

Supporting information for:
Edge, Size, and Shape Effects on WS_2 , WSe_2 ,
and WTe_2 Nanoflake Stability: Design
Principles from an Ab Initio Investigation

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Methodology

Binding energies and stability function

As defined in Refs. ? and ? , the method we used to calculate the binding energies of our nanoflakes is expressed in the following equation:

$$\Delta^2 E((WQ_2)_n) = E_{tot}^{((WQ_2)_{n-1})} + E_{tot}^{((WQ_2)_{n+1})} - 2E_{tot}^{((WQ_2)_n)} , \quad (1)$$

where each term in the right hand is the total energy of the cluster at each of its respective size. For the calculation of the binding energies, in accordance to Ref. ?

$$E_b^i = E_{tot}^i/n - E_{tot}^W - 2E_{tot}^Q , \quad (2)$$

where each term in the right hand is the total energy of the i -th cluster per formula unit and the isolated atoms of the elements composing our systems.

Results

Convergence tests

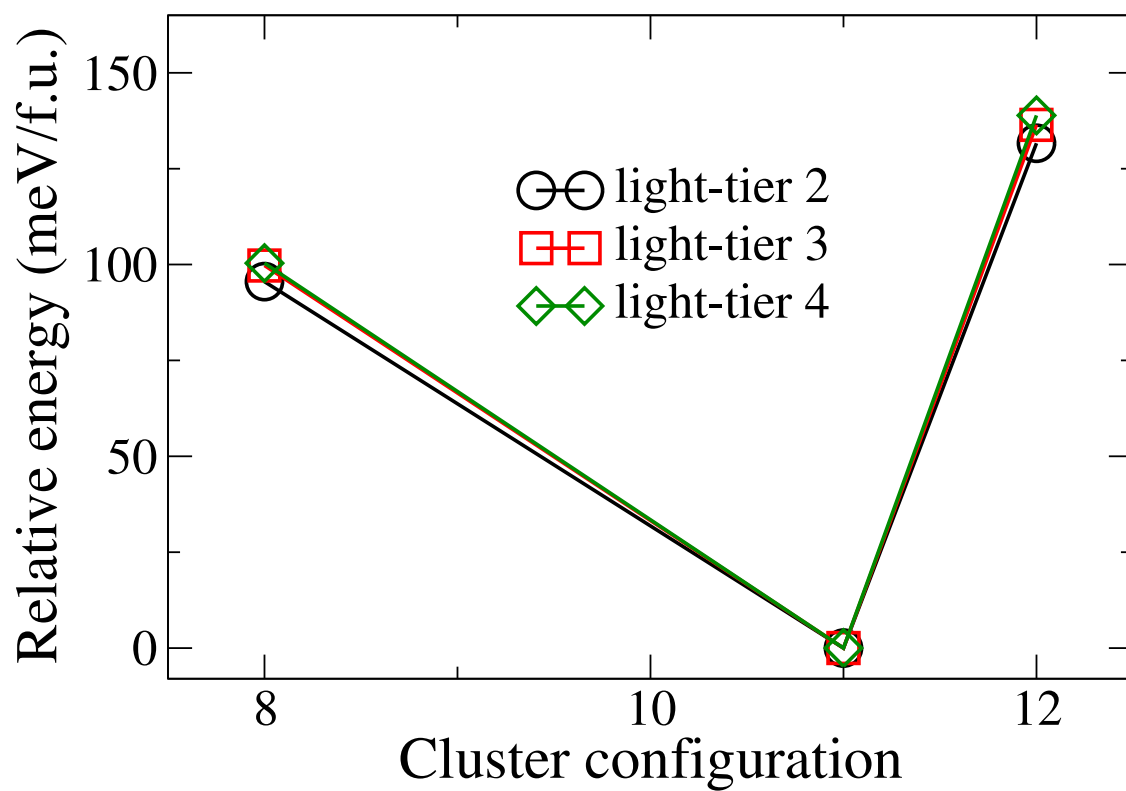


Figure S1: Basis set convergence set within the PBE functional for W_2S_4 clusters. No discrepancies between the basis sets in the determination of the relative energies of the clusters is identified, thus justifying the choice of the *light-tier 2* for our calculations.

Boltzmann probabilities of existence

Table S1: Boltzmann probability of existence of 1D cluster after 1D \rightarrow 2D transitions for our WQ_2 nanoflakes. The number under each probability are the sizes of the 1D clusters belonging to that probability for each species.

WS ₂	1.00%	5.00%	10.00%	20.00%	30.00%	40.00%	50.00%
1098.15 K	8, 10	8, 10	8, 10	8, 10	8, 10	8	–
1148.15 K	8, 10	8, 10	8, 10	8, 10	8, 10	8	–

WSe ₂	1.00%	5.00%	10.00%	20.00%	30.00%	40.00%	50.00%
1098.15 K	10, 11	10, 11	10, 11	10, 11	10	10	10
1148.15 K	10, 11	10, 11	10, 11	10, 11	10	10	10

WTe ₂	1.00%	5.00%	10.00%	20.00%	30.00%	40.00%	50.00%
1098.15 K	–	–	–	–	–	–	–
1148.15 K	–	–	–	–	–	–	–

Electronic Properties

Atomic configurations

Geometric coordinates, in Å, for our gas-phase $(WQ_2)_n$, $Q = S, Se, Te$ with $n = 1 - 16, 36, 66, 105$ nanoflakes after relaxation in FHI-aims. At each (x, y, z) coordinate there are the respective chemical formula, total energy (E_{tot}), in eV, and relative energy (E_{rel}), in meV per formula unit.

W₁S₂; $E_{tot} = -474\,451.059\,545\,12$ eV; $E_{rel} = 0$ meV/f.u.

W	-0.7269190000000000	2.8710260000000001	0.0847810000000000
S	1.3782220000000001	2.6845119999999998	0.2836080000000000
S	-1.5976220000000001	1.2657290000000001	-0.9973720000000000

W₂S₄; $E_{tot} = -948\,906.774\,793\,07$ eV; $E_{rel} = 95.543\,130\,500\,0$ meV/f.u.

W	0.9526780000000000	0.1947310000000000	-0.7979920000000000
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S	2.6248730000000000	1.2992120000000000	-0.0769370000000000
S	-0.8300880000000000	1.6421950000000001	-0.5904100000000000
W	-0.9526019999999999	-0.1947510000000000	0.7979100000000000
S	0.8301330000000000	-1.6422669999999999	0.5902400000000000
S	-2.6249959999999999	-1.2991210000000000	0.0771880000000000

W₂S₄; $E_{tot}=-948\,906.965\,879\,33$ eV; $E_{rel}=0$ meV/f.u.

W	1.1228480000000001	0.2487090000000000	-0.6229620000000000
S	1.1801759999999999	2.3327369999999998	-0.1277900000000000
S	-0.6043420000000000	-0.4260310000000000	-1.9978670000000001
W	-0.7923450000000000	-1.0150920000000001	0.2260310000000000
S	1.3155749999999999	-1.2266400000000000	1.1416299999999999
S	-2.2219120000000001	0.0863150000000000	1.3809560000000001

W₃S₆; $E_{tot}=-1\,423\,364.105\,712\,06$ eV; $E_{rel}=202.006\,980\,333\,3$ meV/f.u.

W	-1.3198010000000000	-0.4041110000000000	-0.4309280000000000
S	-1.7462489999999999	-1.8231599999999999	-1.9644189999999999
S	-3.1690730000000000	0.3152400000000000	0.3538020000000000
W	1.2998080000000001	-0.4220620000000000	1.1803669999999999
S	1.6212930000000001	1.7959480000000001	1.9451700000000001
S	-0.5052560000000000	-1.7763469999999999	1.3339319999999999
W	1.2922959999999999	1.2181460000000000	-0.3318350000000000
S	3.0459120000000000	-0.3698850000000000	-0.4225320000000000
S	-0.5189290000000000	1.4662310000000001	-1.6635570000000000

W₃S₆; $E_{tot}=-1\,423\,364.711\,310\,29$ eV; $E_{rel}=0.140\,903\,666\,6$ meV/f.u.

W	-1.4379280000000001	0.2009710000000000	0.1584800000000000
S	-3.4809030000000001	-0.3646950000000000	-0.2386290000000000
S	-0.3728710000000000	-0.7367790000000000	1.9993559999999999
W	1.1677249999999999	-0.8358700000000000	0.2619370000000000
S	-0.9717290000000000	2.4950160000000001	0.1955200000000000

S	2.2897270000000001	-2.6574279999999999	-0.0114070000000000
W	0.6030550000000000	1.4116540000000000	-1.0423810000000000
S	2.4021140000000001	1.1522440000000000	0.3294000000000000
S	-0.1991890000000000	-0.6651130000000000	-1.6522760000000001

$\mathbf{W}_4\mathbf{S}_8$; $E_{tot}=-1\,897\,821.286\,917\,26\text{ eV}$; $E_{rel}=30.466\,027\,750\,0\text{ meV/f.u.}$

W	-1.6733730000000000	1.5207409999999999	-0.8663330000000000
S	-2.4991469999999998	3.4977589999999998	-0.7270010000000000
S	-0.4200760000000000	1.1515359999999999	-2.7803710000000001
W	-0.8957760000000000	-0.4791420000000000	0.9498140000000000
S	-3.0202810000000002	-0.1786100000000000	-0.0525160000000000
S	0.4228670000000000	-1.1538700000000000	2.7806139999999999
W	1.6728440000000000	-1.5217440000000000	0.8643020000000000
S	-0.0150980000000000	1.6604479999999999	0.8258310000000000
S	2.5040070000000001	-3.4970690000000002	0.7209280000000000
W	0.8948690000000000	0.4790810000000000	-0.9467480000000000
S	3.0173990000000002	0.1812820000000000	0.0550390000000000
S	0.0117620000000000	-1.6604120000000000	-0.8235610000000000

$\mathbf{W}_4\mathbf{S}_8$; $E_{tot}=-1\,897\,821.408\,781\,37\text{ eV}$; $E_{rel}=0\text{ meV/f.u.}$

W	1.1786960000000000	-1.6297210000000000	-0.0496010000000000
S	1.4378110000000000	-3.7468300000000001	-0.3355640000000000
S	2.4022310000000000	-0.4791210000000000	-1.6484829999999999
W	-1.9069270000000000	0.5964380000000000	-0.2386350000000000
S	-3.9693269999999998	0.1550140000000000	-0.6658950000000000
S	-1.7267859999999999	1.4418359999999999	1.9130799999999999
W	0.4274620000000000	0.7134960000000000	1.4285150000000000
S	-1.0698820000000000	2.0256590000000001	-1.8617690000000000
S	1.7480000000000000	-1.0681780000000001	2.1269960000000001
W	0.8385629999999999	1.0827110000000000	-0.9281290000000000
S	1.7393289999999999	2.4682270000000002	0.6893440000000000
S	-1.0991720000000000	-1.5595310000000000	-0.4298590000000000

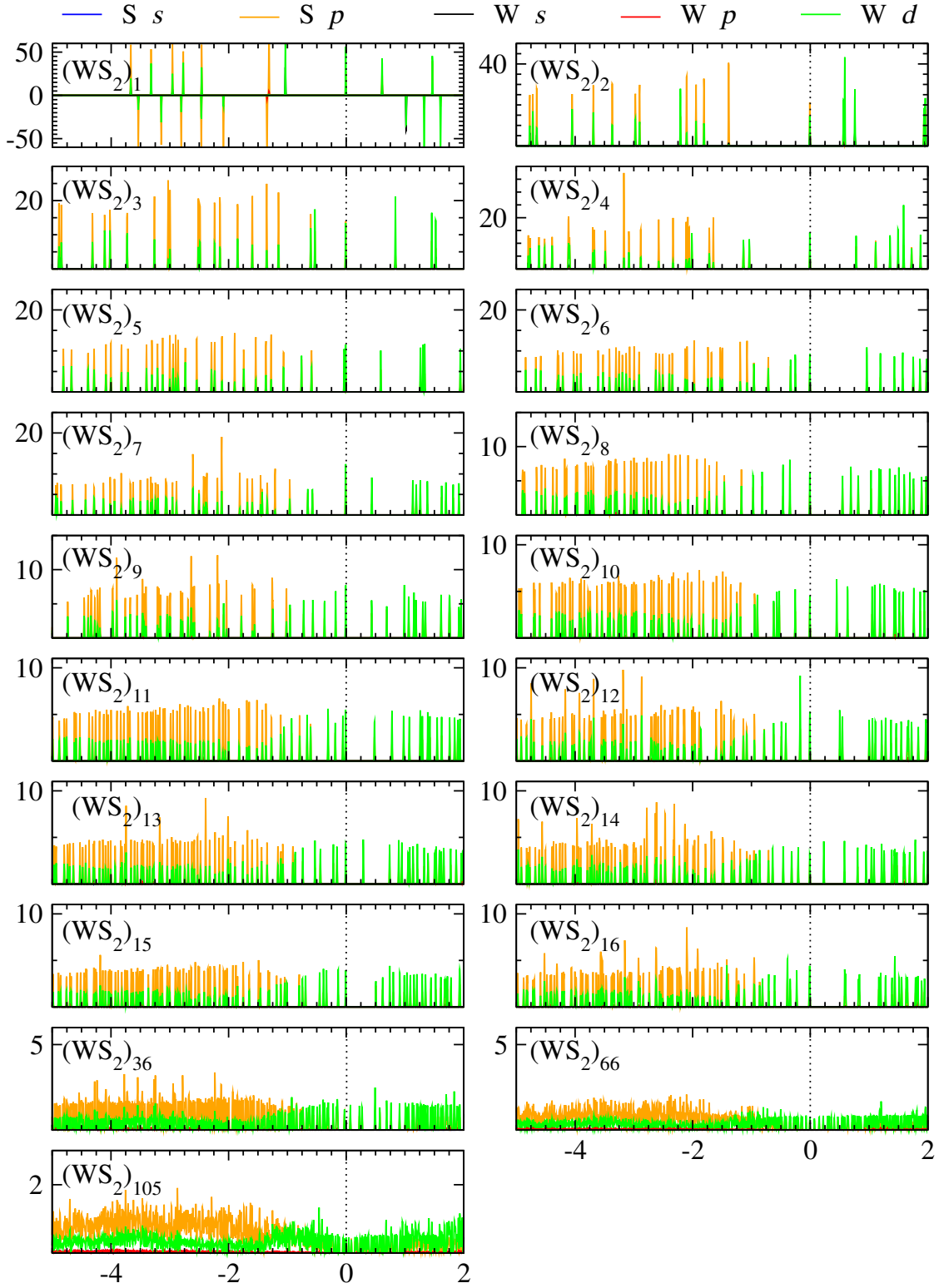


Figure S2: Projected density of states (PDOS) per f.u. of all our WS₂ pGMCs.

W₅S₁₀; $E_{tot}=-2\,372\,277.087\,965\,27$ eV; $E_{rel}=144.923\,088\,200\,0$ meV/f.u.

W	-0.3441030000000000	2.2073499999999999	-1.8017460000000001
S	0.5230220000000000	0.5155860000000000	-2.9548070000000002
S	1.2292590000000001	3.0661550000000002	-0.5406220000000000
W	-2.2117059999999999	0.9700500000000000	0.1523090000000000
S	-2.6239370000000002	2.4024589999999999	-1.6598820000000001
S	-3.4809530000000000	1.8188470000000001	1.6468900000000000
W	-0.6016030000000000	-1.3068390000000001	0.8890400000000001
S	-2.8043420000000001	-1.2652310000000000	0.0835070000000000
S	0.7754280000000000	-2.1354410000000001	2.5996400000000000
W	2.0645150000000001	-1.9949190000000001	0.6879630000000000
S	-0.2507470000000000	0.9421600000000000	1.4918670000000001
S	3.2691599999999998	-3.7504130000000000	0.3920190000000000
W	0.9229110000000000	0.3800590000000000	-0.4901180000000000
S	3.0351979999999998	0.0982450000000000	0.5475740000000000
S	0.4978980000000000	-1.9480700000000000	-1.0436380000000001

W₅S₁₀; $E_{tot}=-2\,372\,277.812\,580\,71$ eV; $E_{rel}=0$ meV/f.u.

W	-1.9880080000000000	2.2704420000000001	0.4966530000000000
S	0.1825190000000000	2.8636610000000000	0.6934590000000000
S	-3.4059390000000000	3.7289310000000002	-0.1977180000000000
W	-1.9209000000000001	-0.4315430000000000	0.8987090000000000
S	-1.9062280000000000	0.6330880000000000	-1.1786930000000000
S	-2.7924300000000000	1.1162710000000000	2.3567640000000001
W	0.4378400000000000	-2.1156920000000001	0.1327330000000000
S	-1.8243389999999999	-2.7231220000000000	0.3661990000000000
S	2.6000909999999999	-2.7352650000000001	0.6038750000000001
W	2.6814279999999999	-1.0610310000000001	-1.0180439999999999
S	0.2611540000000000	-0.4669230000000000	1.8291489999999999
S	4.0282760000000000	-1.5769310000000001	-2.6114009999999999
W	0.3388330000000000	0.5909030000000000	-0.2542900000000000
S	2.7666960000000000	1.0198259999999999	-0.1445230000000000

S 0.5410090000000000 -1.1126100000000001 -1.9728690000000000

W₆S₁₂; $E_{tot} = -2\,846\,734.204\,447\,47$ eV; $E_{rel} = 6.433\,733\,500\,0$ meV/f.u.

W -3.6537880000000000 1.4638899999999999 0.6429009999999999
S -5.3803570000000001 2.0806010000000001 1.7654970000000001
S -3.7093569999999998 -0.6539350000000000 -0.1684260000000000
W -1.0256310000000000 2.1270549999999999 -0.1591910000000000
S 1.0943360000000000 2.7041789999999999 0.4824570000000000
S -3.0564060000000000 2.9883500000000001 -0.9985870000000000
W -1.3379239999999999 -0.3550930000000000 0.3675750000000000
S -0.6321270000000000 0.5043950000000000 -1.7671980000000000
S -1.7920689999999999 1.4286820000000000 1.9935639999999999
W 1.0248850000000000 -2.1271010000000001 0.1569150000000000
S -1.0948979999999999 -2.7040340000000000 -0.4852870000000000
S 3.0546739999999999 -2.9889720000000000 0.9984120000000000
W 3.6540830000000000 -1.4637540000000000 -0.6416040000000000
S 0.6313560000000000 -0.5052780000000000 1.7657470000000000
S 5.3836740000000001 -2.0790500000000001 -1.7602869999999999
W 1.3373480000000000 0.3547280000000000 -0.3686410000000000
S 3.7081149999999998 0.6534440000000000 0.1710390000000000
S 1.7940849999999999 -1.4281050000000000 -1.9948859999999999

W₆S₁₂; $E_{tot} = -2\,846\,734.243\,049\,87$ eV; $E_{rel} = 0$ meV/f.u.

W -1.4642679999999999 -2.6256759999999999 1.6214919999999999
S 0.6470470000000000 -2.9072110000000002 2.2739539999999998
S -3.1331419999999999 -1.3877550000000001 2.4950160000000001
W -1.7143310000000000 2.6316359999999999 -0.0370290000000000
S 0.4163510000000000 3.3061280000000002 0.1384270000000000
S -2.9427409999999998 4.1668360000000000 -0.8799310000000000
W -1.7030660000000000 -0.2413200000000000 0.8526690000000000
S -1.7041379999999999 0.7849040000000000 -1.4219269999999999
S -2.6245940000000001 1.7552500000000000 1.8514900000000001

W	0.6918110000000000	-1.6224430000000001	0.1035300000000000
S	-1.5352090000000000	-2.3856090000000001	-0.6298690000000000
S	3.0579550000000002	-1.9914810000000001	0.2493630000000000
W	2.8962409999999998	-0.5317460000000001	-1.4872230000000000
S	0.4995900000000000	0.2454290000000000	1.5469670000000000
S	4.2917389999999997	-0.8887190000000000	-3.0789390000000001
W	0.6135050000000000	0.9868470000000000	-0.6652600000000000
S	2.9462050000000000	1.5898040000000000	-0.6968000000000000
S	0.7610420000000000	-0.8848720000000000	-2.2359290000000001

W₇S₁₄; $E_{tot}=-3\,321\,189.857\,279\,90$ eV; $E_{rel}=52.979\,845\,857\,1$ meV/f.u.

W	-1.2846550000000001	-2.9130950000000002	1.8144279999999999
S	0.9361990000000000	-3.0640230000000002	2.2590080000000001
S	-1.6912330000000000	-1.0067150000000000	3.2595580000000002
W	-1.8337319999999999	2.5834890000000001	-0.0488910000000000
S	0.2898160000000000	3.2975720000000002	0.0921440000000000
S	-3.0625079999999998	4.0928170000000001	-0.9313920000000000
W	-1.7577469999999999	-0.4057780000000000	0.9096360000000000
S	-1.7416959999999999	0.7065540000000000	-1.3827190000000000
S	-2.6930420000000002	1.7767350000000000	1.8491810000000000
W	0.7844580000000000	-1.6134500000000001	0.2528130000000000
S	-1.3695090000000001	-2.4753550000000000	-0.4337750000000000
S	3.2249200000000000	-1.7580330000000000	0.4159630000000000
W	2.9447470000000000	-0.4650730000000000	-1.4152819999999999
S	0.5047330000000000	0.3168870000000000	1.5533079999999999
S	4.3605760000000000	-0.8191980000000000	-2.9900060000000002
W	0.5759960000000000	0.9699090000000000	-0.6512010000000000
S	2.8359709999999998	1.7224390000000001	-0.8066000000000000
S	0.8362610000000000	-0.9967690000000000	-2.1172270000000002
W	-3.5996120000000000	-1.9779119999999999	2.4554440000000000
S	-3.1543619999999999	-4.2286359999999998	2.5140899999999999
S	-4.1363630000000002	-1.1135839999999999	0.4996020000000000

W₇S₁₄; $E_{tot}=-3\,321\,190.228\,138\,82$ eV; $E_{rel}=0$ meV/f.u.

