Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Electronic Supplemental Information

A Computational Survey of Semiconductors for Power Electronics

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Table S1: Candidate *n*-type Materials for Power Electronics

Computed lattice thermal conductivity (κ_L) and Baliga **FOM** of *n*-type candidate materials. SG denotes the space group number. The calculated energy above the convex hull (ΔE_{hull}) is extracted from the NREL Materials Database (materials.nrel.gov) and the Materials Project database (materialsproject.org). Materials that lie on the convex hull (ΔE_{hull} = 0) are stable against decomposition into competing phases. The Baliga FOM values are normalized by the Baliga FOM of *n*-type Si, the most widely used power electronic material.

Material	SG no.	κ_L (W/mK)	FOM (*n*)	FOM (*p*)	ΔE_{hull} (meV)
Al_2O_3	167	35.1	1.7×10^7	9.3×10^4	0
MgO	225	41.2	2.4×10^6	1.9×10^4	0
$HfGeO_4$	88	20.8	1.3×10^6	3.1×10^3	0
Al_2MgO_4	227	23.0	1.1×10^6	3.2×10^3	0
$Y_2Si_2O_7$	12	35.0	7.6×10^5	5.2×10^3	0
$MgSiN_2$	33	40.0	3.5×10^5	7.5×10^3	0
Al_4CaO_7	15	21.3	3.3×10^5	2.1×10^3	0
$NaSi_2N_3$	36	57.3	3.1×10^5	3.4×10^3	0
$ZnSiO_3$	148	46.8	2.6×10^5	7.4×10^2	50
Si_3N_4	159	60.2	7.2×10^4	7.5×10^3	0
Si_3N_4	176	132.6	6.5×10^4	1.6×10^4	0
$In_2Si_2O_7$	12	40.0	4.5×10^4	8.2×10^1	10
$Ca_2Si_5N_8$	9	24.4	3.1×10^4	1.4×10^3	0
SnC	216	64.1	2.9×10^4	1.6×10^2	816
Be_2C	225	87.7	2.5×10^4	7.4×10^3	0
CaO	225	26.0	2.3×10^4	3.0×10^3	0
Al_4C_3	166	42.7	2.1×10^4	3.5×10^2	0
$ScAl_3C_3$	186	20.0	1.6×10^4	7.4×10^3	0
$ScAl_3C3$	194	20.0	1.6×10^4	7.4×10^3	0
$CaZrSi_2O_7$	5	55.8	1.6×10^4	6.4×10^3	0
$HfSiO_4$	141	28.7	1.4×10^4	1.9×10^4	0
Ba_2ZrO_4	139	35.8	1.3×10^4	2.4×10^3	0
Ge_3N_4	159	20.6	1.2×10^4	4.6×10^1	0
GeC	216	134.5	1.1×10^4	1.5×10^3	436
$ZnGeN_2$	33	25.2	1.0×10^4	7.0×10^1	0
$ZrGeO_4$	88	33.2	8.6×10^3	1.0×10^3	0
Al_2MgC_2	164	22.4	8.4×10^3	9.0×10^2	7
B_4C	166	27.8	8.0×10^3	8.1×10^3	38
$Sc_2Si_2O_7$	12	60.4	7.9×10^3	1.3×10^3	0
BeB_2C_2	59	27.4	6.8×10^3	2.4×10^2	7
ZnS	216	38.0	6.1×10^3	7.6×10^1	0
$ZrSiO_4$	141	38.4	5.1×10^3	6.4×10^3	0
RuC	216	155.9	4.3×10^3	5.5×10^2	456

Table S2: Candidate *p*-type Materials for Power Electronics

Computed lattice thermal conductivity (κ_L) and Baliga **FOM** of *p*-type candidate materials. SG denotes the space group number. The calculated energy above the convex hull ($\mathbf{\Delta E_{hull}}$) is extracted from the NREL Materials Database (materials.nrel.gov) and the Materials Project database (materialsproject.org). Materials that lie on the convex hull ($\mathbf{\Delta E_{hull}} = 0$) are stable against decomposition into competing phases. The Baliga FOM values are normalized by the Baliga FOM of *n*-type Si, the most widely used power electronic material.

Material	**SG**	κ_L (W/mK)	**FOM (*n*)**	**FOM (*p*)**	$\mathbf{\Delta E_{hull}}$ **(meV)**
Al_2O_3	167	35.1	1.7×10^7	9.3×10^4	0
Sc_4C_3	220	25.1	8.2×10^2	2.0×10^4	0
MgO	225	41.2	2.4×10^6	1.9×10^4	0
$HfSiO_4$	141	28.7	1.4×10^4	1.9×10^4	0
Si_3N_4	176	132.6	6.5×10^4	1.6×10^4	0

Table S3: Comparison of Electronic Structure Properties Calculated with DFT-PBE Functional and GW Method

Electronic structure properties of 7 *n*-type candidate materials from Table S1 calculated with DFT-PBE functional and many-body GW method. SG denotes the space group number. E_g is the band gap in eV, m^*_{DOS} (CB) is the conduction band density-of-states effective mass in units of electron mass, and N_b (CB) is the conduction band degeneracy. Both m^*_{DOS} (CB) and N_b (CB) are calculated within an energy window of 100 meV from CB minimum. Compared to PBE values, GW-calculated E_g are significantly larger, and m^*_{DOS} (CB) are smaller.

Material	**SG**	**PBE**			**GW**		
		E_g	m^*_{DOS} **(CB)**	N_b **(CB)**	E_g	m^*_{DOS} **(CB)**	N_b **(CB)**
$HfGeO_4$	88	3.99	0.116	1	6.62	0.067	1
$Y_2Si_2O_7$	12	4.66	0.170	1	7.55	0.077	1
$MgSiN_2$	33	4.03	0.077	1	6.13	0.044	1
Al_4CaO_7	15	4.02	0.136	1	7.28	0.058	1
$ZnSiO_3$	148	3.61	0.083	1	6.46	0.048	1
$In_2Si_2O_7$	12	2.74	0.090	1	5.47	0.049	1
$HfSiO_4$	141	5.69	7.393	3	8.34	4.053	4

Table S4: Dependence of Calculated Effective Masses and Band Degeneracies on Energy Window

Calculated electronic structure properties using different energy windows (100 meV, 150 meV, 200 meV) from the relevant band edges. E_g is the band gap in eV, m^*_{DOS} is the density-of-states effective mass, N_b is the band degeneracy, and m^*_b is the band effective mass. Effective masses are reported in units of electron mass.

Energy window: **100 meV**

Material	E_g	m^*_{DOS} (VB)	m^*_{DOS} (CB)	N_b (VB)	N_b (CB)	m^*_b (VB)	m^*_b (CB)
Si	0.62	0.65	0.64	3	6	0.31	0.19
SiC	2.23	1.71	0.25	3	3	0.82	0.12
GaN	1.76	2.08	0.03	3	1	1.00	0.03
Ga_2O_3	2.01	10.86	0.04	2	1	6.84	0.04
d-C	4.13	0.30	0.49	3	6	0.15	0.15
AlN	4.08	1.27	0.06	1	1	1.27	0.06

Energy window: **150 meV**

Material	E_g	m^*_{DOS} (VB)	m^*_{DOS} (CB)	N_b (VB)	N_b (CB)	m^*_b (VB)	m^*_b (CB)
Si	0.62	0.83	0.84	3	9	0.40	0.20
SiC	2.23	1.84	0.38	3	6	0.88	0.11
GaN	1.76	2.33	0.05	3	1	1.12	0.05
Ga_2O_3	2.01	10.53	0.06	2	1	6.63	0.06
d-C	4.13	0.45	0.69	3	6	0.22	0.21
AlN	4.08	1.56	0.09	1	1	1.56	0.09

Energy window: **200 meV**

Material	E_g	m^*_{DOS} (VB)	m^*_{DOS} (CB)	N_b (VB)	N_b (CB)	m^*_b (VB)	m^*_b (CB)
Si	0.62	0.92	0.98	3	9	0.44	0.23
SiC	2.23	1.98	0.52	3	6	0.95	0.16
GaN	1.76	2.44	0.06	3	1	1.17	0.06
Ga_2O_3	2.01	9.08	0.08	2	1	5.72	0.08
d-C	4.13	0.66	0.87	3	6	0.32	0.26
AlN	4.08	1.81	0.12	1	1	1.81	0.12

Figure S1: Native Defect Energetics of $HfGeO_4$

Defect formation energy ($\Delta H_{D,q}$) as a function of the Fermi energy (E_F) for $HfGeO_4$ grown under the most Hf- and Ge-rich and O-poor conditions allowed by the phase stability of $HfGeO_4$. E_F is referenced to the valence band edge. The equilibrium Fermi energy is pinned around the mid-gap, which suggests that $HfGeO_4$ is an insulator.

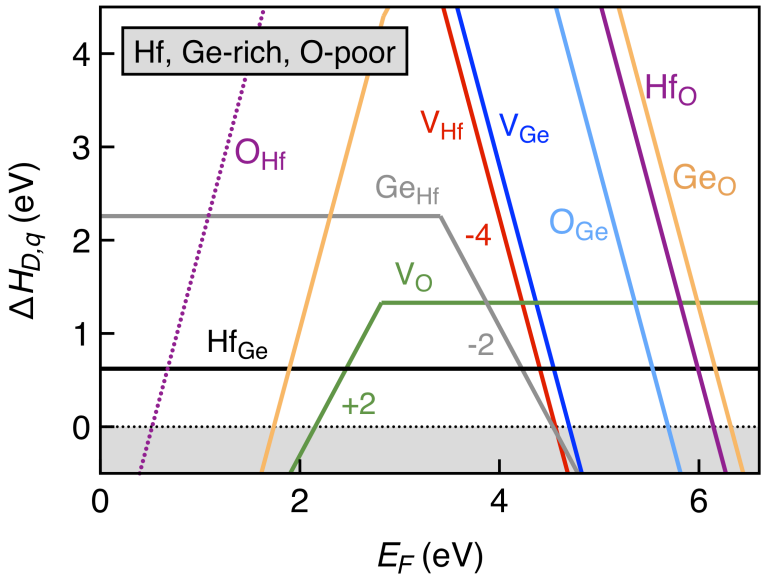


Figure S2: Native Defect Energetics of $MgSiN_2$

Defect formation energy ($\Delta H_{D,q}$) as a function of the Fermi energy (E_F) for $MgSiN_2$ grown under the most Mg-rich and N-poor conditions allowed by the phase stability of $MgSiN_2$. E_F is referenced to the valence band edge. The equilibrium Fermi energy is pinned around the mid-gap, which suggests that $MgSiN_2$ is an insulator.

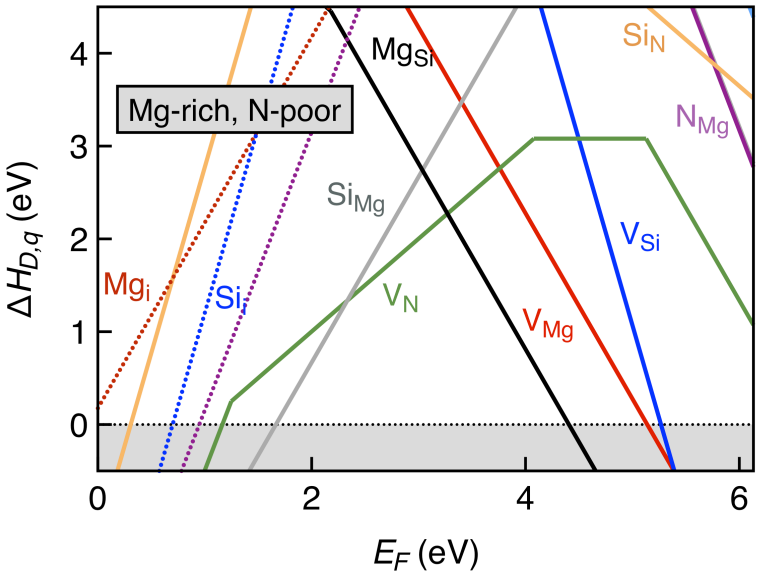
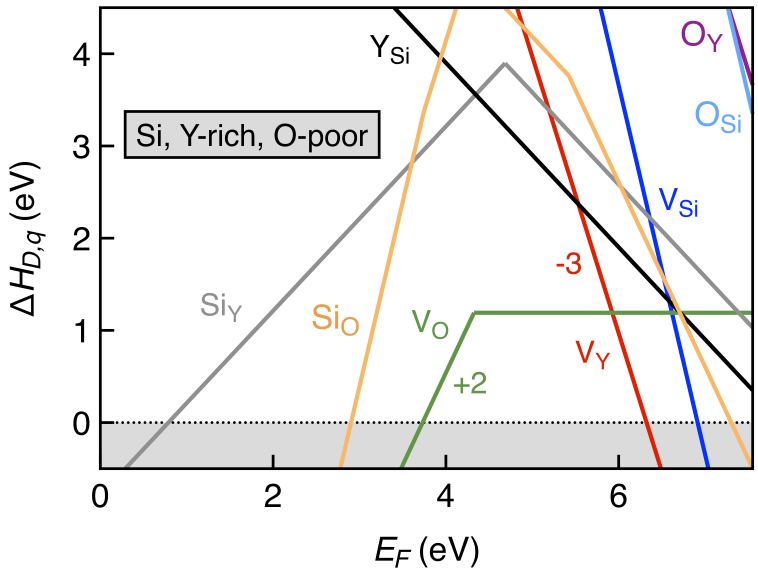


Figure S3: Native Defect Energetics of $Y_2Si_2O_7$

Defect formation energy ($\Delta H_{D,q}$) as a function of the Fermi energy (E_F) for $Y_2Si_2O_7$ grown under the most Y-rich and Si-rich, and O-poor conditions allowed by the phase stability of $Y_2Si_2O_7$. E_F is referenced to the valence band edge.



Methods: Defect Calculations

The native defect formation energies are calculated using density functional theory (DFT) and the standard supercell approach. Within the supercell approach[1], the formation energy ($\Delta H_{D,q}$) of a point defect D in charge state q is calculated as:

$$\Delta H_{D,q} = \left(E_{D,q} - E_H\right) + \sum_i n_i \mu_i + qE_F + E_{corr}$$

where E_H and $E_{D,q}$ are the total energies of the defect-free, host supercell with no net charge and the supercell with defect D in charge state q, respectively. The chemical potential of element i is represented by μ_i and n_i is the number of atoms of element i added (n_i <0) or removed (n_i >0) from the supercell. E_F is the Fermi energy and the term qE_F is the characteristic energy of exchanging charge between the defect and the reservoir of charge (Fermi sea). The supercell approach to calculating defect formation energies suffers from artefacts arising due to finite size effects. Additional artefacts are introduced due to the limitations of DFT, notably, the underestimation of the band gap with standard DFT functionals such as GGA-PBE. Various corrections schemes are applied to correct for the finite size and inaccurate electronic structure artefacts; these corrections are represented by the term E_{corr} and described in more detail in Ref. 1.

We calculate the total energies of the supercells using the generalized gradient approximation of Perdew-Burke-Ernzerhof (PBE)[2] within the projector augmented wave (PAW) formalism as implemented in the VASP software.[3] Supercells containing 96, 128, and 88 atoms is used to calculate the defect energetics of $HfGeO_4$, $MgSiN_2$, and $Y_2Si_2O_7$, respectively. The total energies are calculated with a plane-wave energy cutoff of 340 eV and Γ-centered 4×4×4 Monkhorst pack k-point grid to sample the Brillouin zone. The defect supercells are relaxed by allowing ionic relaxations, while keep the volume constant.

The elemental chemical potentials are expressed relative to those of the elements in the reference elemental phases as: $\mu_i = \mu_i^o + \Delta\mu_i$, where μ_i^o is the reference elemental chemical potential under standard conditions and $\Delta\mu_i$ is the deviation from the reference. The values of reference elemental chemical potentials are obtained from the FERE approach.[4]

The underestimation of the band gap in DFT is corrected by applying individual valence and conduction band edge shifts (relative to the DFT-computed band edges) as determined from GW quasi-particle energy calculations (see Ref. 1 for more details). The finite size corrections that are included in the term E_{corr}, following the methodology in Ref. 1, are: (1) image charge correction for charged defects, (2) potential alignment correction for charge defects, (3) band filling correction for shallow defects, and (4) correction of band edges for shallow acceptors/donors. The calculations are organized, and the results are analysed using our software package for automation of defect calculations, pyladadefects.[5]

References:

[1] S. Lany and A. Zunger, *Phys. Rev. B.*, 2008, **78**, 235105.
[2] J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865.
[3] G. Kresse and J. Furthmuller, *Phys. Rev. B*, 1996, **54**, 11169.
[4] V. Stevanovic, S. Lany, X. Zhang, and A. Zunger, *Phys. Rev. B*, 2012, **85**, 115104.
[5] A. Goyal, P. Gorai, H. Peng, S. Lany, and V. Stevanovic, *Comp. Mat. Sci.*, 2016, **130**, 1.

Table S5: Calculated Properties of 863 Materials from the Inorganic Crystal Structure Database

Computed lattice thermal conductivity (κ_L) in W/mK, band gap (E_g) in eV, hole (μ_h) and electron (μ_e) mobilities in cm^2/Vs, dielectric constant (ε), cutoff frequency (ω_{max}) in meV, critical breakdown field (E_b) in V/cm, and Baliga figure of merits FOM of assumed *p*- and *n*-type materials. ICSD denotes the Inorganic Crystal Structure Database identification number and SG denotes the space group number. The Baliga FOM values are normalized by the Baliga FOM of *n*-type Si, the most widely used power electronic material.

