700000	-8.14500000
O	12.57700000	-5.33400000	-16.50100000

O	9.14700000	-10.10300000	-9.39800000
O	17.33400000	-9.29800000	-15.24900000
O	8.72700000	-7.48800000	-11.92300000
O	17.75400000	-11.91400000	-12.72400000
O	11.00800000	-7.00800000	-9.15600000
O	15.47300000	-12.39300000	-15.49100000
O	10.72900000	-6.88800000	-14.87600000
O	15.75200000	-12.51300000	-9.77000000
O	11.66200000	-12.70400000	-9.30800000
O	14.81900000	-6.69700000	-15.33900000
O	11.38300000	-12.58400000	-15.02900000
O	15.09800000	-6.81800000	-9.61800000
O	13.59500000	-14.02700000	-10.99800000
O	12.66200000	-8.21000000	-16.56600000
O	13.81900000	-11.19100000	-8.08000000
O	12.88600000	-5.37500000	-13.64900000
O	13.23100000	-11.03000000	-16.65400000
O	13.25000000	-8.37100000	-7.99300000
O	12.85600000	-5.45500000	-10.78100000
O	13.62500000	-13.94600000	-13.86600000
O	15.26600000	-9.32400000	-12.28000000
O	11.21500000	-10.07700000	-12.36600000
O	12.94100000	-8.33100000	-10.84600000
O	13.54000000	-11.07000000	-13.80100000
O	12.97100000	-8.25100000	-13.71400000
O	13.51000000	-11.15000000	-10.93300000
Sn	13.05300000	-6.91300000	-9.38700000
Sn	13.70700000	-12.60900000	-9.53900000
Sn	12.77400000	-6.79200000	-15.10800000
Sn	13.24100000	-9.70100000	-12.32300000
Sn	13.42800000	-12.48800000	-15.26000000
Sr	8.82900000	-10.16600000	-12.09400000
Sr	11.54900000	-10.02100000	-9.35500000
Sr	11.07000000	-7.01900000	-12.18600000
Sr	11.27100000	-9.90100000	-15.07500000
Sr	11.72400000	-12.71400000	-12.33800000
Sr	15.21000000	-9.50000000	-9.57100000
Sr	14.75700000	-6.68700000	-12.30900000
Sr	15.41100000	-12.38200000	-12.46100000
Sr	14.93200000	-9.38000000	-15.29200000
Sr	17.65300000	-9.23500000	-12.55300000