W	-3.3798230000000000	3.1140340000000002	1.0217390000000000
S	-4.7457880000000001	4.7203889999999999	0.6036160000000000
S	-1.2863880000000001	3.6215340000000000	1.6348750000000001
W	-3.1118869999999998	0.3689020000000000	0.8444700000000001
S	-4.3935279999999999	1.5370830000000000	2.3993859999999998
S	-3.1385079999999999	-1.5109360000000001	-0.4712340000000000
W	-0.8129040000000000	1.4752749999999999	0.2983350000000000
S	1.4642260000000000	1.8971780000000000	0.8792830000000000
S	-2.8782040000000002	1.9766580000000000	-0.9321840000000000
W	-0.7426660000000000	-1.2301750000000000	0.1372280000000000
S	-0.3187960000000000	0.2739450000000000	-1.6936549999999999
S	-1.2412510000000001	0.0168240000000000	2.1545220000000000
W	1.7103580000000000	-2.7025579999999998	-0.5557350000000000
S	-0.4019760000000000	-3.2559849999999999	-1.2633559999999999
S	3.7550379999999999	-3.6502699999999999	0.0325260000000000
W	4.2157159999999996	-1.7254550000000000	-1.1900780000000000
S	1.2820000000000000	-1.5865450000000001	1.4216320000000000
S	5.8883010000000002	-2.0588410000000001	-2.4986959999999998
W	1.6550819999999999	-0.0966480000000000	-0.4207000000000000
S	4.1738629999999999	0.1465050000000000	0.0393560000000000
S	2.3071280000000001	-1.3309120000000001	-2.4413299999999998

W₈S₁₆; $E_{tot}=-3\,795\,646.593\,541\,49$ eV; $E_{rel}=10.220\,920\,125\,0$ meV/f.u.

W	-5.0116440000000004	1.7690030000000001	0.7363700000000000
S	-6.8426879999999999	1.9071290000000001	1.8522870000000000
S	-4.8370179999999996	0.1247290000000000	-0.7852120000000000
W	-2.3958550000000001	2.8844259999999999	0.6231570000000000
S	-4.3723060000000000	3.8183600000000002	-0.1594280000000000
S	-0.3857660000000000	3.5576379999999999	1.4076670000000000
W	-2.5371869999999999	0.2315450000000000	0.1513200000000000
S	-3.2702439999999999	1.3787190000000000	2.2022889999999999

S	-2.285655999999999	-1.736836000000000	-1.190785999999999
W	0.211486000000000	1.342275000000001	0.268413000000000
S	2.288049000000000	1.739104000000000	1.189954000000000
S	-1.679972999999999	1.857688999999999	-1.320524999999999
W	-0.210191000000000	-1.339838000000001	-0.267201000000000
S	0.763947000000000	0.189766000000000	-1.741638999999999
S	-0.762952000000000	-0.187297000000000	1.742512000000001
W	2.395246000000002	-2.883162000000000	-0.620126000000000
S	0.385186000000000	-3.555368000000001	-1.405867999999999
S	4.370326999999996	-3.819121000000000	0.162375000000000
W	5.010602999999997	-1.772192999999999	-0.738127000000000
S	1.680984000000000	-1.854425999999999	1.323236000000001
S	6.839026999999997	-1.917475000000000	-1.857661999999999
W	2.538368999999999	-0.230498000000000	-0.151155000000000
S	4.839938000000001	-0.124070000000000	0.780312000000000
S	3.268317999999998	-1.380100000000001	-2.202160000000001

$\mathbf{W}_8\mathbf{S}_{16}$; $E_{tot} = -3\,795\,646.675\,308\,85$ eV; $E_{rel} = 0$ meV/f.u.

W	-1.297086000000000	-2.907241000000000	1.645000999999999
S	0.887452000000000	-3.366915000000001	2.064335999999999
S	-1.605304000000001	-1.095971999999999	3.083397999999999
W	-1.604139999999999	2.620177000000000	-0.116898000000000
S	0.501576000000000	3.320682000000001	0.021076000000000
S	-2.841310000000000	4.090326000000001	-1.043404999999999
W	-1.738051000000000	-0.287180000000000	0.798411000000000
S	-1.504161000000001	0.792847000000000	-1.494880999999999
S	-2.361136999999998	1.911864999999999	1.984358000000001
W	0.932465000000000	-1.647713000000000	0.234569000000000
S	-1.295787000000000	-2.291939000000002	-0.572670000000000
S	3.300625999999998	-1.922159000000000	0.534025000000000
W	3.137833999999998	-0.591486000000000	-1.300051000000001
S	0.601608999999999	0.273463000000000	1.512991000000000

S	4.5710430000000004	-1.0471550000000001	-2.8329130000000000
W	0.7901500000000000	0.9508380000000000	-0.6718650000000000
S	3.0829540000000000	1.6116539999999999	-0.7075470000000000
S	1.0397780000000001	-0.9986400000000000	-2.1099660000000000
W	-3.6679539999999999	-1.7948960000000000	2.2800199999999999
S	-3.2716409999999998	-4.1008570000000004	1.9158040000000001
S	-4.0526540000000004	-0.8181000000000000	0.1898080000000000
W	-4.4703480000000004	0.8333940000000000	1.7691269999999999
S	-6.3002089999999997	1.7764690000000001	1.1758450000000000
S	-4.7732250000000001	-0.2855730000000000	3.7278639999999998

$\mathbf{W}_9\mathbf{S}_{18}; E_{tot}=-4\,270\,102.435\,138\,63\text{ eV}; E_{rel}=156.430\,601\,222\,2\text{ meV}/\mathbf{f.u.}$

W	4.6380260000000000	-4.1325170000000000	-0.8093340000000000
S	5.8236049999999997	-5.8404949999999998	-0.2624290000000000
S	2.6888570000000001	-4.4892979999999998	-1.8411139999999999
W	-5.6308350000000003	2.6391659999999999	0.7533879999999999
S	-7.5054080000000001	2.9420720000000000	1.7612550000000000
S	-5.4415139999999997	0.8826640000000000	-0.6135850000000000
W	-3.0129670000000002	3.5484390000000001	0.6509000000000000
S	-4.8884939999999997	4.6305810000000003	-0.1954550000000000
S	-1.0516250000000000	3.9581979999999999	1.7237220000000000
W	-3.0369750000000000	0.9585980000000000	0.3059480000000000
S	-3.9851990000000002	2.0687160000000002	2.2796409999999998
S	-2.7461750000000000	-0.9956170000000000	-0.9732229999999999
W	-0.4650710000000000	1.9591820000000000	0.2722200000000000
S	1.7126729999999999	2.3358639999999999	1.1222390000000000
S	-2.2295140000000000	2.5612800000000000	-1.2888850000000001
W	-0.4986560000000000	-0.7319920000000000	-0.1020010000000000
S	0.3034090000000000	0.8558540000000000	-1.6999979999999999
S	-1.3423860000000001	0.3774000000000000	1.8585970000000001
W	2.0593219999999999	-2.4033899999999999	-0.4691430000000000
S	-0.0857270000000000	-2.7557469999999999	-1.3719159999999999

S	3.8348490000000002	-3.0757900000000000	1.0883130000000001
W	4.4646160000000004	-1.3826099999999999	-0.4999060000000000
S	1.2311850000000000	-1.3146730000000000	1.4666260000000000
S	5.9587430000000001	-2.5306060000000001	-1.8614390000000001
W	2.0021390000000001	0.3321670000000000	-0.1082450000000000
S	4.3352849999999998	0.4139550000000000	0.8868970000000000
S	2.8678340000000002	-0.8114070000000000	-2.0730740000000001

$\mathbf{W}_9\mathbf{S}_{18}$; $E_{tot}=-4\ 270\ 103.843\ 014\ 04\ \text{eV}$; $E_{rel}=0\ \text{meV}/\mathbf{f.u.}$

W	32.7824680000000015	12.9218869999999999	2.6901809999999999
W	31.3731909999999985	15.3993640000000003	3.0398939999999999
W	29.9854610000000008	18.0260989999999985	3.4576850000000001
W	34.1920289999999980	15.3989740000000008	3.0401300000000000
W	32.7828179999999989	18.0252699999999990	3.4566450000000000
W	31.3732429999999987	20.6520370000000000	3.8727469999999999
W	35.5798660000000027	18.0259980000000013	3.4576650000000000
W	34.1918480000000002	20.6519159999999999	3.8731650000000002
W	32.7827819999999974	23.1300239999999988	4.2213060000000002
S	32.7825810000000004	14.2008720000000004	4.5988689999999997
S	31.2148210000000006	16.8472609999999996	4.9889070000000002
S	29.1117440000000016	19.7181500000000014	4.6514400000000000
S	34.3505570000000020	16.8470440000000004	4.9889150000000004
S	32.7825729999999993	19.5827789999999986	5.3650409999999997
S	30.8479519999999994	22.5052459999999996	5.2752260000000000
S	36.4539180000000016	19.7183880000000009	4.6513960000000001
S	34.7166399999999982	22.5052219999999998	5.2753930000000002
S	32.7826009999999997	25.1855909999999987	3.6022059999999998
S	32.7826939999999993	10.8661189999999994	3.3087499999999999
S	30.8479859999999988	13.5473929999999996	1.6362420000000000
S	29.1105780000000003	16.3343449999999990	2.2640660000000001
S	34.7173939999999988	13.5470410000000001	1.6367579999999999
S	32.7824030000000022	16.4689879999999995	1.5481790000000000

S	31.2143149999999991	19.2035380000000018	1.9245360000000000
S	36.4541719999999998	16.3344750000000012	2.2634520000000000
S	34.3511790000000019	19.2036319999999989	1.9245880000000000
S	32.7826359999999966	21.8502690000000008	2.3135750000000002

$\mathbf{W}_{10}\mathbf{S}_{20}$; $E_{tot}=-4\,744\,558.723\,027\,70$ eV; $E_{rel}=11.235\,160\,100\,0$ meV/f.u.

W	6.2286400000000004	-3.1208520000000002	-0.4392050000000000
S	5.9618450000000003	-1.4907090000000001	1.0630800000000000
S	8.2006340000000009	-3.3668360000000002	-1.2498579999999999
W	3.5417529999999999	-4.0177949999999996	-0.6666960000000000
S	5.3343959999999999	-5.1285650000000000	0.3196180000000000
S	1.5868100000000001	-4.4690380000000003	-1.6540400000000000
W	-6.2312989999999999	3.1132010000000001	0.4398480000000000
S	-8.2052709999999998	3.3431370000000000	1.2503690000000001
S	-5.9566299999999996	1.4994410000000000	-1.0782600000000000
W	-3.5458899999999998	4.0137489999999998	0.6811820000000000
S	-5.3399289999999997	5.1310190000000002	-0.2957380000000000
S	-1.5938570000000001	4.4589679999999996	1.6772140000000000
W	-3.7487469999999998	1.4270039999999999	0.1380220000000000
S	-4.7264840000000001	2.5164019999999998	2.1036320000000002
S	-3.4792299999999998	-0.4875570000000000	-1.2608410000000001
W	-0.9859690000000000	2.2533219999999998	0.4473230000000000
S	1.1035370000000000	2.5519129999999999	1.2765210000000000
S	-2.6180850000000002	3.0318120000000000	-1.2149870000000000
W	-1.4352320000000001	-0.3349370000000000	-0.1491350000000000
S	-0.1778010000000000	1.1607310000000000	-1.5034250000000000
S	-2.1919040000000001	0.7526250000000000	1.8333210000000000
W	0.9865260000000000	-2.2485089999999999	-0.4455860000000000
S	-1.1008840000000000	-2.5477580000000000	-1.2802659999999999
S	2.6202290000000001	-3.0167540000000002	1.2217499999999999
W	3.7512330000000000	-1.4251280000000000	-0.1469700000000000
S	0.1816910000000000	-1.1482889999999999	1.4997069999999999

S	4.7212240000000003	-2.5351870000000001	-2.1052179999999998
W	1.4395300000000000	0.3407930000000000	0.1400220000000000
S	3.4885210000000000	0.5002770000000000	1.2397170000000000
S	2.1906439999999998	-0.7564800000000000	-1.8411020000000000

$W_{10}S_{20}$; $E_{tot} = -4\,744\,558.835\,379\,30\text{ eV}$; $E_{rel} = 0\text{ meV/f.u.}$

W	3.2490470000000000	1.5876230000000000	1.3964040000000000
S	5.0332699999999999	1.1036770000000000	0.1205120000000000
S	3.7886579999999999	2.7757589999999999	3.0887319999999998
W	4.5853830000000002	-3.7253680000000000	-0.8087490000000001
S	5.7890150000000000	-5.4818009999999999	-0.5341450000000000
S	3.0636619999999999	-3.9023650000000001	-2.4687299999999999
W	-6.1297210000000000	2.1403230000000000	0.5205149999999999
S	-7.8550540000000000	2.5376520000000000	1.7425670000000000
S	-5.9518440000000004	0.2472000000000000	-0.6726950000000000
W	-3.6399960000000000	3.1693009999999999	0.2602870000000000
S	-5.5497980000000000	4.0446569999999999	-0.6993370000000000
S	-1.5753480000000000	3.7714560000000001	1.1934089999999999
W	-3.5049169999999998	0.5184160000000000	0.0518870000000000
S	-4.3671470000000001	1.7253069999999999	1.9945839999999999
S	-3.2379530000000001	-1.5158309999999999	-1.2004859999999999
W	-1.1097180000000000	1.7761979999999999	-0.0193570000000000
S	1.4096640000000000	2.4364330000000001	0.2578010000000000
S	-2.8816359999999999	2.0291180000000000	-1.6330579999999999
W	-0.9643510000000000	-1.2280359999999999	-0.7415240000000000
S	-0.1124890000000000	0.6386020000000000	-1.8933130000000000
S	-1.6830550000000000	0.0089010000000000	1.4509040000000000
W	1.8583310000000000	-2.5362350000000000	-0.8025040000000000
S	-0.1109120000000000	-2.7320970000000000	-2.2808560000000000
S	3.2551990000000002	-3.3664779999999999	1.0200070000000001
W	3.9112809999999998	-1.1153940000000000	0.1913200000000000
S	0.3599930000000000	-2.1215730000000002	0.9909010000000000

S	5.8154339999999998	-1.8353489999999999	-1.0902810000000001
W	1.2318009999999999	0.0226890000000000	0.0749600000000000
S	2.6500420000000000	-0.4733880000000000	2.1852950000000000
S	2.6731549999999999	-0.4993950000000000	-1.6950449999999999

$\mathbf{W}_{11}\mathbf{S}_{22}$; $E_{tot}=-5\,219\,014.599\,834\,32\text{ eV}$; $E_{rel}=52.585\,018\,272\,7\text{ meV/f.u.}$

W	-6.3009360000000001	3.2116340000000001	0.4595980000000000
W	-3.6186270000000000	3.9546299999999999	0.6346090000000000
W	-3.7847290000000000	1.4006330000000000	0.1414160000000000
W	-1.1405060000000000	2.2168580000000002	0.3672190000000000
W	-1.3486700000000000	-0.4331610000000000	-0.1690050000000000
W	1.2959989999999999	0.4612420000000000	0.0692350000000000
W	1.1934849999999999	-2.2912759999999999	-0.4243540000000000
W	3.7223980000000001	-1.3162750000000001	-0.2298940000000000
W	3.6935169999999999	-4.0603590000000001	-0.6314290000000000
W	6.1341109999999999	-3.1428110000000000	-0.5267300000000000
W	6.1954890000000002	-5.9063049999999997	-0.8564700000000000
S	-8.2474570000000007	3.5770170000000001	1.2929170000000001
S	-5.3537169999999996	5.1948499999999997	-0.2988130000000000
S	-4.8312210000000002	2.4655350000000000	2.0873719999999998
S	-6.0930840000000002	1.5350220000000001	-0.9972520000000000
S	-1.7405690000000000	4.2184100000000004	1.8625020000000001
S	-2.7279040000000001	3.0174349999999999	-1.2879900000000000
S	-2.2576250000000000	0.6280460000000000	1.7832220000000001
S	-3.5144050000000000	-0.4989510000000000	-1.2252840000000000
S	0.9708430000000000	2.4947100000000000	1.3180250000000000
S	-0.2864290000000000	1.1599870000000001	-1.5943080000000001
S	0.2600280000000000	-1.1625120000000000	1.4912639999999999
S	-1.0405300000000000	-2.5478220000000000	-1.2186570000000001
S	3.5198220000000000	0.6871980000000000	0.9533740000000001
S	2.1443289999999999	-0.6659770000000000	-1.8883630000000000
S	1.5905579999999999	-4.3197830000000002	-1.6596109999999999

S	6.056060999999997	-1.3408190000000000	0.8376160000000000
S	2.7915719999999999	-2.9505080000000001	1.2580340000000001
S	4.6383109999999999	-2.4753219999999998	-2.1655139999999999
S	4.2931140000000001	-6.1612700000000000	-1.9955099999999999
S	5.3532450000000003	-4.8201099999999997	1.0089180000000000
S	7.6354139999999999	-4.3557769999999998	-1.8242010000000000
S	7.2719129999999996	-7.6734200000000001	-0.2760280000000000

$\mathbf{W}_{11}\mathbf{S}_{22}$; $E_{tot} = -5\,219\,015.178\,269\,52\text{ eV}$; $E_{rel} = 0\text{ meV/f.u.}$

W	2.1273789999999999	2.9397869999999999	1.5089079999999999
S	1.8618420000000000	5.0361349999999998	1.1581889999999999
S	2.8085990000000001	2.0636830000000002	-0.5297550000000000
W	4.1445090000000002	1.0729439999999999	1.1037330000000001
S	5.8856580000000003	0.1790820000000000	-0.0252430000000000
S	3.9141940000000002	2.5360350000000000	2.9050099999999999
W	4.1255309999999996	-4.2291759999999998	-0.9523580000000000
S	5.0270469999999996	-6.1427040000000002	-0.6004090000000000
S	2.4598499999999999	-4.2368810000000003	-2.4363419999999998
W	-6.6454100000000000	1.4734200000000000	-0.1793680000000000
S	-8.6367639999999994	1.4065220000000000	0.6292860000000000
S	-5.9993930000000004	-0.0820040000000000	-1.6674359999999999
W	-4.2852309999999996	2.7873199999999998	0.2791830000000000
S	-6.0983190000000000	3.6320209999999999	-0.8630530000000000
S	-2.4942760000000002	3.3761990000000002	1.6240660000000000
W	-3.8691970000000002	0.2323770000000000	-0.3636900000000000
S	-5.1779000000000002	1.0252110000000001	1.5680419999999999
S	-3.1180330000000001	-1.4137350000000000	-1.9188950000000000
W	-1.4783329999999999	1.5451660000000000	0.4482210000000000
S	0.3622000000000000	1.5200089999999999	2.0355680000000000
S	-2.9384519999999998	2.0837029999999999	-1.4851600000000000
W	-1.2381660000000001	-1.0031159999999999	-0.6588700000000000
S	-0.0587980000000000	0.8907020000000000	-1.3516619999999999

S	-2.4096400000000000	-0.4091560000000000	1.3812500000000001
W	1.5651430000000000	-2.5327039999999998	-0.7761690000000000
S	-0.3023080000000000	-2.7244739999999998	-2.1251620000000000
S	2.9793159999999999	-3.5609050000000000	0.9271230000000000
W	4.0923809999999996	-1.5457850000000000	0.0043390000000000
S	0.2490080000000000	-1.8678800000000000	1.0680820000000000
S	5.6867369999999999	-2.6512730000000002	-1.4028700000000001
W	1.6378029999999999	0.0594160000000000	0.3073200000000000
S	3.1098279999999998	-0.7144800000000000	2.1062710000000000
S	2.7131910000000001	-0.7454560000000000	-1.7181439999999999

$\mathbf{W}_{12}\mathbf{S}_{24}$; $E_{tot} = -5\,693\,470.788\,661\,38\text{ eV}$; $E_{rel} = 198.180\,940\,916\,6\text{ meV/f.u.}$

W	-6.2404289999999998	3.0913789999999999	0.4280510000000000
W	-3.5703140000000002	3.9778680000000000	0.6493560000000000
W	-3.7146460000000001	1.3911080000000000	0.1225140000000000
W	-0.9953260000000000	2.2451099999999999	0.4463730000000000
W	-1.3669070000000001	-0.3518530000000000	-0.1489620000000000
W	1.4996330000000000	0.3497390000000000	0.1456350000000000
W	0.9981470000000000	-2.2360820000000001	-0.4448860000000000
W	3.8643010000000002	-1.5346560000000000	-0.1415640000000000
W	3.4940790000000002	-4.1308579999999999	-0.7425910000000000
W	6.2118320000000002	-3.2795320000000001	-0.3938390000000000
W	6.0716749999999999	-5.8643169999999998	-0.9333790000000000
W	8.7382700000000000	-4.9793789999999998	-0.6727710000000000
S	-8.1979900000000008	3.3551980000000001	1.2699900000000000
S	-5.3605869999999998	5.1129619999999996	-0.3094150000000000
S	-4.7357570000000004	2.4746009999999998	2.0809709999999999
S	-5.9730270000000001	1.4607330000000001	-1.0663800000000001
S	-1.6610360000000000	4.3810050000000000	1.7550990000000000
S	-2.6081460000000001	3.0124450000000000	-1.2355440000000000
S	-2.1903999999999999	0.7184680000000000	1.8288100000000000
S	-3.4293360000000002	-0.4575680000000000	-1.3092729999999999

S	1.0912860000000000	2.5688029999999999	1.2645240000000000
S	-0.1243330000000000	1.1683269999999999	-1.4964990000000000
S	0.2448540000000000	-1.1209920000000000	1.5158480000000001
S	-1.0763910000000001	-2.4774759999999998	-1.3642010000000000
S	3.5746660000000001	0.5951270000000000	1.0636049999999999
S	2.2560169999999999	-0.7668360000000000	-1.8136040000000000
S	1.4102610000000000	-4.4545990000000000	-1.5655209999999999
S	5.9170080000000000	-1.4321660000000001	1.0367059999999999
S	2.6177750000000000	-3.0569440000000001	1.1995199999999999
S	4.7016910000000003	-2.6030470000000001	-2.1134949999999999
S	4.1720569999999997	-6.2589530000000000	-2.0584009999999999
S	5.0927319999999998	-4.9071970000000000	0.9474669999999999
S	8.4520959999999992	-3.3594430000000002	0.8288450000000001
S	7.2561650000000002	-4.3540120000000000	-2.3431530000000000
S	7.8494029999999997	-7.0059399999999998	0.0405430000000000
S	10.7093059999999998	-5.2361839999999997	-1.4855820000000000

$W_{12}S_{24}$; $E_{tot} = -5\,693\,473.166\,832\,67$ eV; $E_{rel} = 0$ meV/f.u.