Compound	ICSD	SG	κ_L	E_g	μ_h	μ_e	ε	ω_{max}	E_b	FOM (*p*)	FOM (*n*)
C1	52054	227	1106.1	4.135	945.15	898.07	5.9	160.1	1.31E+07	9.26E+06	8.82E+06
B1N1	614864	216	830.7	4.47	109.02	1038.61	6.9	127.5	9.86E+06	5.86E+04	5.58E+05
C1	27422	194	543.5	3.36	713.35	2186.41	5.8	160.7	8.94E+06	5.79E+04	1.77E+05
C1Si1	181128	216	388.5	1.379	27.54	969.48	10.5	96.2	1.46E+06	6.54E+02	2.30E+04
C1Si1	28389	216	388.4	1.379	27.21	992.63	10.5	96.2	1.46E+06	6.46E+02	2.35E+04
C1	66466	194	267	4.558	651.55	155.29	5.9	161.4	1.63E+07	1.22E+07	2.90E+06
C1Si1	24261	186	191.8	2.37	28.32	188.63	10.6	101.1	2.69E+06	5.21E+02	3.47E+03
C1Ru1	188286	216	155.9	0.888	21.82	171.82	55.3	73.2	8.52E+05	5.49E+02	4.32E+03
Al1N1	42001	186	153	4.08	16.56	1521.23	8.7	87.8	4.58E+06	2.15E+04	1.98E+06
C1Ge1	182363	216	134.5	1.652	57.2	443.63	11.4	79.9	1.45E+06	1.46E+03	1.13E+04
N4Si3	74740	176	132.6	4.25	33.95	139.3	8.1	127.6	9.00E+06	1.58E+04	6.50E+04
N4Si3	98634	176	132.6	4.25	33.95	139.52	8.1	127.6	9.01E+06	1.58E+04	6.51E+04
Si1	60388	227	130	0.62	60.52	124.69	14.1	62.3	6.40E+05	4.87E-01	1.00E+00
C1Zr1	183162	216	129.3	0.336	25	66.21	25.3	64.1	5.02E+05	5.88E+01	1.56E+02
Be1S1	44724	216	109.7	3.148	2.14	34.6	7.4	69	2.40E+06	1.49E+02	2.42E+03
C1Be2	41567	225	87.7	1.166	414.09	1408.13	15.6	86.4	1.16E+06	7.35E+03	2.50E+04
B1Sb1	184571	216	71.5	0.749	211.99	131.4	12.8	72.7	7.66E+05	8.97E+02	5.58E+02
O2Ti1	93098	141	68.2	2.38	40.85	50.25	31.9	77.1	1.99E+06	2.32E+03	2.86E+03
O2Ti1	202243	141	68.2	2.38	40.8	50.29	31.9	77.1	1.99E+06	2.32E+03	2.86E+03
C1Hf1	185992	216	66	0.508	21.38	3.8	20.1	66.5	6.01E+05	6.87E+01	1.22E+01
N1Sc1	26948	225	64.1	0.47	183.31	496.87	51.2	37.8	4.70E+05	1.01E+00	2.75E+00
C1Sn1	182365	216	64.1	0.655	33.9	6173.68	20.6	66.6	6.80E+05	1.61E+02	2.94E+04
O7Sc2Si2	75925	12	60.4	4.7	1.16	7.16	10.6	139.4	1.29E+07	1.29E+03	7.94E+03

Ge1O8Zr3	29263	121	60.2	4.13	6.14	3.48	22	86	4.53E+06	6.51E+03	3.69E+03
N4Si3	92156	159	60.2	4.66	9.28	89.16	8.1	124.1	1.01E+07	7.50E+03	7.18E+04
Ga1N1	153890	186	59.8	1.76	20.54	3913.81	11	81.3	1.56E+06	6.09E+01	1.16E+04
O4Si1Ti1	166437	141	57.6	2.78	9.82	1.41	21.9	122.4	4.26E+06	9.71E+02	1.40E+02
N3Na1Si2	72466	36	57.3	4.19	7.64	687.92	8.5	134.7	9.69E+06	3.43E+03	3.09E+05
Al1Cu1O2	32633	166	56.1	2.2	3.51	128.19	8.7	89.6	2.15E+06	3.39E+01	1.24E+03
Ca1O7Si2Zr1	203131	5	55.8	4.88	1.03	2.55	10.8	126.3	1.14E+07	6.40E+03	1.58E+04
O7Sc2Si2	16214	12	54.4	4.69	1.13	7.15	10.6	139.4	1.28E+07	1.24E+03	7.79E+03
C1Si1	24630	186	48.3	1.784	28.36	428.72	10.5	115.3	2.25E+06	2.51E+03	3.79E+04
O3Si1Zn1	167186	148	46.8	3.61	2.51	870.52	13.6	93	4.17E+06	7.35E+02	2.55E+05
Ge1O2	158598	58	46.4	1.2	19.88	3140.25	14.9	97.7	1.31E+06	4.48E+00	7.07E+02
Ge1O2	158590	136	46.3	1.2	20.23	3158.76	14.9	97.6	1.31E+06	4.56E+00	7.12E+02
C3Al4	14397	166	42.7	1.328	6.66	402.37	20.4	105	1.52E+06	3.53E+02	2.13E+04
N4Si3	16752	159	41.6	2.43	6.74	16.37	16.5	238.3	1.02E+07	2.25E+02	5.46E+02
Mg1O1	157528	225	41.2	4.54	5.45	668.21	10.6	46.2	2.30E+06	1.93E+04	2.37E+06
In2O7Si2	409452	12	40	2.74	1.2	659.92	9.2	138.4	4.99E+06	8.24E+01	4.54E+04
Mg1N2Si1	642668	33	40	4.03	20.59	965.37	8.8	115.7	6.93E+06	7.50E+03	3.52E+05
O4Si1Zr1	69644	141	38.4	4.86	4.3	3.42	11.7	120.1	1.03E+07	6.44E+03	5.12E+03
S1Zn1	41985	216	38	2.02	10.6	850.77	9.5	32.2	8.53E+05	7.65E+01	6.13E+03
Zn1O1	76641	186	37.2	0.73	9.88	2761.21	12.4	63.2	7.00E+05	4.41E-02	1.24E+01
Ba2O4Zr1	39707	139	35.8	3.4	4.53	24.7	35.3	66.4	2.50E+06	2.41E+03	1.32E+04
Sn1O2	56674	136	35.3	0.66	12.97	4093.29	12.7	87.9	7.95E+05	2.77E-02	8.75E+00
Al2O3	151589	167	35.1	5.87	3.8	698.63	10.6	89.4	8.49E+06	9.26E+04	1.71E+07
O7Si2Y2	281313	12	35	4.66	1.53	223.47	8.3	129.9	1.10E+07	5.18E+03	7.57E+05
Ge1O4Zr1	29262	88	33.2	3.93	1.68	13.9	17.2	91	4.57E+06	1.04E+03	8.60E+03
N1Y1	644875	225	31	0.62	62.53	435.26	48.4	30.1	4.77E+05	1.72E+00	1.20E+01
Al2O5Ti1	27681	63	29.8	3.25	25.85	15.48	14.8	106.9	4.39E+06	4.38E+03	2.63E+03
O1Cu2	173983	224	29.6	0.72	4.6	41.29	8.1	72.6	7.49E+05	1.21E-02	1.08E-01
Hf1O4Si1	59111	141	28.7	5.69	5.04	3.69	11.2	121.9	1.45E+07	1.86E+04	1.36E+04

C1B4	29093	166	27.8	1.5	19.45	19.3	9.2	214.6	3.94E+06	8.09E+03	8.01E+03
Na2O19Ti9	62766	12	27.5	2.46	6.07	4.52	47.7	117.4	3.40E+06	6.29E+02	4.69E+02
Hg1O3Ti1	19005	161	27.4	1.37	4.77	334.85	157.4	88.6	1.35E+06	3.07E+01	2.15E+03
C2B2Be1	418618	59	27.4	0.283	83.61	2362.54	12.4	154.7	6.80E+05	2.39E+02	6.76E+03
C3B12	612562	166	26.3	1.5	19.42	19.32	9.2	214.6	3.94E+06	8.09E+03	8.01E+03
Ca1O1	60704	225	26	3.64	8.07	61.31	16.5	31.9	1.30E+06	3.01E+03	2.29E+04
N2Si1Zn1	656276	33	25.5	3.22	7.66	1330.77	10.1	113.1	4.70E+06	8.46E+02	1.47E+05
Ge1N2Zn1	155462	33	25.2	1.7	28.81	4203.72	11.7	91.5	1.69E+06	7.01E+01	1.02E+04
C3Sc4	42760	220	25.1	0.692	541.13	21.74	131.3	71.9	7.29E+05	2.02E+04	8.16E+02
Ca2N8Si5	79070	9	24.4	3.35	8.78	195.54	11.7	132.2	6.37E+06	1.41E+03	3.15E+04
O3Ti2	647544	167	24	0.44	23.11	9.73	29.5	67.1	5.67E+05	4.97E-02	2.10E-02
Ge2N4Si1	183103	227	23	1.68	36.46	1028.15	16.2	103.1	1.88E+06	1.12E+02	3.15E+03
Al2Mg1O4	56116	227	23	5.17	2.09	691.89	8.4	91.1	7.05E+06	3.24E+03	1.07E+06
C2Al2Mg1	85739	164	22.4	1.755	15.16	141.88	22.9	79.3	1.52E+06	8.97E+02	8.38E+03
Al4Ca1O7	16191	15	21.3	4.02	1.72	268.96	9.2	112.9	6.62E+06	2.11E+03	3.30E+05
Ge1Hf1O4	202080	88	20.8	3.99	1.5	622.92	16.5	91.8	4.74E+06	3.13E+03	1.29E+06
Ge3N4	637158	159	20.6	2.01	7.11	1779.94	10	105.3	2.33E+06	4.63E+01	1.15E+04
Ga2O3	166198	12	20.5	2.01	1.06	2292.91	12.1	87.6	1.91E+06	8.31E+00	1.79E+04
Si1C1Ga1N1	183047	31	20	0.57	75.58	209.16	13.6	117	8.66E+05	3.53E-01	9.78E-01
C3Al3Sc1	660402	194	20	0.304	115.51	255.9	467.6	97.4	5.68E+05	7.27E+03	1.61E+04
C3Al3Sc1	43477	186	20	0.304	116.08	254.69	472.9	97.4	5.68E+05	7.43E+03	1.63E+04
S1Pt1	654379	131	19.8	0.91	21.31	23.53	13	55.7	7.36E+05	5.25E-01	5.79E-01
Mg1O3Ti1	169652	148	19.7	3.63	2.76	1.16	18.3	82.9	3.59E+06	1.13E+03	4.72E+02
B12	94429	166	19.3	1.451	746.22	8.2	9.8	144.9	2.31E+06	6.65E+04	7.31E+02
Mg1S1	53939	225	19.1	2.74	4.88	161.45	16.4	27.7	9.43E+05	3.31E+02	1.10E+04
Ge2N3Na1	47100	36	17.9	2.34	6.74	1149.01	10	107.2	2.84E+06	1.08E+02	1.85E+04
Ge1Mg1N2	23502	33	17.8	2.66	18.57	1806.32	9.5	92.6	2.78E+06	1.06E+03	1.03E+05
Ca1O5Si1Ti1	9839	15	17.4	3.2	2.8	2.84	24.1	117	4.90E+06	7.07E+02	7.16E+02
Al1Au1O2	95663	194	16.9	0.88	4.28	215.06	11.2	92.8	9.91E+05	2.22E-01	1.12E+01

Ge1Mg2O4	1086	227	16.6	3.08	2.64	796.79	8.7	88.9	3.17E+06	4.16E+02	1.26E+05
B1Bi1	184569	216	16.6	0.243	125.36	7038.98	276.9	64.1	4.50E+05	2.33E+03	1.31E+05
Ca1O5Si1Ti1	89769	15	16.5	3.2	2.81	2.85	24.1	117	4.89E+06	7.10E+02	7.21E+02
O3Sr1Zr1	173398	62	16.4	4.06	1.55	97.13	27.8	92.4	4.91E+06	1.88E+03	1.18E+05
Al1O3Sc1	86931	62	16.3	4.95	10.29	6.86	20	85.8	5.95E+06	2.93E+04	1.96E+04
N8Si6Sr1	391265	44	16.1	3.22	4.72	8.16	14.2	134	6.10E+06	7.29E+02	1.26E+03
Ga1In1O3	30339	194	16.1	1.36	2.81	3148.53	13.1	77.9	1.20E+06	2.31E+00	2.59E+03
Ga4O8Ti1	155638	12	16.1	2.58	1.87	92.48	16.8	93.7	2.72E+06	9.04E+01	4.49E+03
Al2Ge2O7	201750	15	15.8	3.41	3.08	408.53	7.9	114.9	5.25E+06	9.41E+02	1.25E+05
O3Ti1Zn1	22382	148	15.3	3.16	2.16	0.82	25.8	81	2.91E+06	5.43E+02	2.06E+02
C3Al3Y1	606289	194	15.3	0.168	103.25	430.7	133.4	101.9	4.64E+05	1.01E+03	4.23E+03
N2Sr1Zr1	82537	166	15.2	0.45	73.37	408.38	75.8	70.1	5.83E+05	4.64E-01	2.58E+00
C3Mg2	71941	58	15.2	1.644	8.58	93.8	11	217.5	4.57E+06	6.62E+03	7.24E+04
Zn1Li1N1	16790	216	15.1	0.52	14.8	3969.62	35.7	56.5	5.66E+05	1.49E-02	3.99E+00
Al1Na1O6Si2	162531	15	15	5.22	2.87	402.11	7.6	129.6	1.37E+07	2.07E+04	2.90E+06
O2Zr1	80050	14	14.9	3.79	3.15	5.73	18.2	88.8	4.19E+06	1.65E+03	3.01E+03
C2B12Li2	415556	38	14.9	1.381	146.58	1064.19	8.8	184.3	2.89E+06	2.30E+04	1.67E+05
Al2Cd1O4	183382	227	14.8	2.7	5.16	981.27	9.9	92.7	2.83E+06	1.93E+02	3.67E+04
Mg1O2	35479	205	14.7	3.57	1.45	0.78	6.7	110.3	5.28E+06	1.97E+02	1.06E+02
Ge1Mg2O4	86505	227	14.7	3.08	2.65	823.29	8.7	88.9	3.17E+06	4.18E+02	1.29E+05
Ga4Ge1O8	202044	12	14.6	2.03	1.91	1441.36	11.2	94.3	2.08E+06	1.46E+01	1.11E+04
Ca1Mg2N2	79123	164	14.6	2.05	15.35	1354.77	18.3	60.5	1.37E+06	2.38E+02	2.10E+04
C1B1Li1	78731	194	14.3	1.023	62.04	74.61	14	144.5	1.61E+06	2.65E+03	3.19E+03
Mg1O2	41732	205	14.1	3.57	1.45	0.78	6.7	110.3	5.28E+06	1.97E+02	1.06E+02
Ca1O4Ti2	51183	63	13.5	0.2	7.34	7.33	25.2	78.2	4.51E+05	1.21E-04	1.21E-04
B1Li1	236959	227	13.4	1.436	1484.25	399.75	18.5	84.9	1.35E+06	4.98E+04	1.34E+04
Na2O5Si1Ti1	166623	129	13.3	3.35	1.42	1.23	9.1	116.5	5.21E+06	1.78E+02	1.54E+02
Ca1Hg1O2	80717	166	13.3	2.08	3.58	24.84	8	77.4	1.74E+06	2.29E+01	1.59E+02
Ga2Mg1O4	157769	227	13.3	3.15	1.06	1212.51	10.5	82	2.95E+06	2.38E+02	2.72E+05

Na1O6Sc1Si2	74553	15	12.9	5.11	3.09	138.38	8.7	123.3	1.19E+07	2.18E+04	9.78E+05
Ca1S1	619529	225	12.7	2.37	11.94	41.02	12.1	26.9	8.42E+05	2.51E+02	8.60E+02
Ca1Ga4O7	10351	15	12.6	2.54	1.13	321.89	10.5	92.6	2.63E+06	5.03E+01	1.43E+04
Au1O2Sc1	95669	194	12.5	2.15	6.99	45.24	14.4	81.3	1.89E+06	9.71E+01	6.30E+02
Au1Ga1O2	95666	194	12.4	0.05	36.72	570.61	11.9	82	3.34E+05	7.07E-08	1.10E-06
La1N1	162195	186	12.3	1.17	3.33	99.26	17.4	42.5	7.28E+05	1.47E+00	4.40E+01
N2Sr1Ti1	85770	129	12.1	1.29	40.91	46.91	28	97	1.38E+06	2.99E+01	3.43E+01
Cd1O3Ti1	262708	148	12	3.02	1.66	2.51	21.5	79.3	2.69E+06	2.65E+02	4.01E+02
B3Si1	412621	74	12	1.424	36.51	33.45	12.5	131.4	2.03E+06	2.81E+03	2.57E+03
Ge1O3Zn1	33722	148	12	2.09	0.87	1940.6	16.2	80.7	1.83E+06	1.15E+01	2.57E+04
Ca1O5Si1Ti1	36184	15	11.9	3.2	2.77	2.9	24.1	117	4.89E+06	7.00E+02	7.33E+02
Ga2O4Zn1	81112	227	11.9	2.33	1.17	2061.26	11.7	81.7	2.07E+06	2.15E+01	3.79E+04
Ca1O5Si1Sn1	96819	2	11.9	3.2	0.67	258.13	19.3	112.6	4.63E+06	1.36E+02	5.23E+04
C2B12Mg1	416800	15	11.9	2.501	74.77	615.42	10.2	135	4.21E+06	4.17E+04	3.43E+05
Na1O6Si2Ti1	281612	2	11.8	0.96	0.94	0.51	9.1	126.2	1.34E+06	6.68E-02	3.63E-02
C2B12Mg1	416801	74	11.8	2.153	29.29	86.01	12.4	150.9	3.99E+06	1.69E+04	4.97E+04
O1Sr1	181274	225	11.7	3.28	4.18	53.12	20.3	23.9	9.63E+05	1.03E+03	1.31E+04
Ca2N2Zn1	69049	139	11.6	0.74	9.61	7.09	16.2	80.7	8.09E+05	2.54E-01	1.88E-01
Ba1O3Ti1	161341	38	11.6	3.29	0.7	5.09	6.8	101.4	4.14E+06	5.88E+01	4.28E+02
Sc1S2Cu1	15298	156	11.5	1.5	13.11	8.46	19.9	43.4	8.53E+05	2.93E+01	1.89E+01
C2B13Li1	415557	74	11.5	2.58	28.51	36.69	14.3	205.4	8.64E+06	1.93E+05	2.49E+05
B1Li1Si2	425643	137	11.4	1.138	591.43	13.05	24.5	84.7	1.12E+06	1.49E+04	3.29E+02
Na1O6Si2Ti1	166310	15	11.3	0.95	2.82	0.52	9.1	126.2	1.33E+06	1.88E-01	3.47E-02
Mg2O4Sn1	167815	227	11.3	1.9	2.56	968.64	10	84.2	1.73E+06	1.23E+01	4.65E+03
O2Pb1	34234	136	11.2	0.01	4.65	14.46	22	72.8	2.79E+05	1.09E-12	3.38E-12
S1Cd1	67776	186	11.1	1.12	7.33	1054.04	10.4	34.8	6.42E+05	6.84E-01	9.85E+01
Ga1O3Y1	1999	185	11.1	2.73	12.46	436.44	12.6	84.5	2.57E+06	1.15E+03	4.02E+04
O7Ti2Y2	160111	227	10.9	3.06	31.69	24.91	43.6	91.2	3.25E+06	1.11E+04	8.68E+03
O7Pb1Ti3	2104	11	10.8	2.18	11.03	3.75	39.7	97.4	2.34E+06	4.61E+02	1.57E+02