W	34.3743949999999998	10.0789430000000007	2.7816130000000001
W	32.9723589999999973	12.6830780000000001	2.9401299999999999
W	31.4471829999999990	15.2473419999999997	3.1340800000000000
W	29.9790509999999983	18.0831850000000003	3.4580220000000002
W	35.7719730000000027	12.5747260000000001	3.0997080000000001
W	34.5902919999999980	15.1236449999999998	3.3394499999999998
W	32.6087350000000029	18.0976099999999995	3.5746920000000002
W	31.4279809999999991	20.6468409999999984	3.8137629999999998
W	37.2204010000000025	15.1377439999999996	3.4566659999999998
W	35.7524969999999982	17.9739620000000002	3.7800419999999999
W	34.2264089999999968	20.5385610000000014	3.9728759999999999
W	32.8248159999999984	23.1428149999999988	4.1291460000000004
S	34.2468720000000033	11.4396459999999998	4.6268620000000000
S	32.7264750000000006	14.1520799999999998	4.7861580000000004

S	31.103246999999996	16.791474999999984	5.0169290000000002
S	29.166668000000014	19.806470000000009	4.634350999999997
S	35.978124999999986	14.045992000000000	5.066474999999996
S	34.234428000000012	16.885847999999993	5.047758000000000
S	32.718392000000015	19.593049000000006	5.479370000000003
S	30.908438000000003	22.541029000000018	5.186239999999997
S	37.982467999999972	17.062017999999984	4.468356000000000
S	36.372740000000003	19.889171000000010	4.891911999999996
S	34.668602999999974	22.548981999999987	5.299386000000002
S	32.777549000000005	25.193915000000005	3.499358000000000
S	34.421354000000009	8.026763000000008	3.409327000000002
S	32.530517000000032	10.673930999999996	1.611607999999999
S	30.826774000000003	13.332815000000001	2.021881000000000
S	29.216504000000005	16.158735000000001	2.446626999999999
S	36.291212000000016	10.681350000000001	1.724701000000000
S	34.481090999999993	13.629336000000003	1.434133000000001
S	32.964767000000019	16.334779999999985	1.866976000000000
S	31.221156000000006	19.174147999999989	1.847155000000001
S	38.032926000000033	13.415051000000001	2.279294000000002
S	36.096640000000007	16.429652000000008	1.897990000000001
S	34.473044999999990	19.068529999999991	2.127822000000001
S	32.952209000000034	21.780191999999996	2.285088000000000

$\mathbf{W}_{13}\mathbf{S}_{26}$; $E_{tot} = -6\,167\,926.743\,056\,58\text{ eV}$; $E_{rel} = 173.213\,740\,846\,1\text{ meV/f.u.}$

W	-6.305866000000000	3.216445999999999	0.437667000000000
W	-3.622027999999998	3.953593999999998	0.641841000000000
W	-3.790448000000000	1.404495000000000	0.116532000000000
W	-1.140973000000000	2.202040000000002	0.388490000000000
W	-1.362779000000000	-0.425044000000000	-0.179348000000000
W	1.299943000000001	0.413115000000000	0.112354000000000
W	1.149334000000001	-2.317117999999998	-0.457208000000000
W	3.769590000000000	-1.383956000000000	-0.159769000000000

W	3.7104970000000002	-4.1502429999999997	-0.6395320000000000
W	6.2191729999999996	-3.1788120000000002	-0.4044000000000000
W	6.1889729999999998	-5.9262649999999999	-0.8157320000000000
W	8.6320150000000009	-5.0278739999999997	-0.6414460000000000
W	8.6769639999999999	-7.7940420000000001	-0.9869090000000000
S	-8.2572910000000004	3.5725020000000001	1.2628360000000001
S	-5.3492300000000004	5.2090079999999999	-0.2856990000000000
S	-4.8506150000000003	2.4541469999999999	2.0689350000000002
S	-6.0911549999999997	1.5589949999999999	-1.0384580000000001
S	-1.7608079999999999	4.1988079999999997	1.8934519999999999
S	-2.7026620000000001	3.0343589999999998	-1.2771340000000000
S	-2.2934860000000001	0.6082360000000000	1.7733140000000001
S	-3.5065170000000001	-0.4556700000000000	-1.2946100000000000
S	0.9457530000000000	2.4628890000000001	1.3649730000000000
S	-0.2469230000000000	1.1660010000000001	-1.5683410000000000
S	0.2115090000000000	-1.2204230000000000	1.4744340000000000
S	-1.0631930000000001	-2.5215260000000002	-1.2848770000000000
S	3.4773170000000002	0.6495800000000000	1.0138670000000001
S	2.2020650000000002	-0.6845450000000000	-1.8353299999999999
S	1.4874000000000001	-4.4281379999999997	-1.4715750000000001
S	2.7284389999999998	-3.0117690000000001	1.2437830000000001
S	4.6711159999999996	-2.5172430000000001	-2.0925210000000001
S	4.1256000000000004	-6.1558760000000001	-1.9200520000000001
S	6.0200430000000003	-1.1609799999999999	0.7229700000000000
S	5.2645790000000003	-4.8212289999999998	1.0666750000000000
S	7.1837010000000001	-4.3331499999999998	-2.3139859999999999
S	6.8097799999999999	-8.0223510000000005	-2.1834389999999999
S	8.5291669999999993	-3.2389250000000001	0.7310210000000000
S	7.8019449999999999	-6.7114979999999997	0.8632060000000000
S	10.1611840000000004	-6.2516129999999999	-1.8979150000000000
S	9.7123380000000008	-9.5805900000000008	-0.3930440000000000

$\mathbf{W}_{13}\mathbf{S}_{26}$; $E_{tot}=-6\ 167\ 928.994\ 835\ 21\ \text{eV}$; $E_{rel}=0\ \text{meV/f.u.}$

W	6.058989999999997	-3.7659129999999998	-0.0624100000000000
S	5.5075979999999998	-2.6162100000000001	1.7632049999999999
S	8.1511189999999996	-3.9704790000000001	-0.4847520000000000
W	-1.5340680000000000	4.2255589999999996	1.1425980000000000
S	-3.1624520000000000	5.4820570000000002	0.2313070000000000
S	0.2635830000000000	4.5338750000000001	2.5348920000000001
W	1.0258160000000001	2.6360869999999998	1.1406050000000001
S	-0.3378740000000000	3.4704470000000001	-0.6813410000000000
S	2.2510249999999998	1.7574030000000000	-0.7366190000000000
W	3.4637030000000002	1.0432310000000000	1.1056889999999999
S	5.2412820000000000	0.2468950000000000	0.0221430000000000
S	3.0432990000000002	2.8023080000000000	2.4978410000000002
W	3.4563709999999999	-4.4426110000000003	-1.1072210000000000
S	5.0289080000000004	-5.8255039999999996	-0.0043970000000000
S	1.7564390000000001	-4.7650150000000000	-2.6051820000000001
W	-6.6857340000000001	2.0751539999999999	-0.3991330000000000
S	-8.7455960000000008	2.0964250000000000	0.1985230000000000
S	-6.1916279999999997	0.5422770000000000	-1.9872240000000001
W	-4.1238720000000004	3.1510880000000001	0.3259990000000000
S	-5.9355110000000000	4.1589609999999997	-0.8842970000000000
S	-2.7467950000000001	2.6416330000000001	2.3033310000000000
W	-4.1918040000000003	0.4602310000000000	-0.5684060000000000
S	-5.4057560000000002	1.3344900000000000	1.3610580000000001
S	-3.6785139999999998	-1.3842360000000000	-2.0392540000000001
W	-1.6968630000000000	1.6860790000000001	0.3159670000000000
S	-0.0494000000000000	0.8113350000000000	1.9425360000000000
S	-3.1105730000000000	2.2382360000000001	-1.5926640000000001
W	-1.7375560000000001	-1.2462240000000000	-0.8203800000000000
S	-0.4426770000000000	0.4555900000000000	-1.5168880000000000
S	-2.8085900000000001	-0.4471110000000000	1.1361019999999999
W	1.1697930000000001	-3.0473309999999998	-1.0232230000000000

S	-1.0422750000000001	-3.2136250000000000	-1.9355530000000001
S	2.4446159999999999	-3.8123170000000002	0.8734270000000000
W	3.6907950000000000	-1.9103910000000000	0.1132560000000000
S	-0.1761400000000000	-2.2253650000000000	0.8126970000000000
S	4.9383379999999999	-2.7829440000000001	-1.8543769999999999
W	1.3276589999999999	-0.3090640000000000	0.1919440000000000
S	2.6867250000000000	-0.8893489999999999	2.1166269999999998
S	2.2976260000000002	-1.1956709999999999	-1.8264250000000000

$\mathbf{W}_{14}\mathbf{S}_{28}$; $E_{tot}=-6\ 642\ 382.836\ 025\ 34\ \text{eV}$; $E_{rel}=233.774\ 790\ 071\ 4\ \text{meV}/\mathbf{f.u.}$

W	-6.2775280000000002	3.1856249999999999	0.4286820000000000
W	-3.5884200000000002	3.9543759999999999	0.6217850000000000
W	-3.7550770000000000	1.3991720000000001	0.1330010000000000
W	-1.0843529999999999	2.1957320000000000	0.4032420000000000
W	-1.3389979999999999	-0.4176580000000000	-0.1437020000000000
W	1.3732100000000000	0.3775710000000000	0.1373030000000000
W	1.1387270000000000	-2.2903419999999999	-0.4316740000000000
W	3.8543029999999998	-1.4860469999999999	-0.1099980000000000
W	3.6234519999999999	-4.1521460000000001	-0.6882120000000000
W	6.3332420000000003	-3.3555809999999999	-0.3740130000000000
W	6.0912910000000000	-5.9635910000000001	-0.9492400000000000
W	8.7544380000000004	-5.1621680000000003	-0.6192720000000000
W	8.6076820000000005	-7.7096520000000002	-1.1474540000000000
W	11.2912149999999993	-6.9311270000000000	-0.8816520000000000
S	-8.2375640000000008	3.5205329999999999	1.2394660000000000
S	-5.3375180000000002	5.1775260000000003	-0.3142900000000000
S	-4.8128739999999999	2.4754640000000001	2.0736750000000002
S	-6.0476869999999998	1.5197650000000000	-1.0332300000000001
S	-1.7301700000000000	4.2374630000000000	1.8592329999999999
S	-2.6511570000000000	3.0069059999999999	-1.2744409999999999
S	-2.2611469999999998	0.6370420000000000	1.8056810000000001
S	-3.4706210000000000	-0.4728730000000000	-1.2630520000000001

S	0.9880380000000000	2.4784799999999998	1.3608760000000000
S	-0.1783950000000000	1.1435569999999999	-1.5387630000000001
S	0.2298180000000000	-1.2031790000000000	1.5158499999999999
S	-1.0354589999999999	-2.5053470000000000	-1.2915930000000000
S	3.5114610000000002	0.6140640000000001	1.0372410000000001
S	2.3034550000000000	-0.7087960000000000	-1.7899369999999999
S	1.4894799999999999	-4.3818390000000003	-1.5968899999999999
S	2.6890670000000001	-3.0728290000000000	1.2426459999999999
S	4.7797060000000000	-2.5671970000000002	-2.0497250000000000
S	4.0296560000000001	-6.2414860000000001	-1.9294860000000000
S	6.0206200000000001	-1.2698069999999999	0.7709920000000000
S	5.1598059999999997	-4.9324649999999997	0.9934960000000000
S	8.4415510000000005	-3.3063729999999998	0.7901830000000000
S	7.2898379999999996	-4.3885699999999996	-2.3146049999999998
S	6.7746680000000001	-7.9794060000000000	-2.4230360000000002
S	7.6304689999999997	-6.7935939999999997	0.7440780000000000
S	11.0180450000000008	-5.2933950000000003	0.6021280000000000
S	9.8602570000000007	-6.2049779999999997	-2.5502170000000000
S	10.3447770000000006	-8.9391660000000002	-0.1948270000000000
S	13.2745560000000005	-7.2367340000000002	-1.6474409999999999

$\mathbf{W}_{14}\mathbf{S}_{28}$; $E_{tot} = -6\,642\,386.108\,872\,40\text{ eV}$; $E_{rel} = 0\text{ meV/f.u.}$

W	36.3953500000000005	1.5089360000000001	3.4338510000000002
W	34.9914109999999994	3.9414970000000000	3.4348390000000002
W	39.5408169999999970	1.3514480000000000	3.6287379999999998
W	37.6350010000000026	3.8459680000000001	3.4762640000000000
W	36.4279879999999991	6.7402460000000000	3.6309320000000000
W	42.3755329999999972	1.2538890000000000	3.8559120000000000
W	41.2380250000000004	3.8040769999999999	3.6445989999999999
W	39.3987860000000012	6.9852069999999999	3.6449159999999998
W	37.7605199999999996	9.2441600000000008	3.8570970000000000
W	45.3447249999999968	1.1739580000000001	3.9479929999999999

W	43.8636880000000033	3.8358599999999998	3.8845700000000001
W	42.4182830000000024	6.6069699999999996	3.8100280000000000
W	40.7403040000000018	9.2430500000000002	3.8854940000000000
W	39.1773609999999977	11.8564010000000000	3.9457369999999998
S	37.6121750000000006	-0.1502720000000000	4.4114540000000000
S	36.1671260000000032	2.9980080000000000	5.2312089999999998
S	34.1609630000000024	5.8228679999999997	4.4122159999999999
S	40.7979419999999990	-0.3280330000000000	4.6132359999999997
S	39.3627779999999987	3.0329419999999998	5.1176820000000003
S	37.7965080000000029	5.7463550000000003	5.1206009999999997
S	35.6035809999999984	8.6696930000000005	4.6207779999999996
S	43.9415109999999984	-0.2418870000000000	4.9982439999999997
S	42.4683300000000017	2.8642770000000000	5.5292500000000002
S	40.8786059999999978	5.7191479999999997	5.2048620000000003
S	39.2020809999999997	8.5210729999999995	5.5311440000000003
S	37.2484540000000024	11.3508399999999998	4.9952959999999997
S	47.1013140000000021	0.1775880000000000	3.2367940000000002
S	45.8606920000000002	2.9907949999999999	5.1459710000000003
S	44.4986930000000029	5.9445690000000004	4.7618250000000000
S	42.8858230000000020	8.7407369999999993	4.7585959999999998
S	41.0072410000000005	11.3948870000000007	5.1458110000000001
S	39.1952500000000015	13.8752279999999999	3.2333599999999998
S	34.3480099999999965	1.9488200000000000	2.3804430000000001
S	37.9888380000000012	2.0485199999999999	1.8304800000000001
S	36.2542520000000010	5.0488379999999999	1.8307340000000001
S	41.0805549999999968	2.0594260000000002	1.9679359999999999
S	39.5000220000000013	4.9227959999999999	2.2780480000000001
S	37.8083340000000021	7.7197940000000003	1.9688779999999999
S	44.1469659999999990	2.0829179999999998	2.2089099999999999
S	42.7711619999999968	4.9868439999999996	2.0890919999999999
S	41.1904790000000034	7.7200240000000004	2.0893280000000001
S	39.3641530000000017	10.3647740000000006	2.2083290000000000

$W_{15}S_{30}$; $E_{tot} = -7\,116\,838.856\,172\,41$ eV; $E_{rel} = 244.009\,221\,400\,0$ meV/f.u.

W	-6.2845510000000004	3.2147929999999998	0.4431240000000000
W	-3.5986340000000001	3.9517009999999999	0.6280520000000001
W	-3.7755740000000002	1.3943660000000000	0.1368770000000000
W	-1.1233280000000001	2.1836890000000002	0.4044500000000000
W	-1.3523060000000000	-0.4413320000000000	-0.1671800000000000
W	1.3162350000000000	0.3691950000000000	0.1488600000000000
W	1.1472110000000000	-2.3274110000000001	-0.4723030000000000
W	3.7829389999999998	-1.4620420000000001	-0.1118670000000000
W	3.6854809999999998	-4.1888379999999996	-0.7308470000000000
W	6.2725749999999998	-3.2562780000000000	-0.3897910000000000
W	6.2431749999999999	-6.0103119999999999	-0.9365520000000001
W	8.7418189999999996	-5.0289729999999997	-0.6611240000000000
W	8.7354219999999998	-7.7686210000000004	-1.1330260000000001
W	11.1723730000000003	-6.8553499999999996	-0.9413480000000000
W	11.2317470000000004	-9.6172850000000007	-1.3369920000000000
S	-8.2281410000000008	3.5939250000000000	1.2763490000000000
S	-5.3255860000000004	5.1899439999999997	-0.3227290000000000
S	-4.8224900000000002	2.4756710000000002	2.0806360000000002
S	-6.0822450000000003	1.5310210000000000	-1.0041009999999999
S	-1.7333060000000000	4.2176349999999996	1.8674940000000000
S	-2.6815519999999999	3.0019149999999999	-1.2759110000000000
S	-2.2794500000000002	0.5984070000000000	1.7930940000000000
S	-3.5042659999999999	-0.4741280000000000	-1.2634909999999999
S	0.9531320000000000	2.4323790000000001	1.3971210000000001
S	-0.2125620000000000	1.1495460000000000	-1.5405180000000001
S	0.2016030000000000	-1.2729930000000000	1.4832390000000000
S	-1.0571310000000000	-2.5056240000000001	-1.3292450000000000
S	3.4645560000000000	0.5817270000000000	1.0811869999999999
S	2.2508539999999999	-0.6840990000000000	-1.7974000000000001
S	1.4871300000000001	-4.3828170000000002	-1.6171210000000000
S	2.6916929999999999	-3.1360150000000000	1.1959439999999999

S	4.7261819999999997	-2.5121240000000000	-2.0648849999999999
S	4.0407419999999998	-6.2614140000000003	-1.8251070000000000
S	5.9754880000000004	-1.2545720000000000	0.8071640000000000
S	5.2370140000000003	-4.9296490000000004	0.9689310000000000
S	7.2038979999999997	-4.3313319999999997	-2.3404500000000001
S	6.6763170000000001	-7.9934089999999998	-2.2437870000000002
S	8.5197979999999998	-3.0630060000000001	0.5370020000000000
S	7.7938320000000001	-6.7121449999999996	0.7668900000000000
S	11.0682880000000008	-5.0878800000000002	0.4554030000000000
S	9.7185539999999992	-6.1367440000000002	-2.5972439999999999
S	9.3685390000000002	-9.8311969999999995	-2.5415139999999998
S	10.3542570000000005	-8.5707310000000003	0.5325970000000000
S	12.7093209999999992	-8.0500290000000003	-2.2164190000000001
S	12.2716270000000005	-11.4145210000000006	-0.7837410000000000

$\mathbf{W}_{15}\mathbf{S}_{30}$; $E_{tot} = -7\,116\,842.516\,310\,73\text{ eV}$; $E_{rel} = 0\text{ meV/f.u.}$

W	5.2850409999999997	-0.5644530000000000	0.9364360000000000
S	5.0642600000000000	0.9132730000000000	2.6044200000000002
S	7.0299730000000000	-1.4318599999999999	-0.1672660000000000
W	5.1693829999999998	-5.8051909999999998	-1.6467870000000000
S	5.9060720000000000	-7.8049099999999996	-1.4033080000000000
S	3.6203820000000002	-5.5461330000000002	-3.2719019999999999
W	5.2449800000000000	-3.2432490000000000	-0.4173660000000000
S	4.2688110000000004	-2.5002939999999998	1.6871760000000000
S	6.8860679999999999	-4.2966939999999996	-1.7552430000000001
W	-2.2666300000000001	4.5603590000000001	1.8994080000000000
S	-3.8714990000000000	5.9597420000000003	1.2055800000000001
S	-0.4468520000000000	4.6526589999999999	3.2536700000000001
W	0.4027440000000000	2.8839470000000000	1.5816960000000000
S	-1.0028840000000001	4.1025669999999996	0.0079680000000000
S	1.5832839999999999	2.3607779999999998	-0.4017620000000000
W	2.8102920000000000	1.3108970000000000	1.3258960000000000

S	4.1219020000000004	0.6806290000000000	-0.6285720000000000
S	2.3267090000000001	2.9172940000000001	2.9444200000000000
W	2.7768030000000001	-4.0514070000000002	-1.5082329999999999
S	4.0025029999999999	-5.2356100000000003	0.2427680000000000
S	0.8678350000000000	-3.9917760000000002	-2.9991479999999999
W	-7.4679279999999997	2.7651759999999999	-0.0304170000000000
S	-9.5340900000000008	2.7180789999999999	0.5490429999999999
S	-6.9690610000000000	1.5591580000000000	-1.8775489999999999
W	-4.8960179999999998	3.6478950000000001	0.8978990000000000
S	-6.6793170000000002	4.8918090000000003	-0.1091180000000000
S	-3.5319900000000000	2.8330530000000000	2.7679469999999999
W	-4.9855820000000000	1.1930799999999999	-0.4779680000000000
S	-6.2136069999999997	1.7107370000000000	1.5805330000000000
S	-4.4454409999999998	-0.3182240000000000	-2.2899840000000000
W	-2.4649790000000000	2.2244929999999998	0.6499360000000000
S	-0.8535490000000000	1.0684229999999999	2.1261209999999999
S	-3.8543509999999999	3.1088469999999999	-1.1437109999999999
W	-2.5707239999999998	-0.4316350000000000	-0.9877650000000000
S	-1.2235080000000000	1.3227869999999999	-1.3820500000000000
S	-3.6302300000000001	0.0170980000000000	1.0799580000000000
W	0.3405570000000000	-2.4277220000000002	-1.4138750000000000
S	-1.7934079999999999	-2.1612209999999998	-2.4574259999999999
S	1.4737960000000001	-3.4273009999999999	0.3987390000000000
W	2.8777629999999998	-1.4001830000000000	-0.0471880000000000
S	-1.0614610000000000	-1.7335190000000000	0.4478360000000000
S	4.0442090000000004	-2.2047970000000001	-2.0930730000000000
W	0.4701390000000000	0.2914630000000000	0.2154150000000000
S	1.7561540000000000	-0.6345520000000000	1.9925020000000000
S	1.4334410000000000	-0.4835200000000000	-1.8856560000000000

$\mathbf{W}_{16}\mathbf{S}_{32}$; $E_{tot}=-7\,591\,294.927\,140\,82\text{ eV}$; $E_{rel}=263.800\,689\,437\,5\text{ meV/f.u.}$

W	-6.2776430000000003	3.2034520000000000	0.4424480000000000
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W	-3.5913719999999998	3.9542459999999999	0.6143540000000000
W	-3.7624260000000000	1.3971070000000001	0.1352320000000000
W	-1.1031839999999999	2.1914159999999998	0.3927820000000000
W	-1.3379440000000000	-0.4287480000000000	-0.1635530000000000
W	1.3461099999999999	0.3690530000000000	0.1476290000000000
W	1.1524410000000000	-2.3104339999999999	-0.4641480000000000
W	3.8234819999999998	-1.4842850000000001	-0.0949200000000000
W	3.6678679999999999	-4.1661789999999996	-0.7220720000000000
W	6.3322529999999997	-3.3355250000000001	-0.3266290000000000
W	6.1628689999999997	-6.0069299999999997	-0.9639870000000000
W	8.8332040000000003	-5.1913060000000000	-0.5917260000000000
W	8.6405189999999994	-7.8052250000000001	-1.1813730000000000
W	11.2865190000000002	-6.9757670000000003	-0.8556750000000000
W	11.1657469999999996	-9.5290330000000001	-1.3622760000000000
W	13.8367389999999997	-8.7330100000000002	-1.1269870000000000
S	-8.2237880000000008	3.5683889999999998	1.2753270000000001
S	-5.3309990000000003	5.1819819999999996	-0.3282400000000000
S	-4.8070170000000001	2.4831750000000001	2.0786590000000000
S	-6.0706400000000000	1.5199769999999999	-1.0037450000000001
S	-1.7257270000000000	4.2281319999999996	1.8491869999999999
S	-2.6697739999999999	2.9984970000000000	-1.2865409999999999
S	-2.2628430000000002	0.6193230000000000	1.7935740000000000
S	-3.4896630000000002	-0.4775890000000000	-1.2576410000000000
S	0.9737460000000000	2.4594410000000000	1.3646910000000001
S	-0.1848040000000000	1.1490840000000000	-1.5462849999999999
S	0.2114730000000000	-1.2524620000000000	1.4880890000000000
S	-1.0313950000000001	-2.4863149999999998	-1.3475379999999999
S	3.4686560000000002	0.5687489999999999	1.1113489999999999
S	2.3027739999999999	-0.6891290000000000	-1.7857689999999999
S	1.4895980000000000	-4.3840599999999998	-1.6011059999999999
S	2.6845870000000001	-3.1190609999999999	1.2157000000000000
S	4.8130750000000004	-2.5287660000000001	-2.0239900000000000
S	4.0568759999999999	-6.1894559999999998	-1.9692879999999999

S	5.9939150000000003	-1.2578590000000001	0.7987020000000000
S	5.1730919999999996	-4.9763159999999997	0.9679150000000000
S	7.3126579999999999	-4.3664670000000001	-2.2692580000000002
S	6.5864430000000000	-8.0767109999999995	-2.2016830000000001
S	8.4924830000000000	-3.1560910000000000	0.6167899999999999
S	7.6677410000000004	-6.7981999999999996	0.7487450000000000
S	10.9578970000000009	-5.1266189999999998	0.5555520000000000
S	9.8133619999999997	-6.2044629999999996	-2.5404380000000000
S	9.3283880000000003	-9.8181290000000008	-2.6379540000000001
S	10.1842170000000003	-8.6066620000000000	0.5233660000000000
S	13.5707380000000004	-7.0684659999999999	0.3314870000000000
S	12.3884989999999995	-8.0257719999999999	-2.7879339999999999
S	12.9082960000000000	-10.7335510000000003	-0.3929920000000000
S	15.8079079999999994	-9.0505720000000007	-1.9195040000000001

$\mathbf{W}_{16}\mathbf{S}_{32}$; $E_{tot} = -7\,591\,299.147\,951\,85$ eV; $E_{rel} = 0$ meV/f.u.

W	32.7302299999999988	7.2552740000000000	2.8445250000000000
W	31.3849100000000014	9.8341019999999997	2.9671609999999999
W	29.8875630000000001	12.4137760000000004	3.1876000000000002
W	28.3291870000000010	15.2309739999999998	3.4236620000000002
W	34.1830470000000020	9.8585560000000001	3.0512839999999999
W	33.0629789999999986	12.3615689999999994	3.2395800000000001
W	30.9091799999999992	15.3181580000000004	3.4814880000000001
W	29.7947910000000000	17.9992990000000006	3.6310769999999999
W	35.7652360000000016	12.3947360000000000	3.2825020000000000
W	34.6493839999999977	15.0745090000000008	3.4295640000000001
W	32.4966289999999987	18.0304970000000004	3.6738430000000002
W	31.3828679999999984	20.5358009999999993	3.8631479999999998
W	37.2308599999999998	15.1604960000000002	3.4866389999999998
W	35.6731989999999968	17.9730430000000005	3.7234189999999998
W	34.1830640000000017	20.5533000000000001	3.9494799999999999
W	32.8488550000000004	23.1345260000000010	4.0703370000000003

S	32.773361999999988	8.658191999999997	4.654891000000001
S	31.236753000000002	11.377808999999992	4.798061999999998
S	29.518934000000016	14.001939000000001	5.027260000000001
S	27.524954000000010	17.018820000000016	4.491566999999999
S	34.498736999999984	11.296815999999997	4.940392000000001
S	32.748212000000023	14.178297000000006	4.772725000000003
S	31.075582000000007	16.923763000000010	5.276473000000002
S	29.217117999999993	19.916567000000006	4.794198999999999
S	36.084097999999973	13.990209000000001	5.142725000000004
S	34.235258000000017	16.863020999999998	5.083148000000004
S	32.787945999999980	19.585401999999984	5.527502000000001
S	30.991581000000000	22.578769999999987	5.204104000000001
S	37.974274999999987	17.156290999999995	4.310436000000002
S	36.339427000000006	19.883234999999991	4.812978000000002
S	34.688741999999977	22.533501999999986	5.244525000000003
S	32.885314999999985	25.188632999999994	3.453625999999999
S	32.711792000000026	5.198159000000004	3.452329999999999
S	30.887010000000001	7.849752999999998	1.672574999999999
S	29.225678999999995	10.499307999999992	2.103756000000002
S	27.589276999999992	13.233202999999996	2.597235000000000
S	34.583205999999970	7.820331999999996	1.708372000000000
S	32.774774999999982	10.804994999999999	1.387655000000001
S	31.324189000000005	13.527931000000006	1.828967000000000
S	29.474575999999990	16.405629999999986	1.769617000000000
S	36.348100999999998	10.479321999999998	2.121535000000002
S	34.483471000000015	13.467854000000009	1.635891000000000
S	32.809373999999983	16.214755000000003	2.138942999999998
S	31.061534999999992	19.099617999999995	1.974553000000000
S	38.038209000000019	13.370945000000007	2.424847999999999
S	36.039932999999978	16.387243999999990	1.881853000000000
S	34.324500999999979	19.011700000000012	2.115591000000002
S	32.797347000000020	21.731048000000013	2.260946000000001

$W_{36}S_{72}$; $E_{tot} = -17\,080\,416.030\,425\,42$ eV; $E_{rel} = 358.704\,861\,138\,8$ meV/f.u.

W	34.090747999999978	25.350412999999996	3.123679999999998
W	35.188974000000018	27.914725000000007	3.008163000000001
W	35.534191999999973	22.660318000000002	3.260076000000002
W	36.690733000000016	25.186740000000004	3.072143000000001
W	37.040658999999980	20.000630999999985	3.372268000000000
W	38.219361999999967	22.543769000000011	3.165242999999998
W	38.583224999999988	17.301625000000014	3.481112000000000
W	39.798434999999978	19.825831999999983	3.273871000000002
W	40.132500999999978	14.577268999999994	3.574307000000001
W	41.349460000000005	17.086707000000005	3.391359000000000
W	41.694540000000035	11.850616000000005	3.643231000000001
W	42.901153999999982	14.355275999999999	3.451954999999999
W	43.262224000000033	9.123763999999995	3.680394999999999
W	44.461460999999999	11.630057000000008	3.489474000000000
W	44.839280000000022	6.401209999999998	3.704813000000001
W	46.031762999999980	8.909499999999995	3.515839000000002
W	46.421365000000015	3.683460000000002	3.729709000000002
W	47.610318999999969	6.191614999999996	3.540925000000001
W	48.003320000000022	0.966534000000000	3.755869000000001
W	49.191996000000032	3.474564000000000	3.567018000000000
W	49.582106000000031	-1.751201000000000	3.781197999999998
W	50.773913999999978	0.756569000000000	3.592058000000002
W	51.152569999999972	-4.471695999999997	3.808047999999999
W	52.350637999999965	-1.966334999999999	3.616811000000002
W	52.712035999999977	-7.197098999999997	3.846016999999998
W	53.917861000000020	-4.693165999999997	3.654780999999998
W	54.262701999999973	-9.928682000000002	3.907296999999998
W	55.479779000000006	-7.420073999999996	3.724543000000002
W	55.812959999999968	-12.668281999999996	4.025431000000002
W	57.028787999999987	-10.144489999999993	3.817650000000000
W	57.391997000000035	-15.386559999999993	4.135069999999998

W	58.5705760000000026	-12.8427740000000004	3.9257909999999998
W	58.9209419999999966	-18.0289630000000010	4.2288769999999998
W	60.0771420000000020	-15.5039449999999999	4.0367470000000001
W	60.4224109999999968	-20.7570529999999991	4.2925849999999999
W	61.5205529999999996	-18.1924540000000015	4.1736129999999996
S	33.3959789999999970	23.5923669999999994	4.3559489999999998
S	35.4500829999999993	26.4478200000000001	4.7794330000000000
S	34.8524310000000028	20.6686090000000000	4.2211829999999999
S	36.9888139999999979	23.6854419999999983	4.8802159999999999
S	36.4062490000000025	17.9267910000000015	4.2702260000000001
S	38.5292150000000007	20.9693000000000005	4.9727790000000001
S	37.9488460000000032	15.1786089999999998	4.3039259999999997
S	40.0747369999999989	18.2416769999999993	5.0850780000000002
S	39.5345160000000035	12.4497199999999992	4.4346990000000002
S	41.6430900000000008	15.4942379999999993	5.1764910000000004
S	41.1068339999999992	9.7103420000000007	4.4861670000000000
S	43.2260500000000008	12.7604109999999995	5.2309900000000003
S	42.6805820000000011	6.9770250000000003	4.5116420000000002
S	44.8014999999999972	10.0311380000000003	5.2631740000000002
S	44.2606219999999979	4.2541229999999999	4.5344290000000003
S	46.3777410000000003	7.3091679999999997	5.2880019999999996
S	45.8434239999999988	1.5373889999999999	4.5627000000000004
S	47.9577760000000026	4.5913149999999998	5.3136130000000001
S	33.2518189999999976	27.1799229999999987	1.9529669999999999
S	34.9474099999999979	29.9254829999999998	3.7238240000000000
S	35.2129260000000031	24.2322150000000001	1.4315899999999999
S	37.0428599999999975	27.4374210000000005	1.8646590000000001
S	36.7657859999999985	21.5445320000000002	1.5472090000000001
S	38.7130480000000006	24.6144469999999984	2.0190070000000002
S	38.3123610000000028	18.8655569999999990	1.6728300000000000
S	40.4026420000000002	21.9477370000000001	2.4069919999999998
S	39.8582400000000021	16.1657229999999998	1.7778430000000001
S	41.9944709999999972	19.2315070000000006	2.5981209999999999

S	41.3803320000000028	13.4410080000000001	1.8570320000000000
S	43.5187340000000020	16.4936749999999996	2.6290730000000000
S	42.9264750000000035	10.7202889999999993	1.9050950000000000
S	45.0605059999999966	13.7692999999999994	2.6564220000000001
S	44.4928200000000018	8.0014769999999995	1.9336260000000001
S	46.6164220000000000	11.0499369999999999	2.6754430000000000
S	46.0728569999999991	5.2840389999999999	1.9578750000000000
S	48.1889559999999975	8.3351109999999995	2.7034479999999999
S	47.4243680000000012	-1.1770870000000000	4.5929960000000003
S	49.5404720000000012	1.8740619999999999	5.3389709999999999
S	47.6556929999999994	2.5667520000000001	1.9830939999999999
S	49.2358499999999992	-0.1511750000000000	2.0087730000000001
S	48.9967200000000034	-3.8918990000000000	4.6212749999999998
S	51.1204200000000029	-0.8433880000000000	5.3635469999999996
S	50.8121390000000019	-2.8731939999999998	2.0338379999999998
S	49.7700249999999969	5.6206600000000000	2.7339620000000000
S	51.3528960000000012	2.9038260000000000	2.7625380000000002
S	52.9329469999999986	0.1806550000000000	2.7857630000000002
S	50.5521269999999987	-6.6110590000000000	4.6409520000000004
S	52.6864180000000033	-3.5621879999999999	5.3928529999999997
S	52.3873839999999973	-5.6024520000000004	2.0664560000000001
S	54.5066509999999980	-2.5529080000000000	2.8117410000000000
S	52.0935369999999978	-9.3353040000000007	4.6691979999999997
S	54.2319040000000001	-6.2830830000000004	5.4416050000000000
S	53.9698830000000029	-8.3363929999999993	2.1216490000000001
S	56.0784779999999969	-5.2924800000000003	2.8637920000000001
S	53.6174230000000023	-12.0732049999999997	4.7013639999999999
S	55.7535820000000015	-9.0082789999999999	5.5210670000000004
S	55.5373269999999977	-11.0842109999999998	2.2135530000000001
S	57.6637249999999995	-8.0213319999999992	2.9952390000000002
S	55.2092680000000016	-14.7895299999999992	4.8936979999999997
S	57.2996860000000012	-11.7081929999999996	5.6259499999999996
S	57.0813190000000006	-13.8125699999999991	2.3262969999999998

S	59.2054660000000013	-10.7694200000000002	3.0279569999999998
S	56.8994470000000021	-17.4559539999999984	5.2830979999999998
S	58.8471139999999977	-14.3868170000000006	5.7509690000000004
S	58.6207050000000010	-16.5292789999999989	2.4192770000000001
S	60.7577110000000005	-13.5120760000000004	3.0742340000000001
S	58.5698790000000002	-20.2793069999999993	5.4378229999999999
S	60.4000729999999990	-17.0739209999999986	5.8665039999999999
S	60.1594849999999965	-19.2920799999999986	2.5206659999999999
S	62.213689999999997	-16.4358840000000015	2.9391409999999998
S	60.6639419999999987	-22.7687850000000012	3.5782010000000000
S	62.3610120000000023	-20.0218479999999985	5.3449720000000003

$W_{36}S_{72}$; $E_{tot} = -17\,080\,419.119\,506\,29$ eV; $E_{rel} = 272.897\,059\,194\,4$ meV / **f.u.**

W	-5.4306000000000001	27.5598179999999999	-11.5798530000000000
W	-3.6108210000000001	28.3828789999999991	-9.2190989999999999
W	-1.8852720000000001	29.1857460000000017	-6.9849600000000001
W	0.2671110000000000	29.7199549999999988	-4.5188709999999999
W	2.1892930000000002	30.1746969999999983	-2.3309000000000002
W	4.0802600000000000	30.6023040000000002	0.0451010000000000
W	-5.4744349999999997	24.8194540000000003	-12.9967939999999995
W	-3.7165130000000000	25.7242980000000010	-10.6792140000000000
W	-1.9748079999999999	26.3533019999999993	-8.3588839999999998
W	-0.1055600000000000	27.1547310000000017	-5.7224409999999999
W	1.6397349999999999	27.2681159999999991	-3.7075429999999998
W	4.0003700000000002	28.1243690000000015	-0.9417740000000000
W	5.7154930000000004	28.7021219999999992	1.0156460000000000
W	-5.5435590000000001	22.1873259999999988	-14.3673110000000008
W	-3.5832950000000001	23.0568460000000002	-12.0329379999999997
W	3.8646530000000001	24.6771710000000013	-2.3838910000000002
W	5.9069320000000003	25.8604459999999996	-0.1324500000000000
W	-5.4234660000000003	19.2499970000000005	-15.4925250000000005
W	-3.6313599999999999	20.0138999999999996	-13.5878979999999991

W	4.185738999999999	22.141418999999991	-3.151243000000000
W	5.989404000000000	23.088079000000005	-1.150541000000000
W	-5.199376000000000	16.385359999999986	-16.366087000000003
W	-3.479166000000002	17.304905000000015	-14.535313000000004
W	4.139672000000000	19.131263000000006	-4.630374999999999
W	6.078112000000000	20.001695000000016	-2.311796999999999
W	-3.269479000000000	14.383905999999996	-15.509415000000006
W	-1.314893000000001	14.524115999999994	-13.152184999999993
W	0.389685000000000	15.127575000000002	-10.628674999999994
W	2.382893000000001	15.781570000000003	-8.263904999999994
W	4.184378999999998	16.449470000000016	-5.923896000000001
W	5.971110000000004	17.350925000000002	-3.629430999999999
W	-1.442580999999999	12.287305999999992	-14.554145000000001
W	0.457797000000000	12.720603999999998	-12.154273999999991
W	2.192105999999999	13.241011999999996	-9.813940000000006
W	4.016439000000001	13.782064000000001	-7.413144000000000
W	5.877098000000002	14.601580000000002	-5.004120999999996
S	-7.218376000000001	26.662921999999982	-12.573036000000001
S	-5.482935000000003	26.839157000000002	-9.354908999999993
S	-3.565767999999998	27.470316000000004	-6.999369999999999
S	-1.840058000000000	28.494852999999991	-4.676769000000002
S	0.230329000000000	28.811112999999989	-2.333405000000000
S	2.091003000000002	29.414445000000006	-0.010045000000000
S	-7.179177000000001	23.879607000000000	-14.293808000000003
S	-5.395361000000003	23.950475999999983	-10.833809000000005
S	-3.204939000000000	24.490726999999997	-8.520450999999996
S	-0.187631000000000	25.318947000000014	-7.185881000000002
S	-0.121416000000000	25.812532000000009	-3.780713000000000
S	2.263183000000002	26.371099999999984	-1.441947000000001
S	4.209168000000000	26.955100000000016	1.242283000000000
S	-7.109827000000001	20.907882000000007	-15.645070999999997
S	-5.409410000000003	21.252718000000016	-12.310577000000003
S	2.184000999999999	23.125257999999988	-2.377943000000001

S	4.2405559999999998	24.1627319999999983	0.0377470000000000
S	-7.0932969999999997	17.6042009999999998	-16.4057040000000001
S	-5.2488809999999999	18.3579229999999995	-13.2930220000000006
S	3.1524999999999999	21.2431440000000009	-5.0686900000000001
S	4.4751729999999998	21.1817349999999998	-0.9478280000000000
S	-5.0583980000000004	15.4200660000000003	-14.2687659999999994
S	-2.5523520000000000	16.4791740000000004	-12.2406269999999999
S	2.3083689999999999	17.9006949999999989	-5.0099780000000003
S	4.2532329999999998	18.4499870000000001	-2.3578329999999998
S	-3.2725919999999999	13.1663800000000002	-13.3965639999999997
S	-1.3955720000000000	13.6007169999999995	-10.9176599999999997
S	0.4909920000000000	14.1027380000000004	-8.4540220000000001
S	2.3648090000000002	14.8142399999999999	-6.1197319999999999
S	4.2822880000000003	15.5974020000000007	-3.6118950000000001
S	-0.7503260000000000	10.6649670000000008	-13.1500869999999992
S	1.2984199999999999	11.1795139999999993	-10.5930079999999993
S	3.3012329999999999	11.7537310000000002	-8.1687360000000009
S	5.1595589999999998	12.5359780000000001	-5.4504390000000003
S	-4.7412169999999998	29.6431530000000016	-11.1718779999999995
S	-3.0118890000000000	30.5394509999999997	-8.5459180000000003
S	-1.0006880000000000	31.1509749999999990	-6.0207280000000001
S	1.3942559999999999	31.7005780000000001	-3.9224570000000001
S	-3.8232070000000000	26.5994059999999983	-12.9849809999999994
S	-1.9236920000000000	27.3749900000000004	-10.4769439999999996
S	-0.1731250000000000	28.1594249999999988	-8.0426190000000002
S	1.8380490000000000	28.4964960000000005	-5.7645039999999996
S	3.6974190000000000	28.8317140000000016	-3.3066819999999999
S	-3.7416290000000001	23.7700229999999983	-14.2876329999999996
S	-1.7961210000000001	24.3249010000000006	-11.5857589999999995
S	3.4348980000000000	25.8528860000000016	-4.4263620000000001
S	5.5648400000000002	26.6564000000000014	-2.2007279999999998
S	-3.9088449999999999	21.0753139999999988	-15.7369990000000008
S	-2.5437010000000000	20.9727180000000004	-11.6748969999999996