O3Sn1Sr1	59161	62	10.8	1.75	34.96	356.85	17.7	84.5	1.61E+06	1.75E+02	1.79E+03
Na1O2Sc1	25729	166	10.8	4.41	1.27	9.6	17.3	64.1	3.30E+06	1.57E+03	1.18E+04
Hf1N2Sr1	82538	166	10.6	0.56	65.67	410.32	55.5	71.7	6.52E+05	1.13E+00	7.04E+00
Al1Na1O2	79404	33	10.5	3.82	0.6	255.01	5.9	104.7	5.42E+06	1.07E+02	4.57E+04
Al1Na1O4Si1	34884	198	10.5	4.5	0.45	126.49	6.1	135.8	1.12E+07	2.23E+02	6.26E+04
Al1B14Li1	606102	74	10.4	1.321	62.33	157.51	25.1	131.1	1.88E+06	7.57E+03	1.92E+04
Al2Ca2O7Si1	24588	113	10.3	4.27	2.2	225.38	10	120.5	8.20E+06	1.29E+03	1.32E+05
Ga1Na1O6Si2	156702	15	10.3	4.21	1.32	332.35	8.2	126.7	8.75E+06	5.84E+02	1.47E+05
Al2Cd1S4	67218	82	10.2	2.73	0.18	179.59	8.2	53.5	1.59E+06	6.00E+00	5.99E+03
Al4O7Sr1	16751	15	10.2	3.76	1.4	237.02	7.6	115.3	6.15E+06	8.68E+02	1.46E+05
Ca6Ga1N5	33795	193	10.1	0.82	3.07	204.54	16.2	83.8	8.82E+05	1.51E-01	1.00E+01
Ga1In1O5Zn2	380305	194	10.1	1.19	9.36	2688.82	11.5	73.6	1.04E+06	1.52E+00	4.38E+02
Au2S1	78718	224	10.1	1.99	3.23	128.78	6.6	45.6	1.07E+06	1.44E+01	5.74E+02
O2Zn1	60763	205	10	2.03	12.84	1.13	10.8	106.4	2.38E+06	9.56E+01	8.38E+00
Cd1Ga2O4	159739	227	10	1.6	1.54	2450.9	12.4	83	1.46E+06	3.17E+00	5.04E+03
Mg1O4Ti2	184695	92	9.9	0.21	0.85	20.01	18.4	81.7	4.64E+05	4.82E-07	1.13E-05
Ca1O3Ti1	180956	62	9.9	2.7	2.37	46	74.1	94.8	2.91E+06	1.18E+03	2.29E+04
Ca1O3Ti1	71915	62	9.9	2.7	2.43	48.74	74.1	94.8	2.91E+06	1.21E+03	2.43E+04
Ca1O3Zr1	167889	62	9.9	4.28	10.77	21.29	33.8	90.7	5.17E+06	7.79E+04	1.54E+05
B15Na1	18319	74	9.8	0.093	130.56	27.22	10.2	140.9	4.28E+05	7.65E+01	1.60E+01
Mg1Na2O4Si1	15619	7	9.8	3.8	0.7	201.12	5.6	113.1	6.06E+06	1.15E+02	3.32E+04
Ga1O6Y3	155086	36	9.8	3.33	1.83	346.49	12.9	78.3	2.98E+06	3.14E+02	5.94E+04
Ca1Mg1O6Si2	9672	15	9.8	4.95	0.66	266.76	8.7	126.7	1.18E+07	3.68E+03	1.49E+06
Hf1O2	57385	14	9.7	4.36	3.76	9.81	16.1	91.6	5.40E+06	4.04E+03	1.05E+04
Zn1S4Ge1Cu2	627794	121	9.6	0.8	12.76	869.77	12.3	44.3	6.14E+05	1.13E-01	7.65E+00
Na4O12Ti5	170677	143	9.6	2.81	0.77	1.51	33.3	106.6	3.57E+06	1.24E+02	2.43E+02
B7Mg1	261234	74	9.6	1.472	46.16	19.01	43.3	125.9	2.01E+06	1.20E+04	4.94E+03
Ga2S4Zn1	53604	82	9.6	2.27	2.66	317.69	9.5	42.6	1.12E+06	4.60E+01	5.49E+03
Ga2S4Zn1	63242	82	9.6	2.27	2.65	318.97	9.5	42.6	1.12E+06	4.58E+01	5.51E+03

N4Sn3	89525	227	9.5	0.27	1.02	10098.07	20.8	85.6	5.15E+05	4.33E-06	4.29E-02
La1O3Y1	419666	62	9.3	4.2	2.85	2.19	66.1	72.1	3.62E+06	1.01E+04	7.72E+03
Ga4O7Sr1	10316	15	9.3	2.44	1	276.13	10.1	95.3	2.59E+06	3.18E+01	8.82E+03
Al2Ca2O5	89708	46	9.3	3.57	6.39	325.6	12.9	98.1	4.44E+06	4.54E+03	2.32E+05
N4Zr3	152050	62	9.1	1.13	64.95	26.48	44.8	92.2	1.19E+06	2.80E+01	1.14E+01
La2Mo1O6	25611	121	9.1	3.22	3.2	0.19	13.8	112.8	4.68E+06	4.79E+02	2.85E+01
C2B2Ca1	88019	140	9.1	0.507	297.43	61.81	17.9	159.7	9.84E+05	3.73E+03	7.72E+02
Al1B14Li1	35336	74	8.9	1.321	62.64	157.12	25.2	131.1	1.88E+06	7.65E+03	1.92E+04
Ca3B1N3	95814	123	8.8	0.53	7.33	155.18	19	210.9	1.26E+06	3.10E-02	6.54E-01
Li2Zr1N2	78790	164	8.8	1.88	35.13	12.96	29.7	74.7	1.53E+06	4.53E+02	1.67E+02
Ca3O7Ti2	86241	36	8.8	2.74	0.93	21.2	39.4	93.1	2.90E+06	1.51E+02	3.46E+03
Ge1Mg1O3	201664	15	8.8	2.5	10.07	531.59	8.9	98.2	2.77E+06	2.14E+02	1.13E+04
Mg2O4Si1	168010	62	8.8	4.67	4.13	530.9	7.4	117.1	9.15E+06	1.26E+04	1.63E+06
C2B2Mg1	79587	64	8.7	1.015	82.09	56.71	14.8	148.5	1.64E+06	3.91E+03	2.70E+03
B4Mg1	23460	62	8.6	0.362	629.82	65.53	26	138.5	7.31E+05	4.71E+03	4.90E+02
Li2S1	642294	225	8.6	3.386	0.94	15.22	7.6	46	1.69E+06	1.05E+02	1.70E+03
Li2S1	657597	225	8.6	3.385	0.94	15.21	7.6	46	1.69E+06	1.05E+02	1.70E+03
In2Mg1O4	157770	227	8.6	1.86	1.44	1016.93	9.6	69.9	1.43E+06	5.64E+00	3.99E+03
Ge1Na2O5Ti1	160148	129	8.5	3.59	1.11	1.97	11.6	101.6	4.71E+06	2.69E+02	4.77E+02
C2Au1Li1	411253	187	8.5	1.682	6.91	315.5	7.1	249	5.82E+06	7.13E+03	3.25E+05
Al1O3Y1	83028	62	8.5	5.78	19.63	19.14	16.9	86.6	7.81E+06	6.80E+05	6.63E+05
La1O3Sc1	99538	62	8.4	4	6.08	6.13	32	79.3	3.86E+06	2.51E+04	2.53E+04
Al1O3Y1	167509	62	8.4	5.78	12.05	19.82	16.9	86.6	7.82E+06	4.18E+05	6.87E+05
Ga1S6Y3	635286	36	8.3	2.29	4.39	11.8	13	43.9	1.15E+06	8.01E+01	2.16E+02
B12Li2Si2	418627	64	8.3	1.745	23.85	49.54	11.3	120.9	2.32E+06	2.48E+03	5.14E+03
Ca1Ge1O5Zr1	154327	2	8.3	3.67	1.83	138.28	14.7	99.6	4.72E+06	6.41E+02	4.85E+04
S4Zn1Cu2Sn1	262388	82	8.1	0.57	18.71	1137.64	16.5	40.5	5.15E+05	1.74E-02	1.06E+00
Ca1In2O4	52390	141	8.1	2.03	1.03	635.26	10	69.8	1.54E+06	8.09E+00	4.98E+03
B6Ca1	26753	221	8	0.043	713.17	187.16	20.8	160.3	3.67E+05	5.39E+02	1.41E+02

Na2O4Si1Zn1	34565	7	8	3.19	0.49	227.57	6.3	113.2	4.64E+06	3.15E+01	1.46E+04
In1Na1O6Si2	183786	15	8	3.55	1.39	269.39	7.8	124.1	6.31E+06	2.12E+02	4.10E+04
Al2Ca3N4	280349	15	7.9	2.54	7.72	13.98	18.8	89.8	2.54E+06	6.15E+02	1.12E+03
N8Si5Sr2	401500	31	7.9	3.2	12.83	79.64	13.8	138.6	6.38E+06	1.86E+03	1.15E+04
O7Y2Zr2	153818	227	7.9	2.89	4.28	103.27	28.8	91.7	3.04E+06	7.04E+02	1.70E+04
Ca5Ga2N4	40372	64	7.8	0.02	4.77	4.57	1611.	64.8	2.92E+05	5.18E-09	4.96E-09
Mg1S4Sc2	37423	227	7.7	1.9	7.49	33.67	16.1	43.5	1.00E+06	5.76E+01	2.59E+02
Ga1Ge1N1Sr2	420413	11	7.6	0.04	45.54	6.96	32	73.8	3.19E+05	6.21E-08	9.49E-09
N3Na1	29380	12	7.6	1.2	1.29	1.27	6.4	189.1	2.52E+06	2.46E-01	2.42E-01
B6Li2	410794	127	7.6	0.018	106.15	564.42	10.7	149.4	3.15E+05	2.63E+01	1.40E+02
B6Ca1	612689	221	7.6	0.043	714.3	186.39	20.8	160.3	3.67E+05	5.40E+02	1.41E+02
K1O2Sc1	34958	166	7.6	3.97	14.6	26.02	18.8	62.9	2.82E+06	1.04E+04	1.86E+04
Al2S4Zn1	15377	227	7.5	2.5	4.21	74.69	11.6	52.8	1.45E+06	1.17E+02	2.07E+03
Al2S4Zn1	76278	227	7.5	2.5	4.21	74.83	11.6	52.8	1.45E+06	1.17E+02	2.08E+03
Ca1O3Sn1	29204	148	7.5	2.92	0.68	366.49	11.2	72.1	2.31E+06	4.61E+01	2.49E+04
C2Ca1	94385	12	7.5	2.219	1.09	38.66	9.5	234	8.33E+06	4.43E+03	1.57E+05
Na2O7Ti3	15463	11	7.4	3.27	0.6	1.65	24.3	107.2	4.44E+06	1.74E+02	4.77E+02
Al2Hg1S4	25635	82	7.4	2.02	0.58	172.52	10.7	53.5	1.22E+06	4.15E+00	1.24E+03
Ca1Ge1O3	31338	62	7.4	2.06	36.86	185.29	21.1	88.3	1.98E+06	5.85E+02	2.94E+03
Cd1Ga2S4	106362	82	7.4	2.13	2.43	271.93	9.6	42.2	1.06E+06	2.64E+01	2.95E+03
O7Sn2Y2	24193	227	7.3	2.64	8.83	859.26	16	85.4	2.50E+06	8.01E+02	7.79E+04
O7Sn2Y2	84805	227	7.3	2.64	8.84	853.39	16	85.4	2.50E+06	8.01E+02	7.79E+04
Ca1Mg1O4Si1	202286	62	7.3	4.66	1.82	241.3	8	114.6	8.77E+06	5.89E+03	7.79E+05
N2Sr2Zn1	80376	139	7.2	0.73	2.97	135.64	18.1	78.3	7.88E+05	8.09E-02	3.71E+00
Ba1N2Zr1	74904	129	7.2	1.43	25.67	91.7	38.5	84.2	1.34E+06	8.38E+01	2.98E+02
C2Ag1Li1	410868	187	7.2	1.768	7.4	91.89	5.1	245.3	6.16E+06	6.51E+03	8.09E+04
S4Sc2Zn1	650850	227	7.1	0.88	13.01	235.91	18.1	45.1	6.48E+05	3.46E-01	6.28E+00
Ba1O1	616005	225	7.1	2.09	14.01	43.22	71.4	11.5	5.23E+05	9.78E+02	3.02E+03
Al2O4Pb1	80128	40	7.1	3.96	0.42	6.23	17.8	106.9	5.92E+06	2.80E+02	4.15E+03

Na2O1	644917	225	6.9	1.89	0.12	150.25	7.6	33.4	8.37E+05	4.10E-01	5.13E+02
S1Sr1	53941	225	6.9	2.5	7.51	33.36	11.9	21.4	7.59E+05	2.14E+02	9.49E+02
La2O7Zr2	51573	227	6.9	3.94	2.81	18.17	24.4	87.6	4.35E+06	7.87E+03	5.10E+04
Ca5N6Si2	414462	15	6.8	2.18	33.53	149.25	25.8	105.8	2.57E+06	9.12E+02	4.06E+03
Ca2O4Sn1	9011	55	6.8	2.73	2.04	448.25	13.1	72.3	2.15E+06	1.08E+02	2.38E+04
N2Si1Sr1	170266	14	6.8	3.15	15.83	262.39	17.6	128.6	5.52E+06	2.65E+03	4.40E+04
Ga1La1O3	73761	62	6.8	3.26	35.28	334.78	27.5	80.3	3.00E+06	1.14E+04	1.08E+05
Ca1O3Si1	33702	2	6.7	4.83	0.74	148.26	7.6	128.4	1.16E+07	6.97E+02	1.40E+05
Ca4N4Ti1	172879	2	6.6	1.48	19.22	76.82	16.9	84.2	1.38E+06	3.36E+01	1.35E+02
K2O13Ti6	25712	12	6.6	3.04	2.82	1.03	25.2	108.7	4.08E+06	5.48E+02	2.00E+02
Ga1La1O3	160235	62	6.6	3.26	34.95	340.25	27.5	80.3	3.00E+06	1.13E+04	1.10E+05
K1O2Y1	49650	166	6.6	3.93	0.91	114.3	12.1	55.8	2.42E+06	1.24E+03	1.56E+05
Ca2Ga2O5	51545	46	6.5	2.18	5.04	727.44	15.3	86.7	2.06E+06	1.04E+02	1.50E+04
Na2O6Si2Zn1	16160	43	6.5	3.87	0.52	128.25	6.2	128.4	7.72E+06	1.05E+02	2.60E+04
Ca1O4Sc2	16886	62	6.5	3.74	8.29	30.05	23.6	82.1	3.69E+06	1.52E+04	5.51E+04
Ge4O9Pb1	201282	5	6.4	3.48	2.08	8.73	15.5	104.3	4.67E+06	5.58E+02	2.34E+03
Ca2O4Si1	81095	62	6.4	4.23	4.31	129.27	8.4	111	7.01E+06	2.02E+03	6.07E+04
Cd2O4Si1	50529	70	6.3	1.49	1.24	1077.89	12.7	110.3	1.78E+06	1.71E+00	1.49E+03
In1O3Y1	251	185	6.3	2.02	3.45	411.06	11.9	74.9	1.64E+06	2.74E+01	3.27E+03
Ga1Na1O2	36652	33	6.3	2.86	0.54	345.51	6.7	87.2	2.82E+06	1.94E+01	1.24E+04
La2O7Sn2	82956	227	6.3	2.56	7.21	692.97	15.9	78.5	2.20E+06	5.18E+02	4.97E+04
Hf2O7Y2	153819	227	6.3	3.4	10.04	189.32	25.1	94.1	3.90E+06	3.80E+03	7.17E+04
Hf1O3Sr1	86830	62	6.3	4.63	0.9	97.01	23.5	95.6	6.36E+06	2.02E+03	2.18E+05
Ba1N8Si6	417444	44	6.2	3.27	16.19	13.15	11.5	136.6	6.45E+06	2.22E+03	1.80E+03
O3Sr1Ti1	27045	221	6.2	2.11	18.32	37.9	120.6	65.9	1.52E+06	1.92E+03	3.96E+03
Al1Li1S2	608360	33	6.2	4.126	5.45	5.66	6.9	56.8	2.62E+06	6.13E+03	6.37E+03
La2O7Sn2	24195	227	6.2	2.57	7.34	658.72	16	78.5	2.21E+06	5.43E+02	4.88E+04
Al2O4Sr1	26466	4	6.2	4.15	2.22	247.42	9.4	107.6	6.45E+06	1.04E+03	1.15E+05
C2Li2	89535	71	6.2	3.207	3.98	27.28	6.3	234.1	1.70E+07	9.12E+04	6.24E+05