S	5.8610829999999998	23.7964419999999990	-3.3848829999999999
S	7.7105119999999996	24.3674199999999992	-0.1746890000000000
S	-3.7338439999999999	18.1534380000000013	-16.8134669999999993
S	-1.7130449999999999	18.9963189999999997	-14.3497540000000008
S	6.0060529999999996	20.9009320000000010	-4.3818640000000002
S	7.5866959999999999	21.2639700000000005	-1.0144010000000001
S	-4.2360559999999996	14.7730920000000001	-17.6889889999999994
S	-1.5811290000000000	15.8656260000000007	-15.3408350000000002
S	-0.4302770000000000	16.6671990000000001	-12.4175950000000004
S	0.6782460000000000	17.0748449999999998	-9.4234449999999992
S	3.5492669999999999	17.6964019999999991	-8.0365050000000000
S	5.9197930000000003	18.1736110000000011	-5.8157150000000000
S	7.6942760000000003	18.2826780000000007	-2.3582980000000000
S	-2.2281490000000002	12.4791150000000002	-16.6798840000000013
S	0.5136960000000000	13.5420719999999992	-14.4441450000000007
S	2.2092299999999998	14.3189949999999993	-11.9656649999999996
S	4.0600069999999997	14.7394099999999995	-9.5928810000000002
S	5.9303260000000000	15.2865310000000001	-7.2370539999999997
S	7.6872639999999999	15.4739459999999998	-4.0395519999999996
S	5.8898390000000003	29.6642760000000010	-1.1179820000000000
S	3.5644540000000000	32.0994079999999968	-1.6442829999999999
S	7.6130370000000003	27.3991140000000009	0.7513350000000000
S	4.8015580000000000	30.4585900000000009	2.2709500000000000

$\mathbf{W}_{36}\mathbf{S}_{72}$; $E_{tot} = -17\,080\,420.538\,546\,65\text{ eV}$; $E_{rel} = 233.479\,271\,416\,6\text{ meV/f.u.}$

W	14.7435050000000007	15.6508699999999994	4.5271660000000002
W	13.6265610000000006	18.4177509999999991	3.7677719999999999
W	12.1594870000000004	21.0008559999999989	3.3494389999999998
W	10.2345240000000004	24.0144069999999985	2.9359920000000002
W	18.3351539999999993	15.6583970000000008	4.0514809999999999
W	16.3655429999999988	18.2876919999999998	3.7777910000000001
W	15.2789730000000006	20.9580130000000011	3.5453600000000001

W	13.5168730000000004	24.0849760000000011	3.2797950000000000
W	12.0090299999999992	26.5913779999999988	3.4073340000000001
W	21.3418689999999991	15.5927190000000007	3.6107440000000000
W	19.9431310000000011	18.2733260000000008	3.4535969999999998
W	18.0081729999999993	20.5159550000000017	3.4648580000000000
W	16.4036049999999989	23.7087719999999997	3.3027929999999999
W	14.8111610000000002	26.5158039999999993	3.0637819999999998
W	13.4050399999999996	29.0591119999999989	3.3683090000000000
W	24.3199509999999997	15.1458940000000002	2.9434499999999999
W	22.7973759999999999	17.8901339999999998	3.2702730000000000
W	21.6683160000000008	20.4269640000000017	3.1883889999999999
W	18.0689859999999989	26.6415149999999983	3.3699010000000000
W	16.2179520000000004	29.0058059999999998	3.2650760000000001
W	14.6565460000000005	31.8554110000000001	2.8886500000000002
W	26.0228999999999999	18.3311489999999999	2.9949050000000002
W	24.4738650000000000	21.0461260000000010	3.1887509999999999
W	23.2816960000000002	23.5159650000000013	3.2525339999999998
W	21.3609510000000000	26.8324409999999993	3.5348860000000002
W	19.7838449999999995	29.0960770000000011	3.5516410000000000
W	18.2399419999999992	31.7538499999999999	3.3282880000000001
W	27.4535319999999992	20.8936519999999994	3.0105080000000002
W	25.9497630000000008	23.6449110000000005	3.2914349999999999
W	24.4256619999999991	26.1490410000000004	3.4728300000000001
W	22.6480929999999994	29.3288620000000009	3.7922460000000000
W	21.2237699999999982	31.7138980000000004	3.7453580000000000
W	29.2661009999999990	23.9838440000000013	3.0339410000000000
W	27.3223219999999998	26.3676889999999986	3.7343370000000000
W	25.8382189999999987	28.8365089999999995	4.0022500000000001
W	24.1769379999999998	32.0252410000000012	4.4843260000000003
S	16.6950560000000010	14.2904830000000000	5.0344030000000002
S	14.8953120000000006	17.5897310000000004	5.7047860000000004
S	13.4397420000000007	20.3154819999999994	5.2161720000000003
S	11.6948240000000006	22.9886769999999991	4.6939970000000004

S	9.991538999999995	25.740245000000016	4.438606000000001
S	19.850491000000017	14.204368000000005	4.934357000000003
S	18.297633999999986	17.548850000000016	5.271283999999996
S	16.677336000000004	20.154025000000007	5.337500000000004
S	14.968322999999998	22.986757000000008	4.921729000000000
S	13.459291999999996	25.704678000000012	4.979461999999998
S	11.402625000000005	28.528311999999997	4.536876000000004
S	22.991748000000012	14.233307999999992	4.637540000000004
S	21.416848000000017	17.324241000000007	5.151235999999999
S	19.969352000000007	20.505597999999991	4.800017999999997
S	18.346645999999998	24.513971000000015	4.188850999999997
S	14.847025999999996	28.181840999999986	4.962589000000004
S	13.045982999999997	31.178070000000017	4.410389999999996
S	24.730944999999984	16.991775000000005	4.582368999999999
S	23.157647000000008	19.763317000000007	4.785654000000001
S	17.896273999999982	28.295021999999995	4.931042999999998
S	16.273292000000014	31.127150000000003	4.662726000000001
S	26.150470999999996	19.954693999999999	4.740240000000000
S	24.568763000000006	22.632633999999995	4.980425999999996
S	22.308088999999989	25.036584999999988	4.735941999999997
S	21.107092000000015	28.225474999999994	5.363405000000002
S	19.460574000000011	30.999075000000013	5.203445000000003
S	27.836342999999994	22.634796999999989	4.629196000000003
S	25.919786999999995	25.267997000000012	5.162981000000003
S	24.204270000000011	27.943110000000008	5.268580000000000
S	22.547800999999998	30.984384999999996	5.683778000000002
S	29.332343999999991	25.513458000000000	4.765703000000002
S	27.932228999999995	28.306107999999983	4.864087999999997
S	26.284666999999989	30.930931999999985	4.990242000000003
S	13.117300999999994	16.247144999999997	2.962864000000002
S	11.562017000000009	18.937480000000008	2.604271999999999
S	9.998644999999998	21.622182999999997	2.651085000000001
S	16.350055000000011	16.047961999999983	2.648177000000000

S	14.9655020000000007	19.0904440000000015	1.9999460000000000
S	13.6040639999999993	21.9316010000000006	1.8861140000000001
S	11.8480629999999998	24.8422459999999994	1.5595170000000000
S	19.5802359999999993	16.1423370000000013	2.0793360000000001
S	18.0130599999999994	18.7438499999999983	2.0247999999999999
S	16.9222810000000017	21.8854129999999998	1.8794480000000000
S	15.1125640000000008	24.6478870000000008	1.5572710000000001
S	13.2550190000000008	27.4790929999999989	1.5473110000000001
S	22.6921180000000007	16.0004799999999996	1.6026290000000001
S	21.3250199999999985	18.8152310000000007	1.5477380000000001
S	16.6121009999999991	27.3065779999999982	1.6156379999999999
S	14.7920470000000002	30.0438839999999985	1.5113019999999999
S	26.4737280000000013	16.1362610000000011	2.3124549999999999
S	24.4044169999999987	19.0341419999999992	1.6032100000000000
S	22.5817049999999995	21.9542849999999987	1.6378060000000001
S	19.7665970000000009	27.2828909999999993	1.8716720000000000
S	18.1304230000000004	30.0370449999999991	1.8736649999999999
S	16.5958340000000000	33.2773340000000033	2.6052439999999999
S	28.1636470000000010	18.8266710000000010	2.2054900000000002
S	26.0554750000000013	21.8906880000000008	1.4957240000000001
S	24.4685069999999989	24.6223090000000013	1.5956360000000001
S	22.9610149999999997	27.5870029999999993	2.0808010000000001
S	21.2969839999999984	30.2025450000000006	1.9978389999999999
S	19.7587520000000012	33.2731560000000002	2.5816659999999998
S	29.6039530000000006	21.6670510000000007	2.3977490000000001
S	27.6128339999999994	24.9097140000000010	1.7632840000000001
S	25.9729419999999998	27.4575589999999998	2.0663520000000002
S	24.5705959999999983	30.3950519999999997	2.6124630000000000
S	22.8852319999999985	33.1768390000000011	2.9150290000000001
S	24.8618279999999992	33.7035160000000005	5.6375909999999996
S	31.1431250000000013	24.4071950000000015	2.0877560000000002
S	25.0058369999999996	13.3232459999999993	2.0368510000000000
S	13.5909899999999997	14.2647829999999995	5.6962859999999997

S	8.3624340000000004	24.1705849999999991	1.8905940000000001
S	13.5364339999999999	33.3636380000000017	1.8454250000000001

$\mathbf{W}_{36}\mathbf{S}_{72}$; $E_{tot}=-17\,080\,420.855\,527\,82\text{ eV}$; $E_{rel}=224.674\,238\,916\,6\text{ meV/f.u.}$

W	11.8685290000000006	15.8011599999999994	3.6173289999999998
W	10.1458040000000000	18.4072649999999989	3.5953219999999999
W	8.6321999999999992	21.0287119999999987	3.5147089999999999
W	6.9645419999999998	23.6688440000000000	3.3486699999999998
W	5.5622650000000000	26.4978790000000011	3.1853210000000001
W	15.0094089999999998	15.7041529999999998	3.4191950000000002
W	13.1438199999999998	18.1051770000000012	3.3085950000000000
W	11.5096260000000008	20.6624100000000013	3.4741430000000002
W	9.6138469999999998	23.7318670000000012	3.5258020000000001
W	8.1834399999999992	26.2811799999999991	3.3586339999999999
W	7.0573399999999999	29.0806639999999987	3.2033510000000001
W	17.9746680000000012	15.7651950000000003	3.4100999999999999
W	16.0949409999999986	18.1611979999999988	2.8925290000000001
W	11.4947210000000002	26.5860820000000011	3.5308139999999999
W	10.1486289999999997	29.3569159999999982	3.3828040000000001
W	8.6798920000000006	31.5837779999999988	3.2436080000000000
W	21.0356400000000008	15.7690599999999996	3.4834200000000002
W	19.8286030000000011	18.2224900000000005	3.3374229999999998
W	13.0540249999999993	29.1508550000000000	3.5763769999999999
W	11.8471949999999993	31.6048359999999988	3.4300649999999999
W	24.2024830000000009	15.7900899999999993	3.6695229999999999
W	22.7337400000000009	18.0150879999999987	3.5301890000000000
W	21.3878710000000005	20.7875370000000004	3.3827300000000000
W	16.7876219999999989	29.2123279999999994	4.0212370000000002
W	14.9078470000000003	31.6086090000000013	3.5036580000000002
W	25.8255499999999998	18.2924809999999987	3.7093020000000001
W	24.7002519999999990	21.0925210000000014	3.5540479999999999
W	23.2688079999999999	23.6413149999999987	3.3871500000000001

W	21.3728079999999991	26.7105210000000000	3.4390109999999998
W	19.7382939999999998	29.2681949999999986	3.6049289999999998
W	17.8730690000000010	31.6690219999999982	3.4940840000000000
W	27.3196539999999999	20.8753220000000006	3.7268100000000000
W	25.9179630000000003	23.7043849999999985	3.5636049999999999
W	24.2508720000000011	26.3443709999999989	3.3977780000000002
W	22.7366059999999983	28.9661049999999989	3.3176909999999999
W	21.0137849999999986	31.5718479999999992	3.2959120000000000
S	13.1723700000000008	14.2233710000000002	4.5121779999999996
S	11.7096780000000003	17.4755320000000012	5.2304259999999996
S	10.0211450000000006	20.1218830000000004	5.2420679999999997
S	8.1903710000000007	22.7033130000000014	5.1649260000000004
S	6.5456719999999997	25.4243710000000007	5.0087330000000003
S	4.8115439999999996	28.5123250000000006	3.9945300000000001
S	16.4711740000000013	14.1147930000000006	4.2597750000000003
S	14.8978459999999995	17.5236100000000015	4.8659739999999996
S	13.5247410000000006	20.3654949999999992	4.4254920000000002
S	11.6768389999999993	22.9370340000000006	4.6450310000000004
S	9.8867650000000005	25.5123530000000009	5.0846250000000000
S	8.3871009999999995	28.2849499999999985	4.8304159999999996
S	6.5336819999999998	31.3511379999999988	3.9937429999999998
S	19.5856600000000007	14.2139249999999997	4.3778759999999997
S	17.8718859999999999	17.5565339999999992	4.7578659999999999
S	11.5458289999999995	28.2594789999999989	5.1739389999999998
S	10.0848650000000006	31.1708779999999983	5.0569059999999997
S	22.9475799999999985	14.1544980000000002	4.5019489999999998
S	21.0872099999999989	17.3879759999999983	5.1910530000000001
S	19.4888399999999988	20.3831950000000006	4.5239969999999996
S	14.9702750000000009	27.9544730000000001	4.6981780000000004
S	13.3082700000000003	30.9867840000000001	5.1967980000000003
S	24.2760660000000001	17.3890050000000009	5.3391310000000001
S	22.8604909999999997	20.1081620000000001	4.9444390000000000
S	20.7426470000000016	23.1005970000000005	3.8415499999999998

S	18.2399950000000004	28.1583089999999991	5.3330789999999997
S	16.4293690000000012	31.1092860000000009	5.3291069999999996
S	25.9456510000000016	20.0260849999999984	5.3879929999999998
S	24.4997390000000017	22.8386059999999986	5.2405260000000000
S	22.7767510000000009	25.4629420000000017	4.9919130000000003
S	21.4298269999999995	28.3550070000000005	5.1558120000000001
S	19.6324700000000014	31.1900270000000006	5.1463250000000000
S	28.1635220000000004	22.7534680000000016	4.5937770000000002
S	26.4778349999999989	25.7842179999999992	4.3565680000000002
S	24.9184139999999985	28.5778250000000007	4.0109740000000000
S	23.1250399999999985	31.4295979999999986	4.0204490000000002
S	9.7574640000000006	15.9436809999999998	2.8927870000000002
S	7.9641330000000004	18.7953809999999990	2.9018039999999998
S	6.4049699999999996	21.5889769999999999	2.5558459999999998
S	4.7193160000000001	24.6196039999999989	2.3180000000000001
S	13.2500640000000001	16.1833680000000015	1.7670920000000001
S	11.4529429999999994	19.0180800000000012	1.7571790000000000
S	10.1061460000000007	21.9103150000000007	1.9207430000000001
S	8.3832290000000000	24.5347730000000013	1.6722610000000000
S	6.9375489999999997	27.3471319999999984	1.5245530000000000
S	16.4530379999999994	16.2642260000000007	1.5845810000000000
S	14.6423919999999992	19.2151759999999996	1.5807410000000000
S	12.1401830000000004	24.2727819999999994	3.0717189999999999
S	10.0226389999999999	27.2650599999999983	1.9682470000000001
S	8.6069099999999992	29.9844769999999983	1.5740620000000001
S	19.5742030000000007	16.3865650000000009	1.7165189999999999
S	17.9122120000000002	19.4189809999999987	2.2157499999999999
S	13.3941479999999995	26.9901200000000010	2.3897260000000000
S	11.7953670000000006	29.9855739999999997	1.7227600000000001
S	9.9349880000000006	33.2192280000000011	2.4114499999999999
S	22.7975719999999988	16.2019120000000001	1.8559639999999999
S	21.3368390000000012	19.1139709999999994	1.7394499999999999
S	15.0109139999999996	29.8167870000000015	2.1553010000000001

S	13.297095999999998	33.1596770000000021	2.5355170000000000
S	26.3487070000000010	16.021665999999997	2.9191259999999999
S	24.4953170000000000	19.088205999999996	2.0827130000000000
S	22.995934999999993	21.860887999999992	1.8282309999999999
S	21.2058940000000007	24.435812999999996	2.2678650000000000
S	19.357473999999998	27.007533999999997	2.4884800000000000
S	17.9845070000000007	29.849721999999999	2.0474980000000000
S	16.4112860000000005	33.258629999999966	2.6537340000000000
S	28.071335999999987	18.860970999999993	2.9179860000000000
S	26.3370670000000011	21.9488820000000011	1.9032570000000000
S	24.6921320000000009	24.6699580000000012	1.7475909999999999
S	22.861053999999993	27.2514730000000007	1.6713039999999999
S	21.172336999999989	29.8976410000000001	1.6828900000000000
S	19.7099930000000008	33.1497340000000023	2.4011140000000002

$\mathbf{W}_{36}\mathbf{S}_{72}$; $E_{tot} = -17\,080\,425.767\,439\,48$ eV; $E_{rel} = 88.232\,248\,361\,1$ meV/f.u.

W	20.425101999999990	1.4082319999999999	3.3768919999999998
W	23.057916999999998	1.3126880000000001	3.6595240000000002
W	21.6609480000000012	3.7308940000000002	3.7044459999999999
W	26.583773999999982	1.3054120000000000	3.7581259999999999
W	24.906245999999994	3.9854930000000000	3.6643020000000002
W	23.3691500000000012	6.8279280000000000	3.8125369999999998
W	29.635291999999997	1.3331610000000000	3.5605530000000001
W	27.823063999999987	3.7047870000000001	3.5693850000000000
W	26.0371050000000004	6.8608010000000004	3.6394810000000000
W	24.9000200000000014	9.544463999999996	3.6081910000000001
W	32.7469400000000022	1.3529050000000000	3.4578080000000000
W	30.859632999999988	3.7453989999999999	3.5472939999999999
W	29.8423230000000004	6.7919369999999999	3.5310169999999999
W	27.5733120000000014	9.5606690000000008	3.6068180000000001
W	26.471070999999985	12.234472999999995	3.5248770000000000
W	35.8969880000000003	1.3176129999999999	3.5398900000000002

W	34.531129999999974	3.625989999999998	3.607450000000000
W	32.737518999999989	6.951966999999998	3.551445999999999
W	31.380483000000017	9.341691000000009	3.527334000000002
W	29.191790999999985	12.320859000000004	3.630166000000000
W	28.117532000000006	14.899967000000002	3.546387999999999
W	39.003250000000013	1.500221000000000	3.704330999999998
W	37.598044999999990	3.752510000000000	3.689960000000001
W	35.748165000000002	7.034385999999996	3.611784999999998
W	34.350904999999974	9.433464000000007	3.664304000000000
W	32.936289000000021	11.974268999999996	3.583826999999999
W	31.126082000000002	15.316442000000003	3.660299999999999
W	29.769543999999998	17.560179000000015	3.687368999999999
W	42.088419000000018	1.565677999999999	3.720174000000001
W	40.500900000000015	4.024733000000003	3.882544999999999
W	39.058608999999970	6.530400000000002	3.901860999999998
W	37.319816000000030	9.634375000000004	3.929970000000000
W	35.903168000000009	12.067510000000004	3.881873999999998
W	34.173946000000008	15.107120999999994	3.806442000000001
W	32.761512000000033	17.576409999999992	3.822079000000000
W	31.367450999999991	20.199798999999987	3.655660999999998
S	21.454830999999987	-0.270128000000000	4.500424999999999
S	19.511772000000006	3.104328000000002	4.572916000000002
S	24.731099000000004	0.011956000000000	4.679693000000003
S	23.171731999999987	2.960512000000000	5.284429000000003
S	21.411030000000002	5.779466000000002	4.827201999999998
S	28.004189000000002	-0.306653000000000	4.468070000000000
S	26.339992999999998	2.989957000000000	5.341037000000000
S	24.759167999999990	5.747080000000004	5.357981999999998
S	22.653214999999994	8.850913999999995	4.493001999999997
S	31.189011000000007	-0.239469000000000	4.339337000000004
S	29.451312999999990	2.919919999999998	5.276660999999998
S	27.939341999999999	5.808980000000000	4.861845999999999
S	26.224395000000012	8.606631999999994	5.329983000000004

S	24.287919999999997	11.627226000000003	4.448400000000004
S	34.347371000000025	-0.341681000000000	4.104148999999996
S	32.696406000000032	2.953298999999999	5.098347999999997
S	31.192430999999991	5.730755000000003	5.087936000000000
S	29.494987999999993	8.617506000000006	4.975869000000003
S	27.777739000000004	11.381111999999999	5.291871999999997
S	25.903787000000012	14.443682000000008	4.239647999999999
S	37.626989000000018	-0.183209000000000	4.478688000000000
S	35.969664000000016	2.836552999999999	5.326602000000003
S	34.351570000000024	5.738868000000001	5.033896000000004
S	32.771793000000024	8.573930000000007	5.330142000000004
S	31.090690999999996	11.316511000000002	4.996350999999998
S	29.547332000000008	14.153650000000007	5.200585000000002
S	27.682054000000008	17.093697999999998	4.568502999999998
S	40.819519999999971	0.115147000000000	4.830290999999999
S	39.118754000000027	3.073554999999998	5.466333999999998
S	37.411675999999999	5.779278999999998	5.229191000000001
S	35.912705000000025	8.615693000000003	5.421736000000001
S	34.355531999999966	11.287867000000003	5.390699999999998
S	32.729545000000017	14.076190999999997	5.188148000000000
S	31.225933999999987	16.956316999999985	5.449662000000000
S	29.470248999999990	19.825299000000011	4.769060999999998
S	43.846325000000002	0.675577000000000	2.881851999999999
S	42.592900000000002	3.392674000000000	4.944492999999996
S	41.085999000000010	6.108026999999999	4.878428000000004
S	39.493861000000025	8.805472000000000	4.526856999999997
S	37.970551000000004	11.616044999999997	4.959569000000001
S	36.377394999999999	14.344281999999998	4.404195999999998
S	34.841484000000012	17.069883000000008	4.811924999999996
S	33.216355999999976	19.756047999999998	4.857872999999997
S	31.434226999999999	22.166138000000001	2.813520000000000
S	21.732117999999998	2.196387999999998	1.734936000000000
S	24.842956000000009	1.953290000000000	2.155778999999999

S	23.061382999999993	5.013942000000001	2.2067169999999998
S	27.984235999999992	1.8942310000000000	1.8871430000000000
S	26.332018999999990	4.9316370000000003	2.0607410000000002
S	24.5156540000000014	7.8365970000000003	1.9458519999999999
S	31.166969999999992	2.0202049999999998	1.8281210000000001
S	29.4582620000000013	4.8514619999999997	2.0242700000000000
S	27.871694999999990	7.6852000000000000	2.1661940000000000
S	26.1556420000000003	10.5636320000000001	1.8535960000000000
S	34.3677690000000027	1.9567340000000000	1.8054920000000001
S	32.7479390000000024	4.7977210000000001	2.3347259999999999
S	31.178530999999996	7.6341359999999998	1.7960730000000000
S	29.501488999999994	10.413959999999994	2.2290760000000001
S	27.803796999999994	13.2605419999999992	1.8303380000000000
S	37.4977779999999967	2.0118950000000000	1.9175500000000001
S	35.9645390000000020	4.9335820000000004	2.2291859999999999
S	34.3411979999999986	7.7020400000000002	1.8871770000000001
S	32.8205510000000018	10.3870400000000007	1.8907400000000001
S	31.1550529999999988	13.1881789999999999	2.3790309999999999
S	29.4735920000000000	15.9602310000000003	1.9179269999999999
S	40.6721530000000016	2.2761320000000000	2.0600220000000000
S	39.1148730000000029	4.9508159999999997	2.1451799999999999
S	37.7090570000000014	7.8075359999999998	2.2946789999999999
S	36.0330719999999971	10.4788549999999994	2.1392859999999998
S	34.5468740000000025	13.2658339999999999	2.2196270000000000
S	32.8438620000000014	15.9276630000000008	2.0418880000000001
S	31.2774329999999985	18.5988749999999996	2.0150910000000000

$\mathbf{W}_{36}\mathbf{S}_{72}$; $E_{tot} = -17\,080\,426.187\,084\,68$ eV; $E_{rel} = 76.575\,437\,250\,0$ meV/f.u.

W	15.0865570000000009	15.5859790000000000	3.4114510000000000
W	13.357269999999998	18.3298610000000011	3.4927800000000002
W	11.8270680000000006	20.9644709999999996	3.5424310000000001
W	10.4185610000000004	23.7485080000000011	3.4986560000000000

W	18.2351710000000011	15.5095290000000006	3.3775430000000002
W	16.4623150000000003	17.7886670000000002	3.4335789999999999
W	14.5158109999999994	20.7983259999999994	3.4226820000000000
W	13.0303710000000006	23.4740740000000017	3.4332750000000001
W	11.9143690000000007	26.4879199999999990	3.4621770000000001
W	21.1942039999999992	15.5120539999999991	3.4571090000000000
W	19.4361120000000014	17.9709649999999996	3.4158990000000000
W	18.3489250000000013	20.9364179999999998	3.4463200000000001
W	16.8191719999999982	23.6343730000000001	3.5241370000000001
W	14.9371170000000006	26.7592110000000005	3.4370669999999999
W	13.3874479999999991	29.0369400000000013	3.4002129999999999
W	24.3019919999999985	15.6113879999999998	3.5080390000000001
W	23.2325090000000003	18.0166949999999986	3.4313460000000000
W	21.1709519999999998	21.1702499999999993	3.4956860000000001
W	18.0251589999999986	26.1767070000000004	3.4402159999999999
W	16.3129780000000011	29.4297690000000003	3.4536920000000002
W	15.0419490000000007	31.7255129999999994	3.4365130000000002
W	25.9984889999999993	18.2227810000000012	3.5404030000000000
W	24.7977029999999985	20.6680209999999995	3.4300809999999999
W	22.6076799999999984	23.7341629999999988	3.4595039999999999
W	21.1406549999999989	26.1735959999999999	3.5233070000000000
W	19.6474849999999996	29.5770160000000004	3.4546350000000001
W	18.2273239999999994	31.8932010000000012	3.4969560000000000
W	27.5234220000000001	20.8387950000000011	3.4773100000000001
W	26.3801820000000014	23.9304549999999985	3.4738159999999998
W	24.8667990000000003	26.6468600000000002	3.5049410000000001
W	23.2672050000000006	29.3242200000000004	3.4956399999999999
W	21.1371639999999985	31.8976539999999993	3.5013709999999998
W	28.9956010000000006	23.7284849999999992	3.3814690000000001
W	27.5544660000000015	26.5118250000000018	3.4037720000000000
W	26.0359130000000007	29.1268829999999994	3.3898809999999999
W	24.3379459999999987	31.7483579999999996	3.3900470000000000
S	16.3280299999999983	13.9332159999999998	4.2558730000000002

S	14.748974999999997	17.173653000000016	5.120389000000003
S	13.091136000000005	19.906038999999998	5.234923000000002
S	11.546925999999991	22.660323999999992	5.235733999999999
S	9.685321000000001	25.709202999999987	4.374177999999997
S	19.704765999999993	13.909898999999993	4.302038999999997
S	18.032876000000017	17.064412000000008	5.136218999999996
S	16.434456999999983	19.907222999999983	4.712722000000003
S	14.839847000000007	22.716629999999985	4.897983000000000
S	13.292116000000000	25.543234000000018	4.953504999999998
S	11.244977000000004	28.589990000000002	4.265939000000004
S	22.978788000000015	13.985277000000000	4.377437999999997
S	21.312357999999997	17.189461999999989	4.938520999999997
S	19.729928999999985	19.870173000000012	5.017258000000000
S	18.116778000000000	22.667971000000014	5.114428000000002
S	16.414394000000015	25.534953000000016	5.031372000000002
S	14.842587999999992	28.444300999999994	5.135989999999996
S	12.971154999999995	31.481165000000007	4.238338999999999
S	24.672412999999988	17.135624000000000	5.239169999999997
S	22.962424999999996	19.952797000000003	4.886084999999996
S	21.292847999999993	22.798565000000000	5.134038999999996
S	19.654208000000006	25.500296999999998	5.078916000000004
S	18.087997000000014	28.325088000000009	4.802260999999997
S	16.557964999999994	31.219065000000005	5.146237000000002
S	26.287663999999995	19.844214000000009	5.230427999999999
S	24.581507999999995	22.758459999999995	4.722648000000004
S	23.039339999999993	25.606266999999990	4.908585000000004
S	21.356470999999991	28.350618999999982	4.757270000000001
S	19.682753000000017	31.236197000000007	5.243336000000002
S	27.782365999999997	22.669108999999988	5.092749000000004
S	26.256909000000003	25.594419999999995	5.176986999999996
S	24.647496000000003	28.384154999999998	5.181498999999996
S	22.855330999999996	31.157948000000011	5.104881999999999
S	29.834756999999997	25.594795000000013	4.278512000000001

S	28.113610000000013	28.567084000000013	4.4445430000000004
S	26.402425999999984	31.5419330000000002	4.2426250000000003
S	13.024421999999995	15.9151600000000002	2.5725699999999998
S	11.2588760000000008	18.808205999999984	2.5983320000000001
S	9.5759720000000002	21.8482260000000004	2.6424829999999999
S	16.5817970000000017	16.0396080000000012	1.6714739999999999
S	14.8553110000000004	18.9629820000000002	1.8663259999999999
S	13.1274730000000002	21.7929780000000015	1.7246079999999999
S	11.6806350000000005	24.719339999999990	1.7882300000000000
S	19.756983999999992	16.236928999999999	1.7170749999999999
S	18.0067120000000003	19.029053999999986	1.8941239999999999
S	16.395855999999984	21.7900160000000014	2.0711860000000000
S	14.8834260000000000	24.5893780000000000	2.2410459999999999
S	13.280452999999996	27.356013999999983	1.7367480000000000
S	22.843251999999997	16.2181740000000012	1.7886820000000001
S	21.3350240000000007	19.0343060000000008	2.2142110000000002
S	19.7123570000000008	21.8655720000000002	1.8305959999999999
S	18.1520730000000015	24.523977999999996	1.8351740000000001
S	16.5715040000000009	27.468896999999983	1.9183760000000001
S	14.7126540000000006	30.1761160000000004	1.7113900000000000
S	26.366372999999994	15.8381290000000003	2.6416200000000001
S	24.6364160000000005	18.9525390000000016	1.7290360000000000
S	22.9977820000000008	21.762043999999995	2.0467670000000000
S	21.261231999999997	24.609007999999993	1.7919210000000001
S	19.7214440000000018	27.4670540000000010	2.0789130000000000
S	18.034673999999990	30.311081999999990	1.8225070000000001
S	16.295688999999994	33.367485999999995	2.5602870000000002
S	28.1454260000000005	18.799690999999993	2.5788370000000000
S	26.222827999999998	21.884275999999998	1.8998910000000000
S	24.5462160000000011	24.658643999999989	2.0728300000000002
S	22.9671950000000002	27.403628999999987	2.0944620000000000
S	21.3976790000000001	30.2633490000000016	1.9189280000000000
S	19.6884310000000013	33.5229130000000026	2.6354280000000001

S	29.746007999999998	21.775220000000009	2.5516480000000001
S	27.8447050000000011	24.8294420000000002	1.6756970000000000
S	26.3111250000000005	27.5371060000000014	1.6830670000000001
S	24.7059870000000004	30.2076579999999986	1.6798720000000000
S	23.0311669999999999	33.3795900000000003	2.5659250000000000

$W_{36}S_{72}$; $E_{tot} = -17\,080\,426.566\,422\,63$ eV; $E_{rel} = 66.038\,271\,972\,2$ meV/f.u.

W	21.1766040000000011	-0.5167890000000001	3.2206920000000001
W	19.6808590000000017	2.0559620000000001	3.1962419999999998
W	18.1058529999999998	4.5811200000000003	3.0799189999999999
W	16.3186479999999996	7.6388249999999998	3.0995650000000001
W	14.9430770000000006	10.1855550000000008	3.2124310000000000
W	13.3586840000000002	12.7795240000000003	3.1532209999999998
W	11.5438469999999995	15.8087759999999999	3.2050730000000001
W	10.0650639999999996	18.1973230000000008	3.2067830000000002
W	8.3388609999999996	21.1967539999999985	3.2147060000000001
W	6.9673249999999998	23.6759050000000002	3.0968170000000002
W	5.2827260000000003	26.7724790000000006	3.0388280000000001
W	3.9322919999999999	29.4371520000000011	3.1464249999999998
W	2.4944660000000001	32.0400490000000033	3.1767699999999999
W	22.3094390000000011	1.9073880000000001	4.2635690000000004
W	20.9605539999999984	4.3925510000000001	4.3982780000000004
W	19.0933419999999998	7.4514009999999997	4.3827879999999997
W	17.7239749999999994	9.7438490000000009	4.4317690000000001
W	15.9339739999999992	12.8568339999999992	4.4419149999999998
W	14.5289490000000008	15.2521380000000004	4.4596309999999999
W	12.6647990000000004	18.3743330000000000	4.5002950000000004
W	11.2876010000000004	20.6250539999999987	4.4873419999999999
W	9.5260330000000000	23.8346200000000010	4.4480019999999998
W	8.2531070000000000	26.1522860000000001	4.3695959999999996
W	6.5890240000000002	29.3288219999999988	4.3607370000000003
W	5.1523370000000002	31.7651910000000015	4.2229460000000003

W	23.444545999999999	4.350301000000000	5.388473000000000
W	21.914093999999998	7.072413000000000	5.553291999999999
W	20.519013000000001	9.542491000000000	5.712876999999998
W	18.734902999999992	12.587877999999999	5.735071999999997
W	17.172339000000000	15.220917999999993	5.654875999999998
W	15.645965999999996	17.777931999999998	5.706603999999996
W	13.893083000000000	20.794314000000000	5.784467000000000
W	12.459034000000000	23.250057000000000	5.741794999999998
W	10.771290000000000	26.325168000000000	5.717717000000000
W	9.368838999999995	28.774792999999990	5.539314000000000
W	7.826684000000000	31.484069000000000	5.356023000000000
S	20.374542999999992	0.625390000000000	5.050131000000000
S	18.748553000000001	3.318423000000000	4.985179999999997
S	17.070291999999998	6.021132999999998	4.785884000000000
S	15.571120000000000	8.773118999999994	5.057578999999996
S	13.973466000000000	11.473696000000000	5.030180999999998
S	12.319817999999997	14.167503999999992	4.870403999999997
S	10.756318000000000	16.968384000000000	5.137076999999997
S	9.055590000000000	19.626169000000000	4.956128999999998
S	7.586739999999998	22.477591000000000	5.071132999999997
S	5.974257999999998	25.165001000000000	4.770709000000000
S	4.524888999999999	27.985292999999986	4.934599000000000
S	3.058752999999998	30.760508999999990	5.002443999999997
S	23.320510999999998	0.168932000000000	2.952204000000000
S	21.736913999999987	3.119422000000000	6.331249999999998
S	20.046545999999993	5.927087000000000	6.118703000000000
S	18.544190000000000	8.625681000000000	6.443414999999999
S	16.908806999999995	11.366441000000000	6.237936999999996
S	15.313743999999998	14.089499000000000	6.446360000000000
S	13.686025000000000	16.794588000000000	6.247011999999998
S	12.086893999999991	19.590039000000000	6.535048999999999
S	10.485582000000000	22.293215000000000	6.257588000000000
S	8.966034000000000	25.107497999999996	6.450528000000000

S	7.4220430000000004	27.7634539999999994	6.0949330000000002
S	5.8909320000000003	30.6506630000000015	6.2911940000000000
S	23.7696949999999987	5.9985900000000001	6.9267839999999996
S	22.2255250000000011	8.8172149999999991	7.1038290000000002
S	20.5404690000000016	11.6241129999999995	6.9363400000000004
S	18.9910129999999988	14.4332949999999993	7.0525810000000000
S	17.3764199999999995	17.1128120000000017	7.0768279999999999
S	15.7499000000000002	19.8193489999999990	6.9458780000000004
S	14.1380839999999992	22.5986669999999989	7.2239420000000001
S	12.6034199999999998	25.3370169999999995	6.9071160000000003
S	10.9983129999999996	28.1620910000000002	7.1190699999999998
S	9.3977170000000001	30.9311700000000016	6.9049519999999998
S	17.9290219999999998	2.7585299999999999	1.6987099999999999
S	16.3152149999999985	5.5470889999999997	1.8696969999999999
S	14.6873629999999995	8.3610609999999994	1.6685890000000001
S	13.1988090000000007	11.0026840000000004	1.7170799999999999
S	11.5789760000000008	13.7959289999999992	1.9186330000000000
S	9.8673830000000002	16.4178530000000009	1.7183800000000000
S	8.1591009999999997	19.1048420000000014	2.0703429999999998
S	6.6980940000000002	21.8662589999999994	1.6825779999999999
S	5.1647379999999998	24.7247260000000004	1.8557360000000001
S	3.6394270000000000	27.5698480000000004	1.6496810000000000
S	2.3946689999999999	30.4840769999999992	1.5409370000000000
S	0.6277250000000000	33.0199080000000009	3.5769199999999999
S	21.5736810000000006	3.1376750000000002	2.3980440000000001
S	19.9043829999999993	5.8323140000000002	2.5818840000000001
S	18.2805029999999995	8.5709149999999994	2.3718029999999999
S	16.8294940000000004	11.3005329999999997	2.6935110000000000
S	15.1580469999999998	14.0065629999999999	2.4455760000000000
S	13.5134179999999997	16.7863970000000009	2.7119000000000000
S	11.8662379999999992	19.4113620000000004	2.4571879999999999
S	10.3097849999999998	22.1622780000000006	2.6959849999999999
S	8.7900630000000000	24.8581700000000012	2.3682390000000000

S	7.2846390000000003	27.6715049999999998	2.5540989999999999
S	5.8370889999999997	30.5025830000000013	2.3581219999999998
S	4.1808779999999999	33.5333019999999991	2.9205909999999999
S	24.6778680000000001	2.7653020000000001	4.3865030000000003
S	22.8515349999999984	5.7929890000000004	3.6838920000000002
S	21.2277309999999986	8.4331589999999998	3.7257940000000001
S	19.7609460000000006	11.1570630000000008	4.0256230000000004
S	18.1224549999999986	13.9373009999999997	3.8634719999999998
S	16.4972600000000007	16.6056799999999996	3.8187060000000002
S	14.8912870000000002	19.3900019999999991	4.0270590000000004
S	13.2058750000000007	22.0141850000000012	3.8516729999999999
S	11.7681869999999993	24.8323320000000010	4.0140289999999998
S	10.1814780000000003	27.4822659999999992	3.7141780000000000
S	8.7651979999999998	30.2304059999999986	3.6581910000000000
S	7.1056090000000003	33.3566130000000030	4.3503759999999998
S	19.7821390000000008	0.1959630000000000	1.5926910000000001
S	21.0667140000000011	-2.6227879999999999	3.6140270000000001

$\mathbf{W}_{36}\mathbf{S}_{72}$; $E_{tot} = -17\,080\,426.610\,979\,78\text{ eV}$; $E_{rel} = 64.800\,573\,361\,1\text{ meV/f.u.}$

W	19.6917839999999984	1.8842200000000000	3.4141270000000001
W	18.0980209999999992	4.5610809999999997	3.2447270000000001
W	16.6432089999999988	6.9797459999999996	3.0795789999999998
W	14.9450310000000002	10.0442879999999999	3.0315740000000000
W	13.4610389999999995	12.4847300000000008	3.0210650000000001
W	11.6840220000000006	15.4256709999999995	3.0799470000000002
W	10.1637050000000002	17.8660679999999985	3.0904210000000001
W	8.4185390000000009	20.8234740000000009	3.0989599999999999
W	6.9950950000000001	23.2784680000000002	2.9848469999999998
W	5.2881030000000004	26.3617479999999986	2.9204509999999999
W	3.9631720000000001	29.0462099999999985	2.9797560000000001
W	2.5329169999999999	31.6547470000000004	3.0023160000000000
W	22.5887719999999987	1.7289260000000000	3.7051319999999999

W	21.115664999999999	4.146195999999998	3.5943170000000002
W	19.4456130000000016	7.3178460000000003	3.5486040000000001
W	18.1439160000000008	9.6192829999999994	3.4658099999999998
W	16.3614590000000000	12.8163560000000007	3.4078080000000002
W	14.9088150000000006	15.0251570000000001	3.4492959999999999
W	13.0719949999999994	18.1953360000000011	3.4637549999999999
W	11.6182750000000006	20.4057120000000012	3.5045329999999999
W	9.8360620000000001	23.6017849999999996	3.4470010000000002
W	8.5345689999999994	25.9034939999999985	3.3646750000000001
W	6.8644179999999997	29.0751969999999993	3.3192919999999999
W	5.3911230000000003	31.4924239999999998	3.2089490000000001
W	25.4470010000000002	1.5662830000000001	3.9118740000000001
W	24.0168500000000016	4.1749530000000004	3.9338970000000000
W	22.6918569999999988	6.8594189999999999	3.9929320000000001
W	20.9851540000000014	9.9427260000000004	3.9284309999999998
W	19.5619410000000009	12.3980139999999999	3.8140730000000000
W	17.8171199999999992	15.3556000000000008	3.8223989999999999
W	16.2967009999999988	17.7957549999999998	3.8326650000000000
W	14.5199189999999998	20.7369079999999997	3.8910710000000002
W	13.0352580000000007	23.1771129999999985	3.8807540000000000
W	11.3368479999999998	26.2415759999999985	3.8332199999999998
W	9.8818570000000001	28.6599819999999994	3.6685400000000001
W	8.2882750000000005	31.3368889999999993	3.4996849999999999
S	20.7365339999999989	0.1926940000000000	4.4571680000000002
S	19.2854120000000009	3.4376289999999998	5.0752449999999998
S	17.8440210000000015	6.1708720000000001	4.9777909999999999
S	16.1670690000000015	8.7683830000000000	4.7189379999999996
S	14.7489559999999997	11.5983979999999995	4.8195220000000001
S	12.9656880000000001	14.1639680000000006	4.7402270000000000
S	11.4674010000000006	16.9686190000000003	4.8797430000000004
S	9.6633300000000002	19.5630990000000011	4.7940529999999999
S	8.2157940000000007	22.4198060000000012	4.8507340000000001
S	6.5168090000000003	25.0558230000000002	4.6039620000000001