Cd1O2	109339	205	6.1	1.3	9.77	2.28	10.1	105.9	1.50E+06	4.69E+00	1.10E+00
Cd1O2	36151	205	6.1	1.3	9.51	2.3	10.1	105.9	1.50E+06	4.57E+00	1.10E+00
La1O3Y1	89455	33	6.1	4.2	2.83	2.63	30.5	69.7	3.46E+06	4.60E+03	4.28E+03
Al1Ca3N3	410579	14	6.1	2.47	0.72	389.81	19.5	83.3	2.25E+06	3.13E+01	1.70E+04
Ba1Hf1O9Si3	183835	188	6.1	4.68	1.83	94.52	8.7	133.7	1.18E+07	1.62E+03	8.31E+04
Cd1S4Sc2	94993	216	6	1.244	8.2	8.53	17.1	44	7.69E+05	2.79E+00	2.90E+00
Hg1O2Sr1	165068	166	6	2.14	2.3	22.92	7.5	76.3	1.77E+06	1.63E+01	1.62E+02
Ge1Na2O4Zn1	76314	7	6	2.61	0.49	295.79	6.7	88.6	2.58E+06	1.01E+01	6.10E+03
Ca1Ga2O4	41662	62	6	3	1.86	1558.66	16.5	78.9	2.65E+06	2.19E+02	1.84E+05
Cd1S4Sc2	620332	227	5.9	1.24	8.76	208.78	17.1	44	7.68E+05	2.90E+00	6.92E+01
Cd1S4Sc2	94994	227	5.9	1.24	8.71	213.29	17.1	44	7.68E+05	2.89E+00	7.07E+01
O3Sr1Ti1	184455	221	5.9	2.11	18.24	36.77	121	65.9	1.52E+06	1.91E+03	3.86E+03
Na2O3Si1	24664	36	5.9	3.88	0.44	124.61	5.7	120.9	7.00E+06	8.31E+01	2.35E+04
In1La1O3	281549	62	5.9	2.66	24	253.47	26.7	70	2.02E+06	3.85E+03	4.07E+04
Ba1O9Si4	80067	188	5.9	4.35	1.52	153.35	8.4	139.4	1.11E+07	8.38E+02	8.46E+04
Na1O4Si1Y1	20161	33	5.9	4.2	4.88	213.27	7.6	122.9	8.25E+06	1.99E+03	8.68E+04
S3Te1Cu3Cl1	88685	160	5.8	1.12	14	22.34	10.9	42.5	7.12E+05	2.99E+00	4.78E+00
Ba1O9Si3Ti1	36185	188	5.8	3.38	1.07	0.77	10.4	134.2	6.62E+06	1.63E+02	1.17E+02
Al1La1O3	153835	221	5.8	3.85	4.57	0.18	29.6	78	3.58E+06	4.29E+03	1.69E+02
B6Sr1	615489	221	5.8	0.039	429.17	591.67	13.8	152	3.57E+05	1.97E+02	2.72E+02
Na2O13Ti6	23877	12	5.8	3.16	0.81	0.98	29.7	113.7	4.60E+06	5.28E+02	6.39E+02
In1Na1O2	34600	166	5.8	1.93	0.41	546.84	11	57.1	1.24E+06	2.29E+00	3.07E+03
O3Pb1Sr1	4121	62	5.7	0.8	11.72	48.82	25.7	67.1	7.60E+05	7.87E-01	3.27E+00
La2O9Si1Ti2	75583	12	5.7	2.88	1.02	1.11	29	124.4	4.58E+06	1.65E+02	1.79E+02
Ge1Na2O5Ti1	20129	129	5.7	3.59	1.11	1.58	11.6	101.6	4.71E+06	2.68E+02	3.82E+02
Ga2Hg1S4	67220	82	5.7	1.58	4.07	357.28	12.5	42.1	8.65E+05	6.07E+00	5.33E+02
Hf2La2O7	153815	227	5.7	4.24	3.09	0.52	21.5	89.4	4.99E+06	1.33E+04	2.24E+03
CaGe1Mg1O4	80455	62	5.7	3.61	2.02	302.55	8.3	89.7	3.97E+06	3.60E+02	5.39E+04
BaCa1Ga4O8	280042	44	5.6	3.06	0.95	332.5	12.9	90.1	3.20E+06	9.85E+01	3.43E+04

Ge1Na1O4Y1	28213	33	5.6	3.53	1.4	234.67	8.2	96.8	4.28E+06	2.18E+02	3.65E+04
S2Zn1	651447	205	5.5	1.42	19.32	35.03	18.6	59.6	1.02E+06	2.92E+01	5.29E+01
Al1La1O3	170772	221	5.5	3.85	5.91	0.18	29.6	78	3.58E+06	5.54E+03	1.69E+02
Ba1Hf1N2	184053	129	5.5	1.48	55.2	117.94	33.8	83.4	1.37E+06	1.93E+02	4.13E+02
Ca1N6	412259	70	5.5	3.19	0.61	7.77	8.1	276.2	2.43E+07	1.15E+02	1.47E+03
La1Na1O4Ti1	81535	129	5.5	2.89	5.19	20.88	29.1	106.6	3.71E+06	8.60E+02	3.46E+03
Ca3Ga2N4	170442	15	5.5	1.94	26.18	1066.58	21.4	78.9	1.66E+06	3.13E+02	1.28E+04
Ge2Na1O6Sc1	22503	15	5.5	3.47	2.74	155.83	10.4	105	4.70E+06	4.85E+02	2.76E+04
O2Rb1Y1	49651	166	5.5	3.66	0.89	125.87	13	55.3	2.21E+06	2.72E+02	3.85E+04
Ge2La2O7	202606	1	5.5	3.6	0.43	161.39	16.7	95.1	4.30E+06	1.53E+02	5.74E+04
C2Au1Rb1	411252	123	5.5	2.431	3.77	10.28	7.4	247.8	1.09E+07	2.68E+04	7.33E+04
Ca2Hf7O16	4136	148	5.5	4.21	2.74	128.21	17.4	95.1	5.42E+06	2.57E+03	1.21E+05
Na2O7Si3	81134	15	5.5	4.69	4.87	239.29	11	130.7	1.13E+07	2.29E+04	1.13E+06
N1Na1Sn1	172471	186	5.4	0.95	2.62	608.93	14.5	62.7	8.08E+05	2.78E-01	6.46E+01
Ge2Na2O7Zr1	20402	2	5.4	3.66	0.35	164.55	11.8	107.7	5.29E+06	2.74E+02	1.29E+05
Ca3O9Si3	4442	2	5.4	4.74	0.97	180.61	9.8	124.7	1.06E+07	4.38E+03	8.16E+05
Ba2In2O5	73937	46	5.3	0.93	8.5	678.87	15.7	73.4	8.79E+05	2.96E-01	2.37E+01
Ba1N7Si4Y1	98276	186	5.3	2.68	2.26	361.22	12.8	125.1	4.17E+06	1.05E+02	1.68E+04
Na2O7Si2Zr1	24866	2	5.3	4.56	0.73	116.5	10.3	130.3	1.07E+07	2.60E+03	4.15E+05
S1Zr2N2	96971	194	5.2	0.9	175.5	93.81	21.5	75.6	8.77E+05	1.99E+01	1.07E+01
Ca1Ga1La1O4	96463	33	5.2	3.41	8.25	221.85	11.5	77.5	3.03E+06	1.46E+03	3.93E+04
Ba2N8Si5	401501	31	5.1	2.89	7.13	20.07	12.2	137.2	5.34E+06	4.96E+02	1.40E+03
O3Sr1Ti1	182763	140	5.1	2.23	15.64	34.03	98.3	97.6	2.40E+06	1.85E+03	4.04E+03
Ba1O7Si2Zn2	88589	36	5.1	3.33	1.44	252.16	8.9	121.7	5.52E+06	1.71E+02	2.99E+04
C2Au1K1	411255	123	5.1	2.272	4.64	27.64	7	248.1	9.67E+06	2.17E+04	1.29E+05
In2S3	12148	167	5	0.33	2.14	5124.51	27.4	39.4	4.27E+05	7.65E-04	1.83E+00
S4Y2Zn1	651411	227	5	0.91	7.59	302.1	13.8	39.9	6.21E+05	1.99E-01	7.87E+00
O13Rb2Ti6	23878	12	5	2.92	4.27	0.73	25.8	106.5	3.75E+06	6.67E+02	1.14E+02
Ca2Ge1O4	173459	62	5	3.59	1.04	196.6	8.8	86.4	3.74E+06	1.90E+02	3.59E+04

O2Si1	75648	122	5	5.75	0.29	22.79	3.8	139.3	1.96E+07	2.18E+03	1.71E+05
Ba1Hg1O2	83411	166	4.9	2.23	0.45	18.56	8.4	74.9	1.81E+06	4.55E+00	1.88E+02
B4Mo1Y1	20081	55	4.9	0.369	48.05	49.52	37.5	103.6	6.37E+05	3.42E+02	3.52E+02
Al2Mg1S4	79672	62	4.9	3.06	3.98	22.86	10.8	60.3	2.01E+06	7.35E+02	4.24E+03
Hf1O3Sr1	89383	62	4.9	4.63	0.91	93.49	23.5	95.6	6.36E+06	2.04E+03	2.10E+05
C7Y4	86049	14	4.8	0.104	55.39	152.39	38.6	221.3	5.15E+05	2.14E+02	5.89E+02
La4O12Ti3	91765	148	4.8	3.08	5.72	1.69	48.3	88.9	3.17E+06	2.30E+03	6.80E+02
Ba1O9Ti4	31783	59	4.8	3.01	5.47	3.25	39.1	104.2	3.80E+06	1.55E+03	9.26E+02
In2Mg1S4	639944	227	4.8	1.79	0.72	259.64	12.6	41.5	9.29E+05	2.77E+00	1.00E+03
Na2S1	644959	225	4.8	2.44	0.31	84.26	7.1	24.5	8.10E+05	6.88E+00	1.87E+03
Ba3Ga2Ge4O14	250124	150	4.8	2.24	1.33	329.1	11.1	95.5	2.35E+06	1.83E+01	4.53E+03
Ge2In1K1O6	65337	15	4.8	2.32	0.89	396.33	8.7	100.2	2.59E+06	1.18E+01	5.26E+03
C2Au1Na1	411254	123	4.8	1.413	61.2	144.92	7.5	249	4.47E+06	3.02E+04	7.15E+04
Ca1O6Si2Zn1	168048	15	4.8	4.04	2.24	289.27	10.1	124.3	7.87E+06	9.56E+02	1.24E+05
In2O5Sr2	22029	46	4.7	1	10.01	473.74	14.5	78.8	9.67E+05	5.56E-01	2.63E+01
N1Li3	156899	194	4.7	1.29	3.43	58.39	14.3	74.2	1.11E+06	2.24E+00	3.81E+01
Cd1S4Y2	620370	227	4.7	1.32	5.56	261.48	12.5	39.2	7.45E+05	2.15E+00	1.01E+02
S3Sc1Y1	23422	33	4.7	2.18	14.89	4.76	22.4	42.7	1.09E+06	3.52E+02	1.13E+02
Ca2O4Pb1	36629	55	4.7	1.5	2.49	312.5	15.3	64.9	1.13E+06	4.29E+00	5.38E+02
In2S4Zn1	15637	227	4.7	1.15	0.97	1933.31	15.1	41.3	7.11E+05	3.35E-01	6.68E+02
Ba1O9Si3Sn1	10385	188	4.7	3.74	0.93	128.05	7.9	132.7	7.70E+06	1.96E+02	2.70E+04
Cd1S4Y2	61697	227	4.6	1.322	7.18	7.46	12.5	39.2	7.46E+05	2.82E+00	2.93E+00
Na6O5Pb1	15102	107	4.6	1.09	0.89	186.09	9.6	63.7	8.89E+05	6.30E-02	1.32E+01
Ca1S3Zr1	23286	62	4.6	1.52	28.6	56.76	33.9	48.1	9.19E+05	8.68E+01	1.72E+02
Ba1S1	616053	225	4.6	2.15	4.47	24.44	15	17	6.23E+05	6.51E+01	3.56E+02
Cd1Ge1O3	20225	15	4.6	1.46	0.73	659.33	11	93.7	1.50E+06	7.65E-01	6.91E+02
Mg2N2Sr1	410826	164	4.6	1.73	6.12	1404.08	18.8	59.4	1.17E+06	2.73E+01	6.25E+03
La2Na2O10Ti3	78487	139	4.6	2.39	1.99	28.48	205.6	107	2.91E+06	7.50E+02	1.07E+04
C2Na2Pt1	411389	164	4.6	0.679	5.79	375.45	16.8	232.8	1.71E+06	3.59E+02	2.32E+04

Na1O2Y1	2740	15	4.6	3.89	1.49	261.01	14.5	65.7	2.91E+06	2.26E+03	3.96E+05
Cu1In1O8W2	74944	15	4.5	1.31	3.17	2.11	17.1	103.9	1.49E+06	2.72E+00	1.81E+00
Ge1Na2O3	23781	36	4.5	2.97	2.06	119.08	6.4	91.6	3.15E+06	8.82E+01	5.11E+03
Ge3La2O9	83341	2	4.5	2.88	2.19	198.94	16.3	97.3	3.27E+06	1.99E+02	1.81E+04
Ge1Na1O4Y1	85497	62	4.5	3.53	1.41	245.48	8.2	96.8	4.28E+06	2.19E+02	3.82E+04
Ca3O5Si1	24625	160	4.5	3.26	0.65	230.02	10.7	114.7	4.88E+06	1.93E+02	6.82E+04
Ba1Ca2Mg1O8Si2	422406	147	4.5	5.02	0.99	352.25	14.3	118.8	1.07E+07	2.19E+03	7.79E+05
Na1Nb1S2	26285	194	4.4	0.72	20.64	5.95	14.2	49.2	6.15E+05	4.07E-01	1.18E-01
Al1La1O3	180417	74	4.4	3.92	19.83	0.24	27.5	91.5	4.59E+06	1.93E+04	2.33E+02
Ga2S3	409550	9	4.4	1.71	0.63	145.54	10.3	47.3	9.85E+05	1.40E+00	3.25E+02
Ga1Li1S2	68465	33	4.4	2.965	5.26	5.47	7.9	47.7	1.54E+06	5.66E+02	5.89E+02
Cd3O5Si1	23170	129	4.3	0.97	14.32	1646.61	21.1	111.9	1.23E+06	9.26E-01	1.07E+02
Al1La1O3	90531	167	4.3	3.94	7.99	0.22	27.2	91.5	4.63E+06	7.94E+03	2.18E+02
Al1La1O3	180415	15	4.3	3.94	8.77	0.22	27.3	91.5	4.63E+06	8.68E+03	2.18E+02
O7Sr3Ti2	34629	139	4.3	2.19	22.32	48.68	50.1	82.3	1.95E+06	1.21E+03	2.64E+03
Ba1O2Zn1	25812	152	4.3	2.28	1.47	221.08	14.4	72.2	1.78E+06	2.92E+01	4.39E+03
Na4O4Si1	15500	2	4.3	3.24	0.34	142.73	6.9	111.2	4.63E+06	2.63E+01	1.10E+04
Ba1O3Zr1	97462	221	4.3	3.42	16.77	79.89	46.1	64.5	2.44E+06	1.21E+04	5.75E+04
K3O7Sc1Si2	413432	194	4.3	3.65	4.59	98.05	9.6	130.5	7.18E+06	2.86E+03	6.11E+04
O4Sn2Ti1	163230	135	4.2	1.34	5.48	6.47	26.1	76.9	1.18E+06	8.24E+00	9.71E+00
Ga3N5Sr3	170443	2	4.2	1.36	5.6	1288.98	19.2	83	1.27E+06	4.16E+00	9.56E+02
O10Sr4Ti3	34630	139	4.2	2.15	2.16	45.34	59.8	88.3	2.07E+06	1.26E+02	2.63E+03
Ba1Ca2O9Si3	24426	2	4.2	4.57	0.33	202.84	11.1	126.5	1.01E+07	3.23E+02	1.99E+05
La1S3Sc1	641844	33	4.1	1.91	25.48	4.13	24.1	42.8	9.91E+05	3.05E+02	4.95E+01
Na2O3Zn2	404913	96	4.1	1.26	2.43	624.78	11.8	74	1.09E+06	6.26E-01	1.61E+02
B4W1Y1	615702	55	4.1	0.299	211.06	85.52	39	104.1	5.80E+05	1.18E+03	4.79E+02
K2O3Sn1	24131	62	4.1	2.15	0.48	106.08	9	80.1	1.87E+06	5.25E+00	1.16E+03
Hf3N4	97997	220	4.1	1.42	45.28	565.67	38.8	82	1.30E+06	9.41E+01	1.18E+03
O4Sn1Sr2	81851	138	4.1	2.66	1.48	248.54	15.4	85.8	2.54E+06	7.94E+01	1.33E+04

O4Sn1Sr2	150383	56	4.1	2.65	1.46	254.63	15.4	85.8	2.53E+06	7.65E+01	1.33E+04
K1La1O2	27001	166	4.1	3.88	0.49	49.11	15.5	49.6	2.10E+06	2.52E+02	2.53E+04
Ba2N2Zn1	80377	139	4	0.48	7.01	13.58	34.9	76.1	6.23E+05	3.01E-02	5.82E-02
O14Si4Sr2Ti2	83362	63	4	4.02	5.51	0.82	10.8	149.5	1.09E+07	2.46E+03	3.65E+02
Cd1In2S4	108215	227	4	1.08	0.9	2004.58	14.6	41.5	6.90E+05	2.07E-01	4.62E+02
Cd1In2S4	620027	227	4	1.08	0.9	2007.02	14.6	41.5	6.90E+05	2.07E-01	4.63E+02
Al1Ba1La1O4	62490	19	4	4.29	2.06	0.94	20.1	93.8	5.46E+06	2.51E+03	1.14E+03
Na2O7Si2Zn2	34325	40	4	3.32	1.58	161.38	7.6	122.1	5.53E+06	1.57E+02	1.60E+04
O2Rb1Sc1	1270	194	4	3.72	2.31	36.83	20.8	70.2	2.99E+06	1.24E+03	1.98E+04
Ga1La2N3	160089	15	3.9	2.03	6.06	9.97	33.7	91.6	2.02E+06	1.40E+02	2.32E+02
GaMg1S4Sc1	81552	62	3.9	2.079	0.85	28.37	13.7	48	1.15E+06	9.26E+00	3.09E+02
Li1S2Y1	44957	166	3.9	2.255	1.05	16.97	18.5	37.6	1.02E+06	2.51E+01	4.05E+02
S3Sc2	654308	70	3.8	1.49	14.91	41.29	23.1	44.6	8.63E+05	3.73E+01	1.03E+02
Na6O4Zn1	6161	186	3.8	1.55	1.51	312.1	10.2	61.2	1.10E+06	1.59E+00	3.28E+02
Na4O4Ti1	69621	2	3.8	3.27	0.28	51.47	6.9	91	3.54E+06	2.29E+01	4.21E+03
O2Sr1Zn1	25556	62	3.8	2.08	2.67	464.53	14.8	74.6	1.68E+06	3.74E+01	6.51E+03
O4Sr1Y2	25701	62	3.8	3.92	4.5	37.27	20.5	74.4	3.45E+06	1.02E+04	8.46E+04
Al2Ba1O4	21080	182	3.8	3.94	0.7	197.25	16.2	116.5	6.75E+06	4.13E+02	1.16E+05
Mg1O7Si2Sr2	261226	113	3.8	4.51	1.3	185.64	8.7	119.5	8.91E+06	9.26E+02	1.32E+05
O4Pb1Sr2	16806	55	3.7	1.42	1.37	253.47	15	61.1	1.03E+06	1.66E+00	3.08E+02
Na1S2Y1	76543	166	3.7	2.64	3.17	14.4	12	33.1	1.04E+06	1.26E+02	5.73E+02
K1La1Na1Nb1O5	94743	129	3.7	3.66	0.52	10.22	14.2	94.7	4.37E+06	1.73E+02	3.40E+03
In1K1O2	380401	166	3.7	2.11	1.35	467.82	10.8	59.6	1.39E+06	1.26E+01	4.40E+03
Ge2K2O6Zn1	65740	20	3.7	2.84	0.44	96.83	9.9	98.1	3.24E+06	4.29E+01	9.41E+03
Ba1O4Y2	78483	62	3.7	3.43	3.72	55.43	16.7	68.4	2.62E+06	2.52E+03	3.76E+04
Na2O8Si3Zn1	20114	4	3.7	3.93	0.24	134.19	7.4	130.4	8.15E+06	1.99E+02	1.12E+05
K2O9Si4	31201	176	3.7	4.62	2.67	155.13	7.7	143	1.31E+07	1.94E+03	1.13E+05
BaGa1La1O4	166167	19	3.7	3.88	1.71	209.68	22.2	81.4	3.84E+06	1.26E+03	1.54E+05
Cd1S2	620305	205	3.6	1.21	15.23	1.39	15	59.2	9.07E+05	7.10E+00	6.47E-01

Ba1S3Sn1	616071	62	3.6	0.87	4.39	11.06	19.2	38.4	5.98E+05	3.63E-01	9.19E-01
Pb1S1	601032	225	3.6	0.45	479.65	449.44	388.5	4.8	3.07E+05	1.76E+00	1.65E+00
Ca1S4Sc2	27181	62	3.6	1.59	9.65	25.58	22.1	47.1	9.34E+05	2.68E+01	7.10E+01
Ba1O5Ti2	281548	5	3.6	2.07	4.23	15.04	38.4	103.5	2.36E+06	1.26E+02	4.47E+02
Ca2O9Pb1Si3	18098	2	3.6	4.39	0.8	5.96	12.7	122.5	8.88E+06	7.04E+02	5.24E+03
Al6Ca4O13	16177	217	3.6	3.6	0.12	124.34	14.3	105.8	5.02E+06	3.65E+01	3.78E+04
O7Si2Sr2Zn1	247476	113	3.6	3.92	2.37	205.07	9.2	119.7	7.00E+06	7.72E+02	6.68E+04
C2Cu1K1	412038	131	3.6	2.522	1.58	82.6	6.3	245.1	1.15E+07	1.11E+04	5.80E+05
S3Sr1Zr1	23287	62	3.5	1.54	54.82	22.02	36.8	48.7	9.34E+05	1.99E+02	8.01E+01
S4Sc2Sr1	27182	62	3.5	1.66	9.8	28.91	19.5	44.4	9.25E+05	3.32E+01	9.78E+01
Na2O2Zn1	404761	14	3.5	1.47	1.67	338.59	10.6	69.9	1.18E+06	1.24E+00	2.50E+02
Ge1Mg2S4	23525	62	3.5	2.31	12.24	24.23	10.4	51	1.31E+06	1.89E+02	3.74E+02
Ge1Na4O4	61496	2	3.5	2.82	0.32	125.69	7	86.4	2.74E+06	1.10E+01	4.32E+03
O2Rb1Sc1	31960	187	3.5	3.72	2.31	36.75	20.8	70.2	2.99E+06	1.24E+03	1.97E+04
Ge2MgO7Sr2	420522	113	3.5	3.58	0.56	181.81	10.1	98.5	4.48E+06	1.15E+02	3.76E+04
C2Ag1K1	410874	123	3.5	2.667	22.51	10.83	5.3	244.9	1.28E+07	1.82E+05	8.75E+04
O4Si1Sr2	36041	14	3.5	4.47	0.67	256.93	13.4	114.7	8.16E+06	6.97E+02	2.67E+05
Pb1S1	68701	39	3.4	0.44	0.79	26.31	2781.8	11.7	3.47E+05	1.76E-02	5.86E-01
S3Sr1Zr1	154104	62	3.4	1.54	50.11	20.97	36.9	48.7	9.34E+05	1.82E+02	7.65E+01
K2O1	60438	225	3.4	1.73	0.14	34.79	9.3	23.3	6.53E+05	3.43E-01	8.53E+01
N3Na1	1144	166	3.4	3.71	0.38	1.51	5.2	275.8	3.47E+07	5.03E+01	2.00E+02
BaGe3O9Sn1	10384	188	3.4	2.76	1.15	238.72	9.5	104.4	3.39E+06	4.74E+01	9.85E+03
O9Si3Sr3	32677	2	3.4	4.37	1.51	163.95	8.8	122.5	8.80E+06	3.32E+03	3.61E+05
Ba1O3Pb1	15933	74	3.3	0.21	16.39	38.47	31.3	68.6	4.40E+05	4.48E-04	1.05E-03
Ba1O3Sn1	181091	221	3.3	0.39	12.25	4529.04	22.5	70.6	5.51E+05	9.78E-03	3.61E+00
Ba1O3Sn1	27049	221	3.3	0.39	12.26	4539.19	22.5	70.6	5.51E+05	9.78E-03	3.62E+00
Hg1In2S4	56081	227	3.3	0.37	0.97	5052.66	28.8	40.5	4.45E+05	7.23E-04	3.76E+00
K2O15Si6Ti1	46012	2	3.3	3.57	1.31	0.19	8	138.7	7.67E+06	2.11E+02	3.07E+01
Cd1Ge1Li2S4	249872	31	3.3	2.272	4.54	4.72	8	49.2	1.26E+06	6.68E+01	6.96E+01

Ca1S4Y2	619557	62	3.3	1.8	7.48	46.53	14.4	40.9	9.23E+05	3.43E+01	2.14E+02
Cd1Na2S4Sn1	281233	5	3.3	1.93	7.46	57.71	7.7	40.5	9.62E+05	3.10E+01	2.40E+02
In1Na1S2	640036	166	3.3	1.84	1.39	62.52	16	34.1	8.33E+05	8.53E+00	3.83E+02
Al2S3	73220	169	3.3	3.13	1.63	9.16	8.7	59.8	2.04E+06	1.31E+02	7.35E+02
Ge2O7Sr2Zn1	420521	113	3.3	3.09	0.36	231.54	10.6	97.2	3.58E+06	3.24E+01	2.09E+04
C2Sr1	91051	15	3.3	2.228	1.14	22.75	9.3	232.6	8.30E+06	4.51E+03	8.97E+04
Ba2MgO7Si2	81117	113	3.3	4.48	0.91	152.87	8.2	116.5	8.42E+06	5.87E+02	9.85E+04
C2Na2	95835	71	3.3	3.435	1.1	5.76	5.9	231.1	1.92E+07	3.40E+04	1.78E+05
Ba1Na1O7Sc1Si2	166998	11	3.3	4.53	2.73	110.34	15.9	124.5	9.67E+06	1.43E+04	5.76E+05
S2Sr1	23640	140	3.2	1.29	51.54	19.64	10.6	57.8	9.31E+05	2.50E+01	9.56E+00
Na2O2	109276	189	3.2	1.64	0.83	15	6.2	104.7	1.86E+06	9.85E-01	1.78E+01
Li2S4Sn1Zn1	419595	7	3.2	2.197	4.39	4.56	8.1	46.2	1.16E+06	5.04E+01	5.24E+01
Ba1S3Zr1	23288	62	3.2	1.38	3.57	91.75	44.3	49.8	8.82E+05	6.83E+00	1.76E+02
Na1S7Si1Y3	412445	173	3.2	2.45	3.07	10.45	15.9	66.3	1.76E+06	1.04E+02	3.51E+02
In1Na5O4	69630	59	3.2	1.79	0.48	217.05	7.6	65.7	1.31E+06	1.18E+00	5.32E+02
Ba1N2Si1	170268	64	3.2	2.87	16.68	12.15	16.3	128.6	4.79E+06	1.49E+03	1.08E+03
Ba1O2	24248	139	3.2	2.32	0.87	36.23	17.1	111.6	2.96E+06	3.19E+01	1.33E+03
Ba1O2	24729	139	3.2	2.32	0.87	36.62	17	111.6	2.96E+06	3.18E+01	1.34E+03
K2O3Ti1	162216	63	3.2	3.64	4.13	2.04	47.2	96.5	4.45E+06	1.24E+04	6.12E+03
O9Si3Sr3	32542	5	3.2	4.61	0.64	92.95	8.1	135.8	1.18E+07	4.81E+02	6.99E+04
Al1K1O8Si3	83534	2	3.2	4.9	0.25	99.39	5.5	137.3	1.36E+07	1.85E+02	7.34E+04
S3Y2	67502	11	3.1	1.82	4.13	16.36	14.1	43.3	9.67E+05	2.02E+01	8.01E+01
Au1Na3O2	62066	136	3.1	2.07	1.23	13.34	7.4	70.7	1.59E+06	8.31E+00	8.97E+01
Ge2N6Sr5	419164	15	3.1	1.36	15.09	378.62	34.6	84.1	1.28E+06	3.26E+01	8.16E+02
Ba1Nb2O6	39272	14	3.1	2.56	10.38	6.14	70.1	97.5	2.83E+06	2.01E+03	1.18E+03
Ga2K2Na4O6	62136	62	3.1	2.52	0.43	177.61	20.1	85.2	2.36E+06	3.45E+01	1.43E+04
C2K2Pt1	421491	164	3.1	1.311	1.18	55.84	13.8	230.1	3.60E+06	5.58E+02	2.65E+04
C2K2Pd1	421490	164	3.1	1.734	1.53	31.2	11.2	229.9	5.38E+06	1.97E+03	4.01E+04
O3Si1Sr1	59308	15	3.1	4.61	0.64	93.92	8.1	135.8	1.18E+07	4.81E+02	7.05E+04

O9Si3Sr3	38271	15	3.1	4.61	0.64	96.43	8.1	135.8	1.18E+07	4.81E+02	7.24E+04
Ge1O4Sr2	56382	14	3.1	3.53	0.46	262.72	14	92	3.98E+06	3.24E+02	1.85E+05
Al1K1O4Si1	83449	159	3.1	4.51	0.95	103.98	8.8	134.1	1.10E+07	2.66E+03	2.92E+05
Ba1O3Pb1	94313	12	3	0.2	13.52	41.83	31.3	68.6	4.34E+05	2.76E-04	8.53E-04
P1Ca3N1	106350	221	3	0.78	82.83	51.95	59.2	45	6.12E+05	2.91E+00	1.82E+00
Ga1N3Sr3	281259	176	3	0.57	1.87	478.72	16.5	68.8	6.45E+05	1.06E-02	2.71E+00
Cd2Na14O9	2195	147	3	1.4	0.32	230.26	8.6	56.6	9.70E+05	1.33E-01	9.56E+01
Ca2Ge1S4	23416	62	3	2.54	1.01	4.37	8.8	48.4	1.36E+06	2.33E+01	1.01E+02
Hg1O2Sr1	69739	154	3	2.14	2.17	32.81	7.5	84.6	1.96E+06	1.54E+01	2.32E+02
Ba1La2O5Zn1	88598	140	3	3.32	7.03	8.88	32.9	74	2.77E+06	3.03E+03	3.82E+03
Ge1N2Sr2	153302	64	2.9	0.01	31.79	16.23	1602.8	75.7	2.80E+05	5.43E-10	2.77E-10
Ca2O6Pd1W1	83259	25	2.9	1.86	7.58	6.63	21.1	98.2	1.98E+06	6.51E+01	5.70E+01
Ga2Ge1Li2S6	161763	43	2.9	2.555	3.38	3.51	10.2	49	1.38E+06	1.53E+02	1.59E+02
Ba2O8Si2Ti1	34453	100	2.9	4.14	0.75	0.54	17.6	122.9	8.05E+06	6.48E+02	4.66E+02
Na4O4Sn1	202818	2	2.9	2.08	0.29	140.2	7.4	77.9	1.76E+06	1.70E+00	8.24E+02
Ca1Ga2S4	619292	66	2.9	2.61	4.77	23.45	12.2	48.5	1.40E+06	1.80E+02	8.82E+02
K1La1O4Ti1	261365	129	2.9	2.79	0.61	10.75	25.3	102.8	3.37E+06	7.13E+01	1.26E+03
K2La2O10Ti3	74193	139	2.9	2.32	0.97	21.11	54.7	102.7	2.67E+06	8.09E+01	1.76E+03
Al2K6O6	74968	12	2.9	2.94	0.26	65.41	9.1	89.3	3.01E+06	1.49E+01	3.76E+03
Ba2Ge2MgO7	419312	113	2.9	3.59	0.69	170.35	9.1	96.5	4.37E+06	1.31E+02	3.22E+04
C6Cu5Na1	55062	62	2.9	2.195	4.98	15.81	8.5	218.1	7.25E+06	1.18E+04	3.76E+04
Cd2K2O3	16223	14	2.8	0.67	3.06	380.77	25.5	63.2	6.70E+05	1.47E-02	1.83E+00
Ba2S4Zr1	69853	139	2.8	0.87	21.14	24.05	62.6	44.9	6.43E+05	5.71E+00	6.50E+00
Hg1Mo1O4	2533	15	2.8	2.12	5.52	3.67	13	111.5	2.65E+06	6.42E+01	4.27E+01
In1Li1S2	53093	33	2.8	2.222	4.11	4.28	8.2	45.2	1.15E+06	5.25E+01	5.46E+01
K1Na1O3Ti1	47177	15	2.8	3.86	0.63	0.22	11.2	94.5	4.71E+06	2.27E+02	7.94E+01
K1La1S2	44942	166	2.8	2.99	0.51	1.77	11.3	28.9	1.03E+06	4.01E+01	1.39E+02
O9Rb2Si3Ti1	19026	176	2.8	3.45	0.78	0.55	10.1	138.3	7.20E+06	3.35E+02	2.36E+02
B1Li3S3	75223	62	2.8	3.053	1.11	6.51	6.9	104.3	3.88E+06	6.05E+01	3.55E+02