S	5.114382000000000	27.904206999999995	4.719047999999999
S	3.667092999999999	30.692772000000015	4.757005999999996
S	23.962258999999995	0.186828000000000	4.928893000000004
S	22.476984000000016	3.313257999999998	5.440967999999998
S	20.961366000000017	6.107632999999999	5.214519000000001
S	19.504187999999992	8.948957999999993	5.366536000000000
S	17.867578000000017	11.580239000000006	5.059820000000002
S	16.343523000000011	14.367869000000007	5.288694999999997
S	14.619590000000005	16.953393999999994	5.083739999999997
S	13.047449000000003	19.741192000000016	5.351746999999996
S	11.335713000000002	22.368670999999991	5.118913000000000
S	9.873725999999996	25.213380000000008	5.277294000000004
S	8.227702000000007	27.809338000000003	4.957690000000004
S	6.756253000000001	30.728583000000004	5.112023999999999
S	27.126871000000013	0.483485000000000	3.131969999999999
S	26.001526999999994	3.378941000000002	5.142297000000001
S	24.704305999999990	6.263666999999999	4.921699000000003
S	23.110340999999982	9.074495000000006	4.718528000000001
S	21.612998000000010	11.963611000000002	4.861144000000004
S	19.999553999999998	14.646919000000005	4.502182000000004
S	18.379083000000014	17.393882000000014	4.794931000000001
S	16.712600999999994	20.035710999999992	4.542845999999999
S	15.081177000000003	22.758161000000012	4.904881999999997
S	13.470290000000003	25.432593000000007	4.557262999999998
S	11.929982000000008	28.285042000000007	4.759186999999998
S	10.270488000000003	31.016497000000011	4.567012000000001
S	17.709500999999995	2.204645000000002	2.346700999999999
S	16.050253000000014	4.936339000000003	2.153699000000000
S	14.509757000000005	7.788578000000002	2.356023000000000
S	12.899597999999992	10.463592999999995	2.006879000000001
S	11.268190999999998	13.185995000000001	2.368474000000000
S	9.601972000000000	15.827785000000004	2.116702999999998
S	7.980598999999998	18.574220000000004	2.411521000000000

S	6.367367999999999	21.257556999999985	2.051822000000000
S	4.869748999999997	24.146595999999988	2.194738000000000
S	3.275707999999998	26.957515999999983	1.991565999999999
S	1.978240000000000	29.842323000000004	1.771463000000000
S	0.853203000000000	32.737262000000012	3.782760999999998
S	21.223780000000014	2.492386999999999	1.801859000000000
S	19.752348000000013	5.411801999999998	1.955619000000000
S	18.106442000000013	8.007865000000007	1.635709000000000
S	16.644870000000009	10.852764999999998	1.794000000000000
S	14.933203999999999	13.480358000000007	1.560478999999999
S	13.361202000000005	16.268090000000008	1.828616000000000
S	11.637062999999995	18.853678999999996	1.624093000000000
S	10.112470999999993	21.641140000000000	1.853078000000000
S	8.475742999999996	24.272349999999994	1.546450000000000
S	7.018519000000004	27.113814000000014	1.698781000000000
S	5.502985999999999	29.908134000000004	1.472507000000000
S	4.017612999999999	33.034525999999996	1.985339000000000
S	24.312970000000000	2.528051000000000	2.156893999999999
S	22.865795999999996	5.316848000000002	2.194217999999998
S	21.463281999999995	8.165468999999999	2.309083999999999
S	19.764378000000007	10.801401000000003	2.062453000000000
S	18.317316000000017	13.658118000000000	2.119162000000000
S	16.513263999999995	16.252586999999983	2.032808999999999
S	15.014388999999995	19.057276999999991	2.171929000000000
S	13.231052999999993	21.622879999999985	2.093138999999999
S	11.812874000000008	24.453018000000001	2.194043999999999
S	10.135887999999996	27.050587000000002	1.935330000000000
S	8.694661000000000	29.783954000000014	1.838230000000000
S	7.243401999999997	33.028711000000013	2.456964999999998

$\mathbf{W}_{36}\mathbf{S}_{72}$; $E_{tot} = -17\,080\,427.310\,997\,10$ eV; $E_{rel} = 45.355\,647\,805\,5$ meV/f.u.

W	15.160078999999996	15.621788000000005	3.480262000000000
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W	13.531060999999993	18.092646999999995	3.404809999999999
W	11.606657999999995	21.059778999999989	3.252942000000000
W	18.252193999999994	15.504334000000001	3.397806000000001
W	16.525200000000017	17.847580000000007	3.444272999999999
W	14.870215000000000	21.215236999999983	3.386712000000002
W	13.232445000000002	23.739574999999985	3.451141999999999
W	11.590360999999997	26.307254000000004	3.754580999999999
W	21.166146999999987	15.542737999999999	3.402530000000001
W	19.555306999999991	17.829360000000012	3.414320000000000
W	18.040973000000010	21.287435999999996	3.313597999999998
W	16.207467000000012	23.689433999999985	3.418737999999998
W	14.725362000000005	26.173255999999985	3.464112000000001
W	13.502648999999999	29.287389999999985	3.486092999999999
W	24.336321000000016	15.652590999999993	3.531626999999998
W	23.233305999999989	18.035657000000005	3.418931000000002
W	21.163354999999993	21.214041999999992	3.431283000000001
W	19.840247000000015	23.643571000000014	3.434117999999998
W	18.267710000000010	26.122485999999985	3.497447000000002
W	16.595684999999996	29.516315999999998	3.435862999999999
W	15.157890000000001	31.686809000000002	3.438254999999998
W	25.993441000000007	18.266632999999988	3.567277999999999
W	24.802644999999983	20.677571000000004	3.423851000000000
W	22.720473999999994	23.873841999999998	3.467280000000001
W	21.179513000000000	26.171019000000011	3.529196999999999
W	19.697487999999999	29.596731999999994	3.437373000000000
W	18.282961000000002	31.851865000000001	3.473765999999999
W	27.501176000000010	20.887626000000009	3.505504000000002
W	26.401503000000017	23.839456999999995	3.447705000000000
W	24.786312999999998	26.332035000000012	3.452017000000001
W	22.817232000000006	29.552315000000001	3.459384000000000
W	21.278005000000003	31.841170999999992	3.540188999999998
W	29.006758000000014	23.741593999999992	3.420716000000001
W	27.518761000000014	26.504981999999983	3.399157000000002

W	26.0486280000000008	29.0534660000000002	3.4767640000000002
W	24.3838989999999995	31.6897079999999995	3.5373420000000002
S	16.3866820000000004	14.0246379999999995	4.4707119999999998
S	14.8846830000000008	17.2434410000000007	5.1628249999999998
S	13.1870600000000007	19.9684279999999994	4.8772679999999999
S	11.5157959999999999	22.6388269999999991	4.8912519999999997
S	9.7557039999999997	26.0246600000000008	4.8484069999999999
S	19.7502700000000004	13.9584530000000004	4.3771459999999998
S	18.0641010000000009	17.0846629999999990	5.1523729999999999
S	16.4760279999999995	19.9955889999999989	4.7260410000000004
S	14.7768510000000006	22.7882379999999998	5.1379140000000003
S	13.1662029999999994	25.4746689999999987	5.2126289999999997
S	11.3046380000000006	28.7048260000000006	4.0757810000000001
S	23.0244280000000003	14.0330899999999996	4.3729120000000004
S	21.3503219999999985	17.2053890000000003	4.9643329999999999
S	19.5900700000000008	19.9573350000000005	4.7546540000000004
S	18.0126379999999990	22.8787249999999993	4.9677670000000003
S	16.4241549999999989	25.5443220000000011	5.0350799999999998
S	14.9053100000000001	28.3261600000000016	4.9530820000000002
S	13.0196850000000008	31.4786549999999998	4.2946270000000002
S	24.6529880000000006	17.1907169999999994	5.2577920000000002
S	22.9083259999999989	19.9976610000000008	4.8457990000000004
S	21.3442599999999985	22.7746199999999988	5.1718890000000002
S	19.7298459999999984	25.4209539999999983	5.2424020000000002
S	18.1524819999999991	28.3125040000000006	4.8637899999999998
S	16.6386360000000018	31.3078700000000012	5.1836349999999998
S	26.2465440000000001	19.8970239999999983	5.2573299999999996
S	24.5638579999999997	22.7654850000000017	4.7352530000000002
S	22.9972500000000011	25.5943620000000003	5.0624479999999998
S	21.2983839999999987	28.3199450000000006	4.8790190000000004
S	19.7565199999999983	31.3120429999999992	5.2463360000000003
S	27.7994489999999992	22.6708169999999996	5.1343560000000004
S	26.2755909999999986	25.5599850000000011	5.1596390000000003

S	24.535425000000000	28.328562999999991	4.968236000000001
S	22.887707999999999	31.245909999999985	5.263625000000002
S	29.838125999999990	25.636759999999989	4.259137000000000
S	28.180402999999983	28.575566999999995	4.320586999999997
S	26.470358999999984	31.373405999999992	4.370759999999998
S	13.037471999999993	15.877931999999995	2.617175000000000
S	11.347533999999996	18.665630000000002	2.817539000000000
S	9.681577000000000	21.299502000000004	2.317796000000000
S	16.594628000000002	16.071697000000003	1.705408000000000
S	14.930628999999997	19.051838000000001	1.915334000000001
S	13.140084999999991	21.894321999999990	1.757989999999999
S	11.405049000000000	24.718837000000006	2.126427000000001
S	19.713169000000006	16.142727000000007	1.642825999999999
S	18.086559000000012	19.080552999999983	1.977379000000000
S	16.384306999999997	21.934653999999983	1.687281000000000
S	14.742074000000006	24.624089000000014	1.723897000000000
S	13.139129000000005	27.416249000000005	2.020389999999999
S	22.878005999999992	16.215619000000002	1.783779000000000
S	21.331908999999996	19.043147000000012	2.154701000000002
S	19.711610000000003	21.867127000000000	1.685923000000001
S	18.066006000000016	24.521924999999995	1.886506999999999
S	16.515668000000016	27.345874999999995	2.202729999999999
S	14.904042000000005	30.054589000000000	1.742667000000000
S	26.409642999999991	15.883499000000005	2.691199999999998
S	24.643256999999984	18.975363999999990	1.725954999999999
S	22.991572000000015	21.786467999999993	2.048347000000001
S	21.258866000000012	24.629153999999998	1.706243000000000
S	19.693584999999988	27.454426999999990	2.087079000000001
S	18.106266999999990	30.231743999999991	1.739300000000001
S	16.379836000000010	33.238081999999986	2.354947000000001
S	28.158531000000000	18.833133000000001	2.641157999999999
S	26.215044999999999	21.872999000000001	1.867904000000000
S	24.549973999999989	24.560320999999983	1.927022999999999

S	22.897953999999986	27.403528999999989	2.2246269999999999
S	21.3116160000000008	30.2577290000000012	1.7576430000000001
S	19.772704999999984	33.3267140000000026	2.4023029999999999
S	29.759194999999983	21.805205999999983	2.5695470000000000
S	27.857178999999986	24.808185999999992	1.6874370000000001
S	26.128443999999982	27.450852999999986	1.7377940000000001
S	24.5719050000000010	30.112027999999987	1.8278950000000000
S	23.1765350000000012	33.360405999999976	2.6488380000000000

$\mathbf{W}_{36}\mathbf{S}_{72}$; $E_{tot}=-17\,080\,427.847\,475\,86\text{ eV}$; $E_{rel}=30.453\,460\,027\,7\text{ meV/f.u.}$

W	20.078489999999986	1.5131580000000000	3.5816550000000000
W	18.4282350000000008	4.2125519999999996	3.3098250000000000
W	16.9433959999999999	6.6239480000000004	3.0428080000000000
W	15.3855339999999998	9.1276600000000006	2.9442210000000002
W	23.2220100000000009	1.3906879999999999	3.6474540000000002
W	21.5458840000000009	3.6960809999999999	3.4859499999999999
W	19.7265140000000017	6.8670939999999998	3.2320250000000001
W	18.4333600000000004	9.1521960000000000	2.9998890000000000
W	26.4884090000000008	1.3129260000000000	3.6379640000000002
W	24.466062999999983	3.8018010000000002	3.5006059999999999
W	23.4253280000000004	6.8030780000000002	3.3091439999999999
W	21.6424810000000001	9.3050400000000000	3.0571419999999998
W	29.6037859999999995	1.3092040000000000	3.6061700000000001
W	28.016846999999985	3.5792299999999999	3.5741380000000000
W	26.388179999999984	7.0005179999999996	3.3209510000000000
W	24.873250999999998	9.2627520000000008	3.1665580000000002
W	32.6878760000000028	1.2842549999999999	3.6716510000000002
W	31.1877360000000010	3.5644749999999998	3.5754929999999998
W	29.4759090000000015	7.0147060000000003	3.3385460000000000
W	27.9752469999999995	9.2933330000000005	3.2413500000000002
W	35.789343999999998	1.3158470000000000	3.7468659999999998
W	34.2748890000000017	3.5773210000000000	3.5922950000000000

W	32.6454370000000011	6.9996029999999996	3.3393130000000002
W	31.0591270000000002	9.2680270000000000	3.3069139999999999
W	39.0205699999999993	1.2730930000000000	3.8561939999999999
W	37.2371380000000016	3.7751269999999999	3.6037520000000001
W	36.1961319999999986	6.7763809999999998	3.4120089999999998
W	34.1743170000000021	9.2647250000000003	3.2751169999999998
W	42.2298150000000021	1.4260340000000000	3.9130579999999999
W	40.9361409999999992	3.7109000000000001	3.6809789999999998
W	39.1172309999999968	6.8809740000000001	3.4267050000000001
W	37.4405900000000003	9.1880220000000001	3.2655699999999999
W	45.2776660000000035	1.4503239999999999	3.9690120000000002
W	43.7195889999999991	3.9543200000000001	3.8702139999999998
W	42.2346999999999966	6.3655320000000000	3.6030590000000000
W	40.5846159999999969	9.0658480000000008	3.3310670000000000
S	21.2436270000000000	-0.1172240000000000	4.5372839999999997
S	19.7628039999999991	3.2283430000000002	5.1301009999999998
S	18.2930819999999983	5.9257400000000002	4.9366810000000001
S	16.7806190000000015	8.5702160000000003	4.6870890000000003
S	24.6362759999999987	-0.1436830000000000	4.5656600000000003
S	23.0235890000000012	3.0673879999999998	5.2854970000000003
S	21.5385199999999983	5.9076160000000000	4.6064850000000002
S	20.0296330000000005	8.8068740000000005	4.7588169999999996
S	27.9019769999999987	-0.2738480000000000	4.4686279999999998
S	26.2745519999999999	3.0205510000000002	5.1551809999999998
S	24.7970779999999991	5.8459479999999999	4.9231939999999996
S	23.1787220000000005	8.7402029999999993	4.8243460000000002
S	31.0940660000000015	-0.1914330000000000	4.6851029999999998
S	29.5643029999999989	2.9877829999999999	5.3006799999999998
S	27.9439729999999997	5.8139120000000002	4.8121349999999996
S	26.3738139999999994	8.8813899999999997	4.9698060000000002
S	34.2904800000000023	-0.1899380000000000	4.7445079999999997
S	32.7225079999999977	3.0001370000000001	5.3317090000000000
S	31.1107160000000000	5.7979969999999996	4.7712599999999998

S	29.496850999999995	8.862664999999998	5.030910999999997
S	37.482109999999987	-0.260221000000000	4.592590000000004
S	35.840476999999999	3.028525999999998	5.382861000000001
S	34.300052999999983	5.805544000000003	4.717664000000001
S	32.651211000000035	8.787302000000004	5.038979999999996
S	40.707769999999965	-0.162115000000000	4.774619000000004
S	39.051267000000028	3.065021999999999	5.226664000000004
S	37.542442999999987	5.798867999999997	5.040638000000004
S	35.832537000000021	8.673736999999991	4.941405999999997
S	43.957762000000024	0.115111000000000	5.182525000000000
S	42.359037999999982	3.109840000000002	5.563457999999998
S	40.666071999999998	5.766074999999998	5.103437999999997
S	39.032353000000005	8.761371000000005	5.054890000000003
S	47.014985000000029	0.418406000000000	3.258138000000002
S	45.804721000000007	3.372663000000002	5.015943000000000
S	44.305523999999984	6.125002000000003	4.600856000000003
S	42.596358999999996	8.815027999999999	4.310979999999998
S	18.066230000000009	1.762618000000000	2.602304000000002
S	16.357549999999998	4.453369999999996	2.311840000000001
S	14.858328999999995	7.205714999999996	1.897087000000000
S	13.648165999999998	10.160071999999995	3.654866000000002
S	21.630411999999998	1.815846000000001	1.857528000000001
S	19.996869000000002	4.811858000000000	1.809441000000001
S	18.303785000000013	7.468555000000003	1.349352000000001
S	16.705282000000004	10.463397000000005	1.730866000000000
S	24.830344000000002	1.904196000000000	1.971471000000000
S	23.120056999999992	4.779246999999998	1.872891000000001
S	21.611039000000017	7.513404999999997	1.686280999999999
S	19.955187999999997	10.740458999999995	2.138895999999999
S	28.011794999999993	1.791257000000001	1.874719000000000
S	26.362477999999994	4.772502000000002	2.195452000000000
S	24.822737000000001	7.549723000000002	1.530807999999999
S	23.180634000000013	10.838514000000000	2.320574999999998

S	31.166226999999992	1.7160040000000001	1.8824470000000000
S	29.5524670000000000	4.7802780000000000	2.1416100000000000
S	27.9407059999999987	7.5780450000000004	1.5816570000000001
S	26.3725929999999984	10.7683250000000008	2.1689229999999999
S	34.2888280000000023	1.6965159999999999	1.9432689999999999
S	32.7191049999999990	4.7650069999999998	2.1012270000000002
S	31.0985779999999998	7.5901880000000004	1.6117159999999999
S	29.5691689999999987	10.7696500000000004	2.2286899999999998
S	37.4841610000000003	1.8374649999999999	2.0888490000000002
S	35.8652569999999997	4.7318930000000003	1.9900420000000001
S	34.3873620000000031	7.5578450000000004	1.7574749999999999
S	32.7609050000000011	10.8520439999999994	2.4446289999999999
S	40.6333229999999972	1.7709960000000000	2.1544210000000001
S	39.1239339999999984	4.6696970000000002	2.3063630000000002
S	37.6390719999999988	7.5099559999999999	1.6280910000000000
S	36.0259519999999966	10.7215170000000004	2.3473639999999998
S	43.8824070000000006	2.0078079999999998	2.2259319999999998
S	42.3698630000000023	4.6522129999999997	1.9764180000000000
S	40.8996429999999975	7.3495860000000004	1.7828649999999999
S	39.4185319999999990	10.6952510000000007	2.3750710000000002

$\mathbf{W}_{36}\mathbf{S}_{72}$; $E_{tot} = -17\,080\,428.943\,800\,42$ eV; $E_{rel} = 0$ meV/f.u.