In4O7Rb2	6321	162	2.8	1.49	0.5	626.4	34	86.2	1.41E+06	1.84E+00	2.30E+03
K2O9Si3Zr1	90684	176	2.8	4.8	0.72	70.98	9.7	137.1	1.30E+07	8.31E+02	8.24E+04
Ba2O7Si2Zn1	409588	15	2.8	3.98	6.26	230.27	9.7	116.6	6.87E+06	2.35E+03	8.68E+04
C2Au1Cs1	411251	123	2.8	2.259	1.41	24.07	8.8	247.5	9.52E+06	7.94E+03	1.35E+05
Ga1N5Sr6	281260	193	2.7	0.31	3.04	247.61	16.6	75	5.16E+05	2.90E-05	2.36E-03
Ca3O1Si1	413382	62	2.7	0.24	171.87	156.87	221.6	50.4	4.19E+05	3.20E-03	2.92E-03
S3Sr1	23638	41	2.7	1.07	7.04	7.72	21.9	57.7	8.25E+05	9.85E-01	1.08E+00
Na4O3Sn1	49624	9	2.7	1.89	1.02	1.45	9.1	68.6	1.43E+06	4.16E+00	5.92E+00
O3Pb1Rb2	1413	36	2.7	1.28	0.11	38.31	10.5	68.2	1.04E+06	2.84E-02	9.85E+00
Ba2Hf1S4	80652	139	2.7	1.16	21.43	26.96	36.3	44.7	7.46E+05	1.88E+01	2.37E+01
Ba1Cd1O2	25555	62	2.7	0.97	2.95	407.4	20.3	55.3	7.60E+05	4.95E-01	6.84E+01
K2O9Si3Ti1	412920	146	2.7	3.66	0.21	0.3	9.9	132.9	7.44E+06	4.87E+01	6.96E+01
Al1K3O3	166540	12	2.7	2.94	0.34	64.59	9.1	89.4	3.01E+06	1.95E+01	3.71E+03
La1O2Rb1	27331	166	2.7	3.57	1.03	49.89	16.3	49.3	1.91E+06	3.40E+02	1.65E+04
O9Rb2Si3Sn1	19028	176	2.7	3.8	1.79	90.98	7.4	137.2	8.40E+06	3.86E+02	1.96E+04
Ba2Ge2O8Ti1	281271	35	2.7	3.72	0.84	46.22	39.1	105.3	5.24E+06	8.46E+02	4.67E+04
Ba1Na2O6Si2	10217	4	2.7	4.19	0.37	107.82	9.4	125.3	8.50E+06	1.83E+02	5.34E+04
Ba3S7Zr2	75241	139	2.6	0.79	19.54	80.51	102.4	45.3	6.17E+05	4.85E+00	2.00E+01
Pb1S4Sc2	154527	62	2.6	1.92	4.51	7.07	51.1	43.5	1.01E+06	1.13E+02	1.78E+02
K2S1	641321	225	2.6	2.33	0.03	20.92	6.4	19.3	6.91E+05	3.00E-01	2.10E+02
S4Sr1Y2	651073	62	2.6	2.08	11.43	33.02	16.6	42.8	1.05E+06	1.79E+02	5.18E+02
Cd1Li2S4Sn1	249873	31	2.6	1.948	3.92	143.51	8.1	47.1	1.08E+06	1.82E+01	6.68E+02
Ge3NbO9Rb1	10382	188	2.6	3.33	1.04	14.01	10.3	112.2	4.88E+06	1.43E+02	1.92E+03
Ge1O3Sr1	59303	15	2.6	3.36	2.12	78.73	9	102.2	4.31E+06	2.67E+02	9.93E+03
C2Cu1Rb1	412039	131	2.6	2.51	1.37	28.45	6	243.6	1.13E+07	8.60E+03	1.79E+05
Al1La3S7Ti1	608322	173	2.5	0.1	1.75	2.56	18.7	58.7	3.56E+05	3.36E-07	4.91E-07
B2Li2S5	401723	63	2.5	2.377	1.94	2.02	6.1	117.5	3.25E+06	2.10E+01	2.18E+01
Na3S4Sb1	44707	217	2.5	1.908	0.9	5.31	18.2	45	1.03E+06	7.79E+00	4.59E+01
Cd4Ge1S6	26214	9	2.5	1.35	4.69	346.79	11.9	50.2	8.75E+05	2.04E+00	1.51E+02

La1Rb1S2	81394	166	2.5	2.96	0.42	2.49	11.2	28.8	1.02E+06	3.10E+01	1.84E+02
Cd4S6Si1	16238	9	2.5	1.44	3.15	357.76	11.6	66	1.11E+06	2.18E+00	2.47E+02
B2S4Sr1	71594	14	2.5	2.82	1.79	10.51	10.5	93.7	3.03E+06	1.75E+02	1.03E+03
Ba3NaNb1O6	72330	167	2.5	3.23	1.55	10.04	21.3	78.9	2.90E+06	8.53E+02	5.54E+03
Ge1Li2Pb1S4	281011	121	2.5	2.249	1.68	9.86	504.3	46.4	1.19E+06	1.07E+03	6.32E+03
K4O18Si6Sn2	151543	146	2.5	3.85	0.57	51.21	7.6	129.6	7.78E+06	1.38E+02	1.24E+04
Ba2O3Zn1	36659	15	2.5	2.68	2.42	186.38	20.3	69.9	2.04E+06	1.78E+02	1.38E+04
C2Ba1	56160	139	2.5	1.571	0.64	23.21	12.2	229.6	4.63E+06	5.66E+02	2.06E+04
K2O6Si2Zn1	79705	20	2.5	3.93	0.32	99.8	8.6	124.3	7.50E+06	9.93E+01	3.09E+04
Ga2Ge1La2S8	262241	36	2.4	1.73	7.6	3.71	14.3	48.3	1.01E+06	2.88E+01	1.40E+01
Bi1Rb1S2	52735	166	2.4	1.347	4.99	5.19	46.7	29.9	6.53E+05	1.38E+01	1.43E+01
La2S3	641807	62	2.4	1.33	2.74	30.03	18.9	36.4	7.18E+05	1.70E+00	1.86E+01
K2O4Zn3	62146	15	2.4	1.42	1.91	241.08	11.4	73.4	1.19E+06	1.17E+00	1.48E+02
Ge1Li4S4	95649	62	2.4	2.511	0.74	12.05	12.7	57.5	1.57E+06	2.30E+01	3.75E+02
Na1O3Rb1Ti1	78753	15	2.4	3.74	0.36	1.51	10.3	94.8	4.51E+06	9.85E+01	4.15E+02
Li1Na1S1	61091	129	2.4	3.051	4.27	4.44	10.1	53.9	1.78E+06	7.28E+02	7.57E+02
K1Na1O2Zn1	38327	14	2.4	1.79	0.78	223.26	15.1	63	1.27E+06	3.80E+00	1.09E+03
K6O7Si2	17064	14	2.4	3.53	0.47	91.78	7.8	113.9	5.46E+06	6.93E+01	1.35E+04
S3Sr1Zr1	154103	62	2.3	0.78	20.37	20.95	21.6	44.8	6.11E+05	2.60E-01	2.68E-01
O3Pb2	23760	14	2.3	1.04	2.17	2.33	28	64.3	8.68E+05	7.65E-01	8.16E-01
La1S2	1435	62	2.3	0.94	17.03	88.66	17.4	51.7	7.20E+05	2.04E+00	1.06E+01
S1Sn1	651025	62	2.3	0.94	4.95	87.43	31.3	34.5	5.90E+05	1.06E+00	1.88E+01
Na4O4Pb1	74859	2	2.3	1.3	0.23	106.57	8.5	68.5	1.05E+06	5.43E-02	2.51E+01
Al1La3Mg1S7	608298	173	2.3	2.44	5.51	1.11	17.3	56.5	1.51E+06	1.97E+02	3.97E+01
Cd1K2O2	25004	60	2.3	1.38	0.26	107.79	10.7	51.5	9.02E+05	1.90E-01	7.87E+01
K2O2	36641	64	2.3	2.4	1.01	8.22	6.3	102.6	2.78E+06	1.19E+01	9.71E+01
Cs1La1S2	73532	166	2.3	2.755	0.81	13.08	11.9	28.6	9.68E+05	4.11E+01	6.63E+02
Ba3O5Si1	1449	140	2.3	3.52	1.46	1.87	28.3	106.6	4.91E+06	7.65E+02	9.85E+02
Al1In1S3	8257	169	2.3	2.36	0.62	108.72	9.6	57	1.47E+06	1.01E+01	1.76E+03

Al2Pb1S4	609026	66	2.3	2.61	2.51	8.37	43.3	61.2	1.73E+06	5.66E+02	1.89E+03
Ba2O4Ti1	15450	14	2.3	4.07	0.69	23.73	15.1	91.5	4.86E+06	4.60E+02	1.58E+04
Ge2K2O7Zr1	88843	15	2.3	3.89	2.29	65.85	10.9	102.9	5.42E+06	2.61E+03	7.50E+04
Ba1O3Si1	6245	19	2.3	4.54	1.03	115.81	12.7	123.7	9.60E+06	1.11E+03	1.25E+05
Al1O4Rb1Si1	4335	33	2.3	4.41	0.59	101.3	8.2	136.3	1.09E+07	1.30E+03	2.24E+05
Ba1O3Pb1	51657	74	2.2	0.2	16.37	38.16	31.3	68.6	4.34E+05	3.34E-04	7.79E-04
O1Si1Sr3	413384	62	2.2	0.47	29.39	70.65	40.6	42.6	4.89E+05	1.57E-02	3.77E-02
Be1Ga1La3S7	616274	173	2.2	1.196	2	11.74	20.2	61.3	9.21E+05	1.17E+00	6.86E+00
Ge1In2Li2S6	262643	9	2.2	2.044	2.95	3.06	9.6	51.6	1.20E+06	2.35E+01	2.43E+01
In2Li2S6Si1	262642	9	2.2	2.144	2.99	3.11	9.5	67.7	1.58E+06	3.35E+01	3.49E+01
Ba10N12Ti4	79102	2	2.2	1.54	1.37	12.31	23.2	92.4	1.55E+06	4.18E+00	3.76E+01
Al1La3S7Zn1	608324	173	2.2	2.39	4.97	1.33	15.8	56	1.47E+06	1.43E+02	3.83E+01
Hg1Na2O2	25511	139	2.2	1.61	0.32	31.37	7.3	73.4	1.32E+06	4.01E-01	3.93E+01
O4Rb2Zn3	40754	15	2.2	1.42	5.39	300.56	11.1	70.3	1.15E+06	3.21E+00	1.79E+02
Au1Li3S2	280535	72	2.2	2.355	1.66	9.79	9.3	48.7	1.28E+06	3.73E+01	2.20E+02
Al1Be1La3S7	606164	173	2.2	2.233	2.09	12.31	17.3	63.4	1.54E+06	4.39E+01	2.59E+02
K4O4Sn1	158	2	2.2	2.34	0.24	35.03	8.1	74.5	1.89E+06	3.12E+00	4.55E+02
Ga2S4Sr1	635274	66	2.2	2.69	3.99	33.18	9.9	47.6	1.41E+06	1.46E+02	1.21E+03
K2O2Zn1	34603	72	2.2	2.01	0.2	119.52	16.7	56.4	1.27E+06	2.44E+00	1.46E+03
Ga2K6O6	2269	12	2.2	2.65	0.15	62.48	9.7	74.2	2.15E+06	8.46E+00	3.54E+03
Ge1K1Na1O3	30910	33	2.2	3.03	0.24	103.47	9.6	96.8	3.47E+06	3.70E+01	1.60E+04
Mo2S3	62486	11	2.1	0.93	5.82	3.96	278.9	55.7	7.46E+05	1.04E+01	7.10E+00
Be1La3S7Sc1	616309	173	2.1	1.394	1.96	11.55	18.8	60.7	1.02E+06	2.68E+00	1.58E+01
Ba1La2S5Zn1	93711	140	2.1	1.74	13.52	12.5	22.5	44.5	9.54E+05	7.50E+01	6.93E+01
K6Mg1O4	2340	186	2.1	1.71	0.48	35.84	10.1	54	1.08E+06	1.05E+00	7.87E+01
S4Sn1Sr2	413024	40	2.1	2.47	1.98	22.41	12.3	42.4	1.19E+06	5.44E+01	6.15E+02
Na6S4Zn1	33236	186	2.1	2.16	1.6	167.61	9.5	36.2	9.62E+05	1.90E+01	1.99E+03
S3Sr2Zn1	421354	33	2.1	2.43	4.65	51.05	13.7	39.2	1.11E+06	1.94E+02	2.13E+03
S3Sr2Zn1	422028	62	2.1	2.43	4.65	51.36	13.7	39.2	1.11E+06	1.94E+02	2.15E+03

Ge1K4O4	37271	2	2.1	2.82	0.18	79.11	8.2	81.4	2.56E+06	7.23E+00	3.18E+03
K2O3Zr1	16264	62	2.1	3.61	0.82	52.27	9.2	87	3.81E+06	1.62E+02	1.03E+04
K6O7Ti2	67396	14	2.1	3.4	0.3	37.41	18.9	97.1	4.08E+06	8.53E+01	1.07E+04
Ge1O1Sr3	413385	62	2	0.44	38.26	61.32	47	41.9	4.75E+05	1.44E-02	2.31E-02
O1Sn1	20624	31	2	0.4	1.69	70.52	18.3	53.5	5.01E+05	1.28E-03	5.33E-02
Hg4S6Si1	95227	9	2	0.45	2.32	715.73	26.8	64.8	5.64E+05	5.90E-04	1.82E-01
S4Ba1Ag2Sn1	41898	23	2	0.63	37.39	235.56	12.3	41.4	5.39E+05	2.88E-01	1.82E+00
Na1S1	644958	194	2	1.23	0.73	21.66	8.3	53.8	8.61E+05	1.10E-01	3.26E+00
Na2S2	43407	194	2	1.23	0.73	21.66	8.3	53.8	8.61E+05	1.10E-01	3.26E+00
K2O3Pb1	15929	193	2	1.16	0.41	126.63	12.6	55.4	8.46E+05	1.24E-01	3.85E+01
Ba5Hf4S13	71936	69	2	1	6.99	91.82	61.3	49.8	7.29E+05	4.26E+00	5.59E+01
Al1Cd1La3S7	606339	173	2	2.38	1.15	1.73	18.4	55.2	1.44E+06	3.76E+01	5.67E+01
Ba6Hf5S16	71935	69	2	0.98	9.35	106.11	66.3	50.5	7.27E+05	5.46E+00	6.20E+01
Cd1K6O4	62053	186	2	1.63	0.23	64.84	11	50.7	9.99E+05	4.67E-01	1.32E+02
S2Bi1Rb1	52735	166	2	1.35	0.53	60.95	46.7	29.9	6.54E+05	1.49E+00	1.71E+02
Ga1In1S3	62929	169	2	2.06	0.51	210.24	10.3	44.2	1.07E+06	3.94E+00	1.63E+03
K1Na1O1	32743	129	2	2.16	0.42	122.93	15.9	38.8	1.01E+06	6.65E+00	1.95E+03
Ba1Ge1O3	23925	19	2	3.51	0.67	97.72	12	92.9	4.01E+06	1.47E+02	2.14E+04
K2S3Ti1	72377	15	1.9	1.54	3.19	0.56	12.2	56.3	1.03E+06	5.14E+00	9.04E-01
As1S2Li1	419061	9	1.9	1.06	12.81	3.92	16.6	48.2	7.40E+05	3.00E+00	9.19E-01
Ba1S2	42134	15	1.9	1.58	3.7	5.26	10.4	56	1.05E+06	5.93E+00	8.46E+00
Au1Li1S1	280534	70	1.9	1.955	4.51	4.68	10	41	9.78E+05	2.68E+01	2.78E+01
Au1Li1S1	165259	15	1.9	1.956	4.51	4.68	10	41	9.78E+05	2.69E+01	2.79E+01
In2Pb1S4	100687	62	1.9	1.42	4.35	7.58	50.8	37.9	7.62E+05	1.79E+01	3.12E+01
K4O4Pb1	37268	2	1.9	1.69	0.18	16.83	8.3	65.7	1.25E+06	3.43E-01	3.21E+01
Be1In1La3S7	616297	173	1.9	1.686	1.86	10.95	18.3	58.1	1.13E+06	7.72E+00	4.53E+01
Bi2Ga2In4S12	410032	11	1.9	1.803	1.28	7.53	22.6	45.7	9.96E+05	9.78E+00	5.76E+01
K1Li1S1	47229	129	1.9	3.065	3.32	3.45	8.6	49	1.63E+06	2.30E+02	2.39E+02
B2S6Sr3	412879	15	1.9	2.312	0.52	17.41	10.2	106.6	2.78E+06	7.94E+00	2.66E+02

Na2S2Zn1	33235	72	1.9	2.37	1.8	208.65	14.3	37.5	1.05E+06	6.48E+01	7.50E+03
S2Ba1Cu2	615832	139	1.8	0.73	9.9	40.41	28.2	34.2	5.30E+05	1.01E-01	4.10E-01
Na2S4	2586	122	1.8	2	0.36	0.32	9.4	56.5	1.27E+06	2.12E+00	1.88E+00
B1Ba1Li1S3	82352	14	1.8	2.164	3.91	4.07	12.8	103.8	2.49E+06	6.36E+01	6.62E+01
Sb1S2Br1Cd1	171723	12	1.8	1.53	4.21	14.17	42.9	39	8.08E+05	2.29E+01	7.72E+01
Ge2Na6S7	25388	15	1.8	2.43	0.53	33.54	11.1	48.1	1.30E+06	1.18E+01	7.50E+02
K1N3	34270	140	1.8	3.96	2.58	1.53	6.3	267	3.76E+07	1.93E+03	1.15E+03
In2Na6S6	300165	15	1.8	2.28	0.41	63.42	10.8	40.4	1.08E+06	8.31E+00	1.29E+03
Al2O6Rb6	74969	12	1.8	2.69	0.22	74.85	10.4	87.2	2.62E+06	1.50E+01	5.11E+03
K4O18Si8	2155	2	1.8	4.4	0.18	19.87	5.2	143.1	1.19E+07	6.54E+01	7.22E+03
C2K2	89528	142	1.8	3.237	0.17	1.52	5.7	228	1.64E+07	3.20E+03	2.82E+04
Ba3S5Ti1	203087	140	1.7	1.38	7.4	1.79	36.5	56	9.53E+05	1.17E+01	2.82E+00
Hg6O7Si2	69123	12	1.7	1.39	1.3	3.81	12.7	134.6	2.03E+06	1.18E+00	3.46E+00
Ge1S1	38165	62	1.7	1.19	1.8	33.11	19.6	40	7.12E+05	5.01E-01	9.19E+00
O1Rb2	180572	225	1.7	1.33	0.17	37.7	11.1	18.9	5.32E+05	1.04E-01	2.29E+01
Cd1O2Rb2	62054	60	1.7	1.32	0.22	109.26	11.2	49.8	8.58E+05	1.29E-01	6.38E+01
P1K1S4Ag2	420033	121	1.7	1.54	48.09	126.98	9.9	62.5	1.12E+06	6.24E+01	1.65E+02
Na4S8Sn3	42031	15	1.7	1.63	0.3	73.49	13.4	43.8	9.05E+05	7.43E-01	1.82E+02
B3Na3S6	79613	167	1.7	2.546	0.37	6.05	12.4	116.8	3.53E+06	1.23E+01	2.01E+02
Ba2S3Zn1	653999	62	1.7	2.02	4.16	18.42	14.5	37.5	9.41E+05	4.57E+01	2.02E+02
B3Li1S6Sr1	79616	9	1.7	2.896	0.84	4.94	7.5	114.8	4.12E+06	3.62E+01	2.13E+02
In1Na5S4	300175	11	1.7	2.02	1.78	107.23	10.7	36.9	9.31E+05	1.44E+01	8.68E+02
Ba2Cd1S3	66654	62	1.7	2.09	3.6	97.26	14.6	35	9.20E+05	5.15E+01	1.39E+03
Ge1O3Pb1	172521	148	1.7	2.67	3.48	26.91	14.9	98	2.99E+06	1.84E+02	1.42E+03
K1Na1S1	62658	62	1.7	2.5	0.88	98.05	9.1	27.3	8.80E+05	3.01E+01	3.36E+03
O7Rb6Si2	411664	14	1.7	3.19	0.48	102.28	9	111	4.51E+06	1.01E+02	2.17E+04
C2Pt1Rb2	94395	164	1.7	1.461	0.79	36.18	14.1	229.4	4.17E+06	5.94E+02	2.72E+04
In6S7	640348	11	1.6	0.28	37.33	52.67	80.3	36.9	4.02E+05	8.01E-04	1.13E-03
Ba2S3	70058	109	1.6	1.6	3.98	1.98	15.7	58.6	1.10E+06	1.04E+01	5.14E+00

Ba2Bi1In1S5	261678	36	1.6	1.444	4.52	4.69	28.4	40.3	7.97E+05	1.15E+01	1.19E+01
Be1La3S7Sb1	616308	173	1.6	1.612	4.24	4.41	18.7	57.6	1.09E+06	1.38E+01	1.43E+01
Au1K1Na2O2	61226	58	1.6	2.14	0.2	1.83	9	70.1	1.63E+06	1.70E+00	1.55E+01
K3S4Sb1	41895	217	1.6	2.134	1.77	1.84	9.4	43	1.08E+06	1.54E+01	1.61E+01
O4Pb3	36253	135	1.6	1.12	1.15	58.2	16.8	65.6	9.22E+05	3.77E-01	1.91E+01
O4Pb3	29094	117	1.6	1.12	1.14	59.14	16.7	65.6	9.22E+05	3.74E-01	1.94E+01
O4Pb3	4107	55	1.6	1.2	0.87	43.09	16.7	65.6	9.66E+05	4.31E-01	2.13E+01
In7Rb1S9	412056	59	1.6	1.624	1.28	7.52	19.5	41.2	8.67E+05	4.51E+00	2.65E+01
Hg1K2O2	27410	139	1.6	2.05	0.24	4.61	6.9	72.3	1.61E+06	1.40E+00	2.69E+01
B6S12Sr3	412878	148	1.6	2.976	0.89	5.26	9.9	115.2	4.30E+06	5.96E+01	3.52E+02
Na6S7Sn2	25389	15	1.6	2.09	0.25	42.78	10.8	44.1	1.08E+06	2.21E+00	3.77E+02
Na6S7Sn2	16242	15	1.6	2.09	0.25	41.98	10.8	44.1	1.08E+06	2.64E+00	4.43E+02
O3Rb2Ti1	6101	64	1.6	3.91	0.25	1.76	9.2	102.3	5.42E+06	7.94E+01	5.61E+02
In5Rb1S8	40877	12	1.6	1.32	2.87	405.64	29.1	41.2	7.66E+05	4.38E+00	6.18E+02
Al4Ba1S7	33237	31	1.6	3.16	1.21	9.91	14.2	66	2.29E+06	1.67E+02	1.37E+03
Ga2O6Rb6	2270	12	1.6	2.44	0.15	72.37	10.8	72.1	1.91E+06	5.10E+00	2.46E+03
C2Pd1Rb2	421494	164	1.6	1.867	0.41	19.54	12	228.9	6.01E+06	7.79E+02	3.74E+04
C2Ag1Cs1	410873	131	1.6	2.886	7.71	19.22	6	245.5	1.51E+07	1.16E+05	2.89E+05
Hg1O2	24774	61	1.5	0.18	3.44	23.76	11.1	104.8	4.79E+05	1.32E-05	9.12E-05
Sr3N1Sb1	152052	221	1.5	0.26	52.15	56.34	45.6	28.6	3.73E+05	3.65E-04	3.94E-04
Sb1S2Na1	71091	15	1.5	0.94	19.5	5.47	27.4	37.8	6.16E+05	3.66E+00	1.03E+00
Na1S2Sb1	71091	15	1.5	0.937	0.49	8.01	27.4	37.9	6.15E+05	9.04E-02	1.48E+00
Ge1Hg2O4	26340	70	1.5	0.93	0.22	61.95	12.5	88.5	9.97E+05	6.12E-03	1.72E+00
Na2S5	38349	62	1.5	1.75	0.56	1.04	7.2	59.4	1.19E+06	1.04E+00	1.93E+00
K2S2Pd1	641296	71	1.5	1.37	1.54	3.32	9.9	37.6	7.43E+05	9.93E-01	2.15E+00
K2S2	43406	189	1.5	1.47	0.58	5.4	6.1	57.7	1.02E+06	3.55E-01	3.31E+00
Au1O1Rb1	409552	139	1.5	1.64	0.17	7.06	7	62.1	1.17E+06	2.28E-01	9.49E+00
Ba1S3	23637	113	1.5	1.37	3.04	15.43	13.7	55.6	9.45E+05	2.71E+00	1.38E+01
Cs1In7S9	409385	59	1.5	1.589	1.28	7.54	16.4	40.5	8.46E+05	3.35E+00	1.97E+01

S2Y1	52216	227	1.5	1.4	8.42	58.27	9.5	42.5	8.08E+05	5.96E+00	4.13E+01
K2S5Sn2	73007	15	1.5	1.41	2.55	56.06	13.1	41.6	8.00E+05	2.59E+00	5.69E+01
Ge1K3S3	636776	12	1.5	2.4	1.78	3.54	9.7	46.4	1.25E+06	3.24E+01	6.45E+01
Ge2K6S6	47111	12	1.5	2.4	1.76	3.58	9.7	46.4	1.25E+06	3.21E+01	6.53E+01
Ba2Hg1S3	32647	62	1.5	1.36	2.25	100.29	18	33.6	6.96E+05	1.57E+00	6.99E+01
K1S4Si1Y1	602576	4	1.5	3.07	0.68	0.9	10	67.4	2.27E+06	5.58E+01	7.35E+01
Ba2S4Ti1	616084	62	1.5	2.07	6.73	7.88	20.4	57.8	1.33E+06	1.25E+02	1.46E+02
Na3S3Sb1	644966	198	1.5	2.402	0.33	10.82	13.9	41.6	1.15E+06	8.60E+00	2.82E+02
B4Ba7S13	170284	15	1.5	2.535	0.69	11.12	11.2	105.1	3.06E+06	2.01E+01	3.24E+02
Al4Bi2S8	408439	126	1.5	2.661	0.43	6.99	13.7	63	1.82E+06	2.04E+01	3.32E+02
O4Rb4Sn1	280293	2	1.5	2.17	0.19	37.63	9.1	72.8	1.71E+06	1.78E+00	3.53E+02
Ba3Ga2S6	201421	15	1.5	2.68	1.58	5.89	13.5	43.5	1.30E+06	1.35E+02	5.04E+02
Na4S4Sn1	42035	114	1.5	2.08	1.32	64.68	8.9	40.8	1.02E+06	1.11E+01	5.45E+02
B1Cs1Li2S3	411530	62	1.5	3.094	0.46	7.45	8.8	106.7	4.08E+06	3.46E+01	5.60E+02
Ge1Na2S3	653637	14	1.5	2.46	1.63	20.02	9.2	50.5	1.37E+06	5.00E+01	6.14E+02
Na1O1Rb1	61092	129	1.5	2.03	0.54	141.13	15.8	35	9.02E+05	5.87E+00	1.54E+03
Au1N1Sr2	95826	63	1.4	0.01	17.67	18.13	38.8	48.7	2.72E+05	7.29E-12	7.50E-12
Ba3Ge1O1	50512	62	1.4	0.39	5.69	8.8	42.2	34.4	4.31E+05	7.79E-04	1.20E-03
In2S7Sn3	68366	11	1.4	0.51	4.04	20.77	58.3	37.1	4.79E+05	4.16E-02	2.14E-01
K2O3Sn2	40463	199	1.4	1.27	135.43	4.15	10.2	74.7	1.11E+06	5.76E+01	1.76E+00
Li1S2Sb1	40457	148	1.4	1.222	2.42	2.51	24.3	42.3	7.44E+05	1.94E+00	2.01E+00
Cs1In3S5	412365	10	1.4	1.226	3.77	3.92	48.9	40.1	7.25E+05	3.27E+00	3.40E+00
Cs1In5S8	40878	12	1.4	1.326	3.92	4.08	24.7	40.2	7.57E+05	5.21E+00	5.42E+00
Ba1Hg1S2	32648	26	1.4	1.16	3.29	31.75	16.1	41.9	7.20E+05	1.28E+00	1.24E+01
Ge1K1S4Y1	603205	4	1.4	2.57	1.01	0.39	10.7	49.8	1.41E+06	5.01E+01	1.93E+01
Ba4In2S8	261680	2	1.4	1.94	3.56	3.16	12.8	58.1	1.27E+06	2.40E+01	2.13E+01
O3Pb1Rb2	62139	62	1.4	1.28	0.3	52.24	10.7	69	1.05E+06	1.40E-01	2.43E+01
Cu1O2Rb3	65446	14	1.4	1.72	0.25	11.14	9.2	71.7	1.37E+06	5.90E-01	2.63E+01
B2K2S7	401097	15	1.4	2.512	0.6	3.51	6.9	90.9	2.54E+06	1.01E+01	5.95E+01

Rb2S1	29208	225	1.4	1.97	0.12	18.03	6.6	16.6	5.93E+05	4.55E-01	6.83E+01
Hg1K6S4	660294	186	1.4	1.72	0.9	39.02	9	30	7.44E+05	1.83E+00	7.94E+01
B2Na2S5	401724	62	1.4	2.543	0.48	2.85	8.3	118.3	3.59E+06	1.70E+01	1.01E+02
In3Rb1S5	59667	10	1.4	1.22	3.72	124.04	48.8	40.6	7.27E+05	3.10E+00	1.04E+02
B1K3S3	411607	14	1.4	2.742	0.36	5.88	8.1	100.7	3.21E+06	1.21E+01	1.99E+02
B2Ba1S4	412516	9	1.4	2.71	0.99	5.85	9.8	109.9	3.54E+06	3.74E+01	2.21E+02
Ba1Hg1S4Sn1	10456	34	1.4	1.85	2.41	54.96	12.5	44.6	9.98E+05	1.18E+01	2.70E+02
Au1Na3S2	202329	167	1.4	2.35	1.22	22.23	8.1	42.6	1.15E+06	1.64E+01	2.99E+02
B3Ba1Li1S6	82353	9	1.4	2.811	0.26	8.63	7.2	114.6	3.94E+06	9.04E+00	2.99E+02
Ba1Cd1S2	66655	62	1.4	1.74	2.03	106.93	16.6	38.1	8.63E+05	8.31E+00	4.39E+02
Ba1Ga4S7	33238	31	1.4	2.6	1.05	19.87	15	49.7	1.42E+06	4.76E+01	8.97E+02
Ba2S4Si1	616062	62	1.4	3	1.91	6.51	17.1	66.3	2.17E+06	4.85E+02	1.65E+03
Rb2S4Zn3	602243	72	1.4	2.59	0.64	131.93	11	39.3	1.17E+06	2.08E+01	4.29E+03
C2Cs2Pt1	94397	164	1.4	1.561	1.22	52.7	13.4	226.8	4.51E+06	1.10E+03	4.76E+04
Bi2Pb3S6	92981	12	1.3	0.579	4.33	4.5	113.7	33.5	4.83E+05	3.11E-02	3.23E-02
O2Rb2	25528	71	1.3	1.81	0.51	5.87	6.3	100.8	1.98E+06	1.12E+00	1.29E+01
K6O5Pb2	74873	2	1.3	2.15	0.32	1.61	9.2	57.5	1.37E+06	2.85E+00	1.43E+01
Hg1O2Rb2	66276	139	1.3	1.99	0.47	4.46	7.4	72.1	1.56E+06	2.36E+00	2.24E+01
AuNa2O2Rb1	411460	58	1.3	2.16	0.12	3.61	10.2	69.8	1.64E+06	1.21E+00	3.66E+01
Li1Rb1S1	67254	129	1.3	2.749	2.82	2.93	8.8	47.4	1.43E+06	1.05E+02	1.09E+02
B3K3S6	79614	167	1.3	2.753	0.3	4.88	7.4	115.3	3.86E+06	9.49E+00	1.54E+02
S2Bi2Ag1Cl3	413938	12	1.3	1.37	1.51	46.39	73	33.4	6.97E+05	7.21E+00	2.21E+02
Ba2Ge1S4	25365	62	1.3	2.29	2.36	7.44	23.1	49.5	1.27E+06	7.72E+01	2.43E+02
Cs2S4Zn3	53242	72	1.3	2.718	3.22	3.35	10.5	38.4	1.19E+06	2.40E+02	2.49E+02
Ba2Bi1Ga1S5	261677	62	1.3	2.33	0.23	20.91	15.2	45.2	1.20E+06	5.49E+00	4.99E+02
N3Rb1	34272	140	1.3	4	1.98	1.34	6.2	266	3.82E+07	1.58E+03	1.07E+03
Ga2K6S6	300169	14	1.3	2.72	0.31	42.39	10.6	42.9	1.30E+06	1.30E+01	1.78E+03
C2Cs2Pd1	94396	164	1.3	2.004	0.83	11.86	13.9	227.7	6.69E+06	2.53E+03	3.62E+04
C2Cs1Na1	189824	57	1.3	3.29	0.22	3.51	8.5	228.3	1.71E+07	6.91E+03	1.10E+05

O7Pb4Rb2	35415	2	1.2	1	1.52	4.51	12	63.5	8.40E+05	1.82E-01	5.39E-01
K2S3	1263	36	1.2	1.29	0.47	2.71	8	55.5	9.06E+05	1.72E-01	9.93E-01
K2S2Pt1	26258	71	1.2	1.59	1.73	3.44	9.5	41	8.54E+05	2.63E+00	5.22E+00
Cs2S3Ti1	49739	36	1.2	1.596	2.65	2.75	11.7	53.8	1.03E+06	5.07E+00	5.26E+00
Bi2Hg1S4	14189	12	1.2	1.218	2.39	2.49	194.3	41.1	7.31E+05	7.87E+00	8.16E+00
Pb1S3Zr1	648497	62	1.2	1.51	3.49	3.29	22.8	40.6	8.22E+05	9.34E+00	8.75E+00
K1La1S4Si1	603184	4	1.2	2.79	0.35	0.15	11.1	66.8	2.02E+06	3.34E+01	1.43E+01
Ba1S2Sn1	2587	14	1.2	1.59	19.06	6.65	16.7	33.7	7.59E+05	5.07E+01	1.77E+01
B18Rb8S18	98521	2	1.2	3.097	1.35	1.4	7.8	123.1	5.03E+06	9.04E+01	9.41E+01
K3S3Sb1	641323	198	1.2	2.688	0.23	7.54	9.7	41.3	1.25E+06	8.24E+00	2.69E+02
Bi2Ga4S8	408441	126	1.2	2.544	0.15	13.4	15.4	47	1.33E+06	6.12E+00	5.46E+02
B1Ba1S4Sb1	248221	62	1.2	2.362	0.15	13.89	26.9	110.6	2.99E+06	6.88E+00	6.37E+02
K1Rb1S1	72326	62	1.2	2.22	1.24	49.23	9.7	23.3	7.44E+05	1.85E+01	7.35E+02
Na1Rb1S1	68489	129	1.2	2.3	0.6	90.02	9.2	26.9	8.26E+05	8.01E+00	1.21E+03
C2Rb2	51532	62	1.2	3.506	0.25	1.13	8.4	226.6	1.92E+07	1.11E+04	4.96E+04
O3Rb1	47164	14	1.1	0.17	0.06	0.1	7.7	131.4	5.08E+05	1.15E-07	1.90E-07
Cs2Hg6S7	260060	102	1.1	0.628	3.28	3.41	25.3	41.8	5.41E+05	5.09E-02	5.29E-02
Au2Ba1S4Sn1	2489	18	1.1	1.059	2.94	3.06	13	40.9	6.77E+05	2.26E-01	2.35E-01
Pb1S3Sn1	23462	62	1.1	1.03	4.22	3.46	23.7	37.4	6.39E+05	1.18E+00	9.71E-01
Rb2S2	73176	189	1.1	1.56	0.29	5.01	6.3	57.8	1.06E+06	2.59E-01	4.47E+00
S2Rb2Pt1	26259	71	1.1	1.59	2.41	3.56	9.3	40.5	8.47E+05	3.57E+00	5.26E+00
K2Mo3O10	24118	15	1.1	3.21	0.07	0.1	10.1	118.8	5.03E+06	7.50E+00	1.07E+01
Ge1K1La1S4	73970	4	1.1	2.51	0.76	0.48	10	48.9	1.36E+06	1.87E+01	1.18E+01
K2O2Pb1	2266	2	1.1	1.92	0.18	4.21	8.5	59.1	1.27E+06	7.87E-01	1.85E+01
Bi2O3	168810	160	1.1	2.34	0.06	0.93	17.9	76.5	1.94E+06	1.73E+00	2.68E+01
Ge2Hg3K2S8	281506	5	1.1	1.52	8.46	23.32	11.3	48.5	9.25E+05	1.16E+01	3.21E+01
B1Rb1S3	73084	14	1.1	2.296	0.58	3.43	8.2	90.9	2.29E+06	6.87E+00	4.07E+01
Cs1Ga3S5	419821	14	1.1	2.652	1.77	1.84	8.5	49.4	1.44E+06	5.13E+01	5.34E+01
B1Rb3S3	411609	14	1.1	2.558	1.74	1.81	7.8	99.1	2.88E+06	6.04E+01	6.29E+01

Ge1Pb2S4	16272	14	1.1	2.05	2.58	4.71	25.1	47.8	1.13E+06	4.71E+01	8.60E+01
B3Rb3S6	79615	167	1.1	2.824	0.48	2.84	7.4	114.6	3.97E+06	1.76E+01	1.04E+02
Au4Cd1K2S4	85583	72	1.1	2.16	3.46	12.97	9.9	40.8	1.05E+06	3.43E+01	1.29E+02
Ba2S4Sn1	42036	14	1.1	1.93	0.39	24.78	14.8	43.6	1.01E+06	3.11E+00	1.98E+02
C1Ba1Si1	168411	62	1.1	0.982	2.14	4.76	18.9	134.6	1.45E+06	9.04E+01	2.01E+02
S3Sn1Zr1	73711	62	1	1.22	1.53	1.27	19.2	40.4	7.25E+05	9.63E-01	7.94E-01
O3Rb2Sn2	24816	166	1	1.21	66.87	12.08	12.1	79.7	1.12E+06	1.31E+01	2.36E+00
K2O3Pb2	1412	199	1	1.68	52.83	2.83	10.9	66.4	1.26E+06	1.28E+02	6.86E+00
Sb1K1S2	60138	15	1	1.59	6.61	2.77	17	40.3	8.45E+05	1.79E+01	7.50E+00
Ge2K2Pb1S6	170601	15	1	2.15	0.41	0.57	14.2	50.5	1.23E+06	5.65E+00	7.87E+00
Bi2Pb1S4	31859	62	1	1.05	1.15	6.74	97.4	35	6.25E+05	1.49E+00	8.75E+00
K2S7Sb4	25329	15	1	1.551	0.6	3.54	18.9	40.9	8.39E+05	1.56E+00	9.19E+00
In1S3Sb1	300207	62	1	1.508	0.6	3.53	28.4	39.7	8.10E+05	1.98E+00	1.16E+01
Ge2Rb4S6	409729	12	1	2.33	0.12	0.95	8.6	50.8	1.32E+06	1.62E+00	1.28E+01
K1S2Sb1	60138	15	1	1.586	0.3	4.9	17	40.3	8.44E+05	8.01E-01	1.31E+01
O2Rb2Sn1	24805	19	1	2.24	0.64	0.84	10.3	70.8	1.72E+06	1.09E+01	1.43E+01
Bi3Cs1S5	200794	62	1	1.426	0.93	8.18	39.1	36.4	7.46E+05	3.02E+00	2.65E+01
Hf1Pb1S3	65668	62	1	1.7	4.64	7.24	20.7	39.3	8.67E+05	2.29E+01	3.57E+01
I1S1Ag3	174095	146	1	0.91	1.13	483.93	14.7	28.9	5.41E+05	9.34E-02	4.01E+01
Ge2Hg3K2S8	281504	41	1	1.52	7.52	35.37	11.3	49.6	9.38E+05	1.03E+01	4.86E+01
Cs1Na1S1	41323	129	1	2.418	2.51	2.61	10.1	25.7	8.29E+05	4.96E+01	5.15E+01
Hg1Rb6S4	639158	186	1	1.61	0.3	33.23	9.3	28	6.92E+05	4.79E-01	5.31E+01
Bi1Rb1S4Si1	281166	14	1	2.049	0.62	3.63	23.8	66	1.48E+06	1.07E+01	6.28E+01
O3Pb1Ti1	61169	99	1	1.99	19.14	1.06	99.8	72.2	1.56E+06	1.17E+03	6.46E+01
Rb4S6Si2	409804	12	1	2.83	0.1	1.66	8.1	69.8	2.16E+06	4.04E+00	6.72E+01
B18Cs8S18	98522	2	1	3.127	1.25	1.3	7.4	122.8	5.08E+06	8.46E+01	8.82E+01
Bi1K1S4Si1	421485	14	1	2.033	0.6	7.56	25.4	66.2	1.47E+06	1.06E+01	1.33E+02
Ge1O5Pb3	100275	4	1	2.32	0.65	8.16	19.5	86.9	2.20E+06	1.94E+01	2.44E+02
In2Rb6S6	23252	12	1	2.28	0.23	32.16	8.6	39	1.05E+06	2.71E+00	3.79E+02

In2Rb4S5	23253	2	1	2.11	0.17	31.79	32	40.8	1.03E+06	4.71E+00	8.82E+02
C2Cs1Rb1	189823	62	1	3.364	0.24	2.33	9.5	225.8	1.75E+07	9.12E+03	8.68E+04
Au1N12Rb1	416488	15	0.9	1.47	0.08	0.11	5.7	269.3	5.33E+06	4.58E-02	6.29E-02
S7Sb4Sn1	169941	11	0.9	0.704	1.33	1.39	51.3	41	5.62E+05	8.31E-02	8.68E-02
S3Sn2	656782	62	0.9	0.73	3.26	3.02	19.2	37.4	5.49E+05	9.49E-02	8.75E-02
Au1K3O1	79086	221	0.9	0.62	0.2	21.12	13.5	26.9	4.60E+05	1.54E-03	1.63E-01
Hg1O1	15890	62	0.9	1.08	1.67	1.58	10.2	69.5	9.35E+05	2.68E-01	2.54E-01
S5Sb2Sn2	35641	62	0.9	0.727	0.31	5.05	111.5	41	5.69E+05	5.10E-02	8.31E-01
Rb2S3	14092	36	0.9	1.33	0.16	2.15	7.7	55.8	9.28E+05	6.76E-02	9.12E-01
Au1O2Rb1	15116	63	0.9	1.66	0.3	0.69	6.5	70.3	1.30E+06	4.01E-01	9.19E-01
S4Pd3Rb2	41886	12	0.9	1.46	1.33	1.04	11	42.1	8.23E+05	1.40E+00	1.10E+00
O4Pb3	97282	55	0.9	0.94	28.02	12.52	24.1	59.3	7.77E+05	4.63E+00	2.07E+00
Hf1S3Sn1	65667	62	0.9	1.42	1.83	1.85	16.9	39.3	7.77E+05	2.50E+00	2.53E+00
S3Sb2	95557	62	0.9	1.296	0.48	2.84	57.2	41.2	7.58E+05	1.29E+00	7.65E+00
Rb3S4Sb1	402363	62	0.9	2.023	1.44	1.49	9	46.5	1.10E+06	9.93E+00	1.03E+01
O2Pb1Rb2	2267	2	0.9	1.89	0.17	3.67	8.7	58.4	1.24E+06	6.78E-01	1.46E+01
Bi2In4S9	2839	11	0.9	1.663	0.6	3.52	26.4	41.3	8.82E+05	3.31E+00	1.94E+01
Hg3Rb2S8Sn2	85599	14	0.9	1.69	0.17	15.4	11.5	44.6	9.39E+05	4.50E-01	4.07E+01
Au2Cd2Rb2S4	85582	54	0.9	2.05	6.49	9.99	10.1	40.1	9.96E+05	4.79E+01	7.35E+01
B1Cs3S3	391170	14	0.9	2.523	0.51	2.98	8.7	97.7	2.78E+06	1.79E+01	1.04E+02
B2Cs2S4	78745	142	0.9	2.773	0.44	2.57	7.2	128.3	4.54E+06	2.60E+01	1.51E+02
Au1O1Rb3	79087	221	0.8	0.25	0.39	23.94	21.2	19.6	3.44E+05	2.04E-05	1.26E-03
P2S6Rb2	416176	71	0.8	1.8	0.61	0.16	7.3	79.8	1.56E+06	1.50E+00	3.93E-01
Au3O2Rb5	91308	55	0.8	0.96	0.64	7.87	9.8	62.7	8.13E+05	4.90E-02	6.02E-01
Rb2S5	100321	19	0.8	1.96	0.16	0.27	7.4	61.1	1.33E+06	6.63E-01	1.12E+00
S4Br2Bi3Ag1	413939	12	0.8	0.73	9.55	6.8	120.5	37.5	5.50E+05	1.74E+00	1.24E+00
Au1K1S5	402875	72	0.8	1.78	0.69	0.55	8.4	55.3	1.14E+06	1.82E+00	1.46E+00
Au1K1S5	84000	72	0.8	1.78	0.66	0.56	8.4	55.3	1.14E+06	1.74E+00	1.48E+00
Cs2S6Sn2	73008	2	0.8	1.71	1.38	1.43	9.7	55.5	1.11E+06	3.28E+00	3.40E+00

Ge1Pb1S3	2090	14	0.8	1.8	3.5	1.08	18.3	49.3	1.05E+06	2.15E+01	6.64E+00
Cs1S2Sb1	200798	14	0.8	1.698	1.45	1.51	20.9	44.9	9.45E+05	7.15E+00	7.43E+00
Rb1S2Sb1	56788	2	0.8	1.941	0.26	0.68	25.8	41.5	9.82E+05	3.52E+00	9.19E+00
Rb1S2Sb1	200263	1	0.8	1.939	0.26	0.7	25.8	41.5	9.81E+05	3.51E+00	9.41E+00
Cs3S4Sb1	409619	62	0.8	2.127	1.33	1.38	9.2	46.2	1.14E+06	1.36E+01	1.41E+01
Cs4Ge2S8	281352	12	0.8	2.34	1.24	1.29	7.9	57.7	1.48E+06	1.58E+01	1.65E+01
Cs2S1	183207	62	0.8	2.09	1.44	1.5	12.5	20.5	6.74E+05	1.76E+01	1.84E+01
Bi1Ge1K1S4	421486	14	0.8	1.931	0.43	2.51	23	49	1.10E+06	5.04E+00	2.94E+01
Bi1Cs1Ge1S4	281168	14	0.8	1.962	0.48	2.82	19.9	48.4	1.11E+06	5.35E+00	3.15E+01
Bi1Ge1Rb1S4	281167	14	0.8	1.938	0.49	2.87	22.3	48.7	1.10E+06	5.69E+00	3.33E+01
Cs4S6Si2	409176	12	0.8	2.944	1.35	0.77	8.6	69.4	2.24E+06	7.43E+01	4.22E+01
Au2Cd2Cs2S4	85581	67	0.8	2.177	1.99	2.07	36.2	38.1	1.00E+06	7.50E+01	7.79E+01
Au6K4S5	202552	190	0.8	1.79	0.29	29.82	9.1	41.5	9.28E+05	8.09E-01	8.31E+01
Pb2S4Si1	16317	14	0.8	2.2	0.47	2.49	32.6	63.8	1.53E+06	1.71E+01	9.04E+01
Cs1Ga1S2	626992	15	0.8	3.064	1.43	1.49	10.1	45.8	1.53E+06	1.17E+02	1.22E+02
Bi1Cs1S4Si1	281169	14	0.8	2.456	0.13	7.4	17.5	67.6	1.80E+06	4.90E+00	2.79E+02
Au5O2Rb7	95825	71	0.7	0.83	0.19	17.15	10.3	65.6	7.66E+05	6.40E-03	5.78E-01
Cs2S3	14094	36	0.7	1.369	1.19	1.24	7.9	56.1	9.50E+05	6.13E-01	6.38E-01
S4Pt3Rb2	26267	69	0.7	1.76	12.46	1.23	10.7	46	9.85E+05	3.90E+01	3.85E+00
Cs2S2	200474	71	0.7	1.729	0.5	2.92	5.8	57.6	1.15E+06	7.65E-01	4.48E+00
Bi1Cs1S2	72975	14	0.7	1.546	1.57	1.63	21.9	37.6	7.97E+05	4.64E+00	4.82E+00
Rb2S7Sb4	2194	2	0.7	1.899	1	1.04	17.8	41.4	9.65E+05	8.16E+00	8.53E+00
In1S1	81339	58	0.7	1.32	6.48	12.64	14.9	39.6	7.49E+05	5.07E+00	9.85E+00
Cs2S5	201073	19	0.7	1.97	0.1	3.48	8.2	61.8	1.35E+06	4.68E-01	1.63E+01
Hg1K1S3Sb1	63623	15	0.7	1.811	0.14	4.75	13.8	43.6	9.68E+05	6.71E-01	2.28E+01
Cs1Ga1S3	281723	14	0.7	2.456	0.33	1.92	11.1	59.3	1.58E+06	7.94E+00	4.60E+01
Au6Rb4S5	82556	190	0.7	1.87	0.22	21.05	8.5	41.5	9.57E+05	7.87E-01	7.57E+01
Al2O11Si4	30119	2	0.7	4.16	0.13	4.55	4.5	137.8	9.97E+06	1.01E+02	3.52E+03
Cd1Ga1In1S4	20785	164	0.6	0.32	0.27	30.48	10.6	52	4.60E+05	3.10E-05	3.49E-03

Cd1Hg1O2	74848	12	0.6	0.52	1.42	7.67	9.4	74.4	6.41E+05	2.65E-03	1.43E-02
In1S1	409645	14	0.6	1.27	6.71	13.36	15	39.6	7.33E+05	4.19E+00	8.31E+00
Au1Rb1S1	71654	63	0.6	2.13	4.89	2.57	11.6	39.3	1.01E+06	5.22E+01	2.74E+01
Au2Cs2S4Sn1	408685	70	0.6	2.151	1.18	9.41	9.1	41.2	1.05E+06	1.04E+01	8.31E+01
S3Ti1	42072	11	0.5	0.59	0.38	0.37	12.7	67.8	6.51E+05	2.03E-03	1.98E-03
S3Zr1	651485	11	0.5	1.41	0.29	0.75	9.2	63.7	1.06E+06	2.08E-01	5.38E-01
Cs2S8Sb4	67976	2	0.5	1.439	0.59	0.62	17.9	57.5	1.00E+06	9.26E-01	9.78E-01
Ge1S3Sn1	637796	14	0.5	1.55	2.74	0.52	15	50.5	9.63E+05	5.61E+00	1.07E+00
Cs1S6Sb1	67977	14	0.5	1.791	0.08	1.29	8.2	58	1.18E+06	2.13E-01	3.43E+00
S1Te2Bi2	26720	148	0.4	0.37	29.76	148.75	56.8	24.5	3.90E+05	3.68E-03	1.84E-02
S2Pd1Cl6	39434	2	0.4	1.98	0.03	0.04	5.4	58.3	1.29E+06	9.63E-02	1.29E-01
Hg2N6	98661	14	0.4	2.14	1.05	0.06	13	273.3	1.03E+07	1.29E+01	7.35E-01
Au1Cs1S1	656712	63	0.4	2.038	0.29	1.73	11	39	9.72E+05	2.24E+00	1.33E+01
S2Ti1	83828	12	0.3	0.43	0.66	0.17	39.7	55.9	5.22E+05	1.66E-03	4.29E-04
S2Ti1	79803	12	0.3	0.42	0.59	0.15	58	47.7	4.89E+05	1.89E-03	4.80E-04
S2Ti1	651214	164	0.3	0.43	0.63	0.18	60.6	47.6	4.93E+05	2.43E-03	6.94E-04
Hf1S3	638846	11	0.3	1.42	0.18	0.42	9.1	63	1.06E+06	1.33E-01	3.10E-01
S2Si1	26858	72	0.3	3.09	0.02	0.2	3.9	75.3	2.60E+06	6.70E-01	6.70E+00
O1Pb1	64778	129	0.3	1.41	0.19	13.32	14.5	48.7	8.83E+05	2.13E-01	1.50E+01
Ga1S1	53587	194	0.3	1.92	0.16	8.71	7.6	43.2	1.00E+06	5.99E-01	3.26E+01
S2Zr1	604434	164	0.2	1.46	0.21	0.2	20.8	40.8	8.08E+05	4.18E-01	3.98E-01
S2Sn1	650993	164	0.2	1.55	0.03	0.32	12.4	41.5	8.47E+05	5.09E-02	5.43E-01
I1Zr1N1	36119	59	0.2	1.83	0.15	0.13	13.1	76.4	1.53E+06	7.24E-01	6.28E-01
Hf1S2	638847	164	0.2	1.69	0.21	0.18	16.9	38.5	8.52E+05	8.16E-01	6.97E-01
B1N1	167799	194	890.9	4.407	21.2	79.28	5.2	167.9	1.65E+07	3.65E+05	1.37E+06
C1Si1	24170	186	235.1	2.23	33.96	606.62	10.54	112.2	2.84E+06	6.01E+03	1.07E+05
C1Si1	15325	186	210.5	2.04	20.41	76.33	10.55	115.2	2.62E+06	2.85E+03	1.07E+05