W	29.7472859999999990	1.4642590000000000	3.4480390000000001
W	28.0221960000000010	4.1000420000000002	3.3717150000000000
W	26.4643079999999991	6.8070639999999996	3.3385520000000000
W	24.9840020000000003	9.5551259999999996	3.2375250000000002
W	23.5187759999999990	12.2867870000000003	3.0336660000000002
W	22.0002549999999992	14.9712060000000005	2.9904410000000001
W	32.9782709999999994	1.4095080000000000	3.6024729999999998
W	30.8770759999999989	3.8236829999999999	3.4005100000000001
W	29.3146720000000016	6.4201509999999997	3.3448669999999998
W	27.7977510000000017	9.1576480000000000	3.2733810000000001

W	26.1377890000000015	12.3543540000000007	3.1593200000000001
W	24.9731139999999989	14.9047719999999995	2.9382779999999999
W	36.0565939999999969	1.3979490000000001	3.6616580000000001
W	34.5743679999999998	4.0388529999999996	3.5856290000000000
W	33.0292519999999996	6.8666410000000004	3.5691090000000001
W	31.4283439999999992	9.6136990000000004	3.4967709999999999
W	29.8873579999999990	12.3270590000000002	3.3559160000000001
W	27.8106870000000015	14.9144480000000001	3.0689799999999998
W	39.1445790000000002	1.4036940000000000	3.7172420000000002
W	37.33812300000000031	3.8333270000000002	3.5921059999999998
W	35.8087629999999990	6.5312210000000004	3.4698359999999999
W	34.1787780000000012	9.3440449999999995	3.3893279999999999
W	32.5900409999999994	12.1764799999999997	3.3428879999999999
W	31.3434309999999989	14.9047350000000005	3.1691050000000001
W	42.26036100000000032	1.4350909999999999	3.8920040000000000
W	41.0472359999999981	3.8067590000000000	3.7593770000000002
W	39.4169309999999982	7.0493030000000001	3.6652740000000001
W	37.8801190000000005	9.7820119999999999	3.5727799999999998
W	36.2930729999999997	12.3940429999999999	3.5111720000000002
W	34.22628300000000022	14.8313340000000000	3.3016350000000001
W	45.28863100000000023	1.3444300000000000	3.9511630000000002
W	43.72883900000000007	3.9736039999999999	3.9896150000000001
W	42.19263300000000007	6.7417840000000000	3.7250869999999998
W	40.69356200000000000	9.4464980000000001	3.5737230000000002
W	39.13837600000000009	12.1232980000000001	3.5175730000000001
W	37.4213799999999992	14.7653909999999993	3.4496099999999998
S	31.1124809999999989	-0.1533870000000000	4.2860509999999996
S	29.30042600000000016	3.0006699999999999	5.1441229999999996
S	27.6895689999999988	5.7148370000000002	5.0804289999999996
S	26.1777499999999996	8.4753380000000007	5.0078410000000000
S	24.68522000000000011	11.2510739999999991	4.8539640000000004
S	23.2855239999999988	14.1144020000000001	4.6868689999999997
S	34.36529300000000012	-0.1814350000000000	4.4606349999999999

S	32.7043350000000004	3.1296170000000001	5.0250300000000001
S	31.0933369999999982	5.7911570000000001	4.8565610000000001
S	29.5185870000000001	8.5061909999999994	4.7540979999999999
S	27.9339049999999993	11.3207819999999995	4.5289310000000000
S	26.3733590000000007	14.1566880000000008	4.7784300000000002
S	37.5831319999999991	-0.1945500000000000	4.5053270000000003
S	35.8691829999999996	2.9829360000000000	5.3533900000000001
S	34.3650250000000028	5.7998580000000004	5.2457789999999997
S	32.7529550000000000	8.5924519999999998	5.2134580000000001
S	31.1214280000000016	11.3559880000000000	5.1197229999999996
S	29.5270030000000006	14.3387659999999997	4.7232630000000002
S	40.7291620000000023	-0.1637020000000000	4.6283240000000001
S	39.1176900000000032	3.1114210000000000	5.2118169999999999
S	37.5887669999999972	5.8656620000000004	4.9934979999999998
S	36.0351360000000014	8.6252510000000004	4.8163479999999996
S	34.4189829999999972	11.3628459999999993	4.7811310000000002
S	32.6989250000000027	14.1098289999999995	4.9497629999999999
S	43.9146100000000033	-0.0348250000000000	5.0494579999999996
S	42.3691269999999989	3.0095000000000001	5.6300710000000000
S	40.7806399999999982	5.8234000000000004	5.2787170000000003
S	39.2482669999999985	8.7495980000000007	5.3302449999999997
S	37.6497680000000017	11.4890770000000000	5.2574810000000003
S	35.8221660000000028	14.2407570000000003	5.0776909999999997
S	47.0190750000000008	0.3126730000000000	3.2270050000000001
S	45.8115779999999972	3.1757939999999998	5.1193010000000001
S	44.3099040000000031	6.0247010000000003	4.8172259999999998
S	42.8501380000000012	8.8500840000000007	4.4781639999999996
S	41.1990279999999984	11.6859559999999991	4.4822379999999997
S	39.4242580000000018	14.5984280000000002	4.3927090000000000
S	27.7611319999999999	1.6184760000000000	2.4774200000000000
S	25.9662900000000008	4.5284009999999997	2.4392269999999998
S	24.3252929999999985	7.3846930000000004	2.4957919999999998
S	22.9376059999999988	10.2376769999999997	2.1078429999999999

S	21.4501740000000005	13.1308729999999994	1.8546680000000000
S	20.2783060000000006	15.9847579999999994	3.7549899999999998
S	31.3644329999999982	1.9805429999999999	1.8300650000000001
S	29.5193159999999999	4.7337410000000002	1.6437210000000000
S	27.9244680000000010	7.4753140000000000	1.5974100000000000
S	26.4312420000000010	10.3960109999999997	1.6546250000000000
S	24.8314360000000001	13.2571080000000006	1.3137939999999999
S	23.3393100000000011	16.3641399999999990	1.8353440000000001
S	34.5112609999999975	2.1004369999999999	1.9506680000000001
S	32.7659599999999998	4.8529710000000001	2.1561240000000002
S	31.1651659999999993	7.5810300000000002	2.1167470000000002
S	29.6209139999999991	10.3623849999999997	1.9617329999999999
S	28.0470690000000005	13.1579599999999992	1.6887120000000000
S	26.4723390000000016	16.4791400000000010	2.0319989999999999
S	37.6682330000000007	1.9949830000000000	1.9649870000000000
S	36.0691249999999997	4.8460869999999998	1.8187519999999999
S	34.4681190000000015	7.6118059999999996	1.7642869999999999
S	32.8226769999999988	10.4044790000000003	1.7081210000000000
S	31.2950939999999989	13.2516269999999992	1.5666679999999999
S	29.6196799999999989	16.4220919999999992	2.5086710000000001
S	40.7861449999999977	2.0149059999999999	2.0831840000000001
S	39.2644919999999971	4.8939709999999996	2.4104450000000002
S	37.6750469999999993	7.6966140000000003	2.1772580000000001
S	36.0773549999999972	10.4259799999999991	2.0698639999999999
S	34.4505920000000003	13.1116039999999998	1.8841030000000001
S	32.8758709999999965	16.4895159999999983	2.3669519999999999
S	43.9872179999999986	2.1439309999999998	2.2356159999999998
S	42.5215299999999985	4.9600239999999998	2.1460059999999999
S	41.0148429999999991	7.7607470000000003	1.9241969999999999
S	39.4776170000000022	10.5047910000000009	1.8179390000000000
S	37.8495089999999976	13.2142970000000002	1.7550170000000000
S	36.0910459999999986	16.3902500000000018	2.5834380000000001

$W_{66}S_{132}$; $E_{tot} = -31\,314\,097.703\,133\,86$ eV; $E_{rel} = 414.921\,751\,227\,2$ meV/f.u.

W	20.242809999999986	0.8844040000000000	3.3459479999999999
W	21.3533930000000005	3.1796350000000002	3.8684520000000000
W	18.6487550000000013	3.4934789999999998	3.2685940000000002
W	17.1115800000000000	6.1399049999999997	3.2569740000000000
W	15.5626599999999993	8.8361239999999999	3.2584000000000000
W	13.9998269999999998	11.5529299999999999	3.2576459999999998
W	12.4384829999999997	14.2774690000000000	3.2436820000000002
W	10.8690359999999995	17.0006069999999987	3.2281949999999999
W	9.2951460000000008	19.7239690000000003	3.2100620000000002
W	7.7186180000000002	22.4480870000000010	3.1904949999999999
W	6.1401859999999999	25.1730850000000004	3.1749170000000002
W	4.5623790000000000	27.8999150000000000	3.1684570000000001
W	2.9836390000000002	30.6270890000000016	3.1726150000000000
W	22.9595939999999992	0.5146590000000000	3.9090159999999998
W	19.8495710000000010	5.8313730000000001	3.8308059999999999
W	18.3090289999999989	8.5705399999999994	3.7959170000000002
W	16.7404270000000004	11.3036449999999995	3.7453699999999999
W	15.1715479999999996	14.0316720000000004	3.7309809999999999
W	13.6000820000000004	16.7603459999999984	3.7217330000000000
W	12.0240790000000004	19.4861180000000012	3.7122080000000000
W	10.4457020000000007	22.2109899999999989	3.6988400000000001
W	8.8679109999999994	24.9350929999999984	3.6863109999999999
W	7.2887089999999999	27.6589640000000010	3.6811650000000000
W	5.7100609999999996	30.3833899999999986	3.6845880000000002
W	1.4046790000000000	33.3534050000000022	3.1837469999999999
W	2.5531760000000001	35.8359090000000009	3.7061069999999998
W	-0.1743100000000000	36.0806520000000006	3.1949730000000001
W	-1.7518490000000000	38.8085730000000027	3.2010779999999999
W	-3.3279839999999998	41.5378809999999987	3.2011180000000001
W	-4.9035409999999997	44.2677100000000010	3.1979489999999999
W	-6.4794960000000001	46.9972089999999980	3.1959320000000000

W	-8.0563819999999993	49.7263390000000030	3.1987730000000001
W	-9.6341370000000008	52.4540429999999986	3.2074189999999998
W	-11.2123469999999994	55.1806089999999969	3.2190370000000001
W	-12.7906519999999997	57.9059799999999996	3.2289599999999998
W	-14.3684890000000003	60.6304409999999976	3.2318560000000001
W	-15.9474309999999999	63.3536810000000017	3.2261150000000001
W	4.1312749999999996	33.1089479999999980	3.6946850000000002
W	0.9751730000000000	38.5637580000000000	3.7147820000000000
W	-0.6019650000000000	41.2928970000000035	3.7178390000000001
W	-2.1777620000000000	44.0224350000000015	3.7159000000000000
W	-3.7529930000000000	46.7524280000000019	3.7126429999999999
W	-5.3290660000000001	49.4817699999999974	3.7127020000000002
W	-6.9066340000000004	52.2095529999999997	3.7187450000000002
W	-8.4851440000000000	54.9365609999999975	3.7296740000000002
W	-10.0638919999999992	57.6627030000000005	3.7407450000000000
W	-11.6429720000000003	60.3892719999999983	3.7453490000000000
W	-13.2213539999999998	63.1153199999999970	3.7398020000000001
W	-17.5257630000000013	66.0772340000000042	3.2134100000000001
W	-16.3758939999999988	68.5638639999999953	3.7049370000000001
W	-19.1040209999999995	68.8015120000000024	3.1997309999999999
W	-20.6800169999999994	71.5266230000000007	3.1898529999999998
W	-22.2517069999999997	74.2545889999999957	3.1802739999999998
W	-23.8204430000000009	76.9820670000000007	3.1649029999999998
W	-25.3893410000000017	79.7148269999999997	3.1135160000000002
W	-26.9295420000000014	82.4538649999999933	3.0781749999999999
W	-28.4333589999999994	85.1052420000000041	3.0405709999999999
W	-30.0399789999999989	87.7700999999999993	3.0000480000000000
W	-14.7992069999999991	65.8402520000000067	3.7245430000000002
W	-17.9499239999999993	71.2864030000000071	3.6865450000000002
W	-19.5194420000000015	74.0090880000000055	3.6705120000000000
W	-21.0810369999999985	76.7327379999999977	3.6565979999999998
W	-22.6437589999999993	79.4490270000000010	3.6564549999999998
W	-24.1929170000000013	82.1450959999999952	3.6585220000000001

W	-25.7305470000000014	84.7909939999999978	3.6477130000000000
W	-27.3246630000000010	87.3997710000000012	3.5703480000000001
S	21.2080300000000008	-0.8937630000000000	4.5019840000000002
S	19.5459959999999988	2.2020510000000000	5.1200020000000004
S	18.0399819999999984	4.9070479999999996	5.0966920000000000
S	16.5405470000000001	7.6132629999999999	5.0793869999999997
S	15.0166719999999998	10.3370920000000002	5.0738219999999998
S	13.4521949999999997	13.0562120000000004	5.0619350000000001
S	11.8788649999999993	15.7780649999999998	5.0482490000000002
S	10.2994819999999994	18.4993249999999989	5.0316609999999997
S	8.7196239999999996	21.2208289999999984	5.0131249999999996
S	7.1386200000000004	23.9410390000000000	4.9951600000000003
S	5.5585420000000001	26.6600310000000000	4.9842550000000001
S	3.9796719999999999	29.3802629999999994	4.9836010000000002
S	24.7050249999999991	-0.6224640000000000	3.3851499999999999
S	23.2341769999999990	2.2027990000000002	5.3367050000000003
S	21.6797980000000017	5.0777580000000002	5.2155839999999998
S	20.3093049999999984	7.9228139999999998	4.8860650000000003
S	18.7894849999999991	10.6837590000000002	4.7699910000000001
S	17.2150150000000011	13.4029760000000007	4.7549549999999998
S	15.6431860000000000	16.1276849999999996	4.7473200000000002
S	14.0621259999999992	18.8520250000000011	4.7498300000000002
S	12.4831579999999995	21.5779089999999982	4.7399180000000003
S	10.9054330000000004	24.3019649999999992	4.7265079999999999
S	9.3265200000000004	27.0232589999999995	4.7198190000000002
S	7.7468620000000001	29.7433130000000006	4.7229369999999999
S	18.5993430000000011	1.3271250000000001	1.8668359999999999
S	16.7476969999999987	4.0330690000000002	2.0704199999999999
S	15.1292550000000006	6.7465159999999997	2.1596350000000002
S	13.5126050000000006	9.4471139999999991	2.2587950000000001
S	11.9585059999999999	12.1822219999999994	2.2307459999999999
S	10.3957549999999994	14.9089089999999995	2.2127479999999999
S	8.8280250000000002	17.6327479999999994	2.1904390000000000

S	7.256378999999999	20.3573430000000002	2.1675300000000002
S	5.6833570000000000	23.0854320000000008	2.1433230000000001
S	4.1076509999999997	25.8159500000000008	2.1264219999999998
S	2.5293019999999999	28.5461489999999998	2.1235019999999998
S	0.9484430000000000	31.2738970000000016	2.1328990000000001
S	22.1362890000000014	1.6818940000000000	2.0863860000000001
S	20.4981259999999992	4.3994759999999999	2.0218639999999999
S	18.9018799999999985	7.0920690000000004	1.9917330000000000
S	17.3135510000000004	9.7958359999999995	1.9556300000000000
S	15.7249459999999992	12.5231490000000001	1.9262740000000000
S	14.1599909999999998	15.2587810000000008	1.9150940000000001
S	12.5924300000000002	17.9882269999999984	1.9057860000000000
S	11.0206680000000006	20.7146149999999984	1.8933460000000000
S	9.4451710000000002	23.4416119999999992	1.8790940000000000
S	7.8690650000000000	26.1714100000000016	1.8694640000000000
S	6.2917259999999997	28.9021480000000004	1.8681890000000001
S	4.7133159999999998	31.6317799999999991	1.8750180000000001
S	2.4018320000000002	32.1038039999999967	4.9921259999999998
S	0.8236370000000000	34.8309980000000010	5.0037070000000003
S	-0.7552740000000000	37.5610300000000024	5.0125070000000003
S	-2.3337200000000000	40.2922239999999974	5.0154389999999998
S	-3.9103289999999999	43.0231479999999991	5.0135240000000003
S	-5.4854900000000004	45.7525380000000013	5.0104530000000000
S	-7.0605219999999997	48.4797069999999977	5.0106580000000003
S	-8.6367709999999995	51.2052649999999971	5.0167109999999999
S	-10.2148040000000009	53.9307889999999972	5.0272759999999996
S	-11.7938829999999992	56.6578299999999970	5.0385830000000000
S	-13.3725989999999992	59.3868980000000022	5.0453450000000002
S	-14.9505830000000000	62.1168699999999987	5.0437979999999998
S	6.1672479999999998	32.4649039999999971	4.7328279999999996
S	4.5881140000000000	35.1895719999999983	4.7445870000000001
S	3.0092690000000002	37.9169940000000025	4.7550770000000000
S	1.4309590000000001	40.6460489999999979	4.7610250000000001

S	-0.1455810000000000	43.3763480000000001	4.7609830000000004
S	-1.7200430000000000	46.1069049999999976	4.7565400000000002
S	-3.2941650000000000	48.8364369999999965	4.7530489999999999
S	-4.8701499999999998	51.5640619999999998	4.7559300000000002
S	-6.4487340000000000	54.2899730000000034	4.7666279999999999
S	-8.0291139999999999	57.0158720000000017	4.7807529999999998
S	-9.6099010000000007	59.7432990000000004	4.7904369999999998
S	-11.1888240000000003	62.4726819999999989	4.7889869999999997
S	-0.6325040000000000	33.9997839999999982	2.1478359999999999
S	-2.2112029999999998	36.7259030000000024	2.1584870000000000
S	-3.7868719999999998	39.4538110000000017	2.1606610000000002
S	-5.3610699999999998	42.1833260000000010	2.1571850000000001
S	-6.9357889999999998	44.9137360000000001	2.1530459999999998
S	-8.5119830000000007	47.6441790000000012	2.1523690000000002
S	-10.0898029999999999	50.3733629999999977	2.1575829999999998
S	-11.6686949999999996	53.1004259999999988	2.1683650000000001
S	-13.2479340000000008	55.8246570000000020	2.1806070000000002
S	-14.8268609999999992	58.5461489999999998	2.1896540000000000
S	-16.4055789999999995	61.2660229999999970	2.1912170000000000
S	-17.9839599999999997	63.9869249999999994	2.1835730000000000
S	3.1339619999999999	34.3590489999999988	1.8863070000000000
S	1.5555410000000001	37.0846829999999983	1.8967980000000000
S	-0.0207990000000000	39.8104259999999996	1.9029229999999999
S	-1.5957230000000000	42.5377200000000002	1.9032960000000001
S	-3.1708940000000001	45.2670630000000003	1.9002829999999999
S	-4.7473640000000001	47.9980019999999996	1.8984049999999999
S	-6.3254609999999998	50.7291949999999972	1.9012910000000001
S	-7.9042770000000004	53.4590219999999974	1.9098860000000000
S	-9.4825350000000004	56.1859589999999969	1.9213570000000000
S	-11.0600869999999993	58.9093879999999999	1.9299109999999999
S	-12.6382220000000007	61.6296210000000002	1.9295850000000001
S	-14.2173490000000005	64.3486819999999966	1.9192389999999999
S	-16.5273690000000002	64.8456170000000043	5.0335989999999997

S	-18.102969000000016	67.571950999999985	5.019110000000004
S	-19.674804999999992	70.297809000000009	5.006311000000002
S	-21.242504000000003	73.026814000000017	4.996545000000002
S	-22.807760999999993	75.761917999999943	4.985011000000001
S	-24.397452999999987	78.488173000000033	4.954659999999996
S	-25.986527999999998	81.191024999999962	4.918040000000004
S	-27.583106999999983	83.882884000000042	4.887749999999996
S	-29.221565999999993	86.599912000000033	4.822862999999999
S	-12.765036000000003	65.202353000000022	4.773634999999996
S	-14.338530999999997	67.929929999999988	4.750156999999997
S	-15.910320999999997	70.654081000000050	4.727267000000003
S	-17.477994999999999	73.377526000000031	4.704152999999998
S	-19.040896000000000	76.103399999999935	4.685886000000000
S	-20.595086999999995	78.837873999999993	4.657983999999999
S	-22.213304000000008	81.537053999999977	4.759631999999999
S	-23.832616000000016	84.249779000000037	4.849859000000004
S	-25.685286999999989	86.954752999999966	5.053395000000001
S	-19.561641999999991	66.710481000000015	2.169490000000001
S	-21.140613999999994	69.435659999999986	2.159284000000000
S	-22.721917999999987	72.159259000000058	2.161754000000002
S	-24.293641000000009	74.883578999999974	2.153303000000002
S	-25.867788000000009	77.602661999999951	2.137065000000002
S	-27.386421999999996	80.364321000000039	2.018892000000001
S	-28.755434999999985	83.209689999999948	1.689033999999999
S	-30.310166999999999	86.084457999999979	1.568765000000000
S	-31.787046000000001	88.905995000000043	3.521119999999998
S	-15.797836000000002	67.068425000000048	1.901667000000000
S	-17.377710000000004	69.789351999999938	1.882835000000000
S	-18.957398000000013	72.509851999999951	1.865907000000000
S	-20.530915000000002	75.231262000000010	1.851849000000001
S	-22.095081000000004	77.950458999999951	1.840085000000000
S	-23.618085000000007	80.674255000000023	1.835242000000000
S	-25.116884999999999	83.380585999999939	1.818321000000001

S	-26.622596999999990	86.085427999999932	1.7959179999999999
S	-28.286968999999991	89.1799180000000007	2.4147080000000001

$W_{66}S_{132}; E_{tot} = -31\,314\,117.993\,238\,29\text{ eV}; E_{rel} = 107.495\,926\,530\,3\text{ meV/f.u.}$

W	38.4265990000000031	3.0678040000000002	3.0587010000000001
W	41.5293559999999999	2.9178389999999998	3.4590500000000000
W	39.6382150000000024	6.0555170000000000	3.4641310000000001
W	36.6443560000000019	6.0911289999999996	3.0285289999999998
W	35.2916030000000021	8.6650399999999994	3.0554670000000002
W	33.6896720000000016	11.2284760000000006	2.9931090000000000
W	31.9047200000000011	14.2735909999999997	3.0264690000000001
W	30.4469020000000015	16.6758929999999985	3.0325720000000000
W	28.7271740000000015	19.6887800000000013	3.0603530000000001
W	27.3143059999999984	22.1434260000000016	2.9883020000000000
W	25.6001259999999995	25.2168640000000011	2.9823960000000000
W	24.2717789999999987	27.8891209999999994	3.0758420000000002
W	22.8420109999999994	30.4980060000000002	3.1235409999999999
W	38.3232590000000002	8.3742009999999993	3.4698069999999999
W	36.5289730000000006	11.4871619999999997	3.4290949999999998
W	35.1333649999999977	13.8660180000000004	3.4133410000000000
W	33.3047880000000021	17.0064039999999999	3.4337640000000000
W	31.9368850000000002	19.2619019999999992	3.4368599999999998
W	30.1674159999999993	22.4624419999999994	3.4127070000000002
W	28.8606960000000008	24.7603310000000008	3.3706670000000001
W	27.1783900000000003	27.9244340000000015	3.3796909999999998
W	25.7019939999999991	30.3365839999999984	3.3039250000000000
W	44.5173580000000015	2.9279630000000001	3.8823699999999999
W	42.7464799999999983	5.9080320000000004	3.8554029999999999
W	41.3350939999999980	8.3722139999999996	3.8872409999999999
W	39.6023670000000010	11.3747249999999998	3.8582649999999998
W	38.0053729999999987	14.0048069999999996	3.7640030000000002
W	36.5118129999999965	16.5580469999999984	3.7790879999999998

W	34.804510999999980	19.582291000000014	3.8272770000000000
W	33.367820000000018	22.033366000000009	3.7968169999999999
W	31.672869999999996	25.093976000000014	3.7960400000000001
W	30.207083000000008	27.510242000000016	3.6827790000000000
W	28.603207999999986	30.185141000000016	3.5614490000000001
S	39.676039000000029	2.134494999999998	4.8584889999999996
S	37.901491999999975	4.793097999999996	4.7187729999999997
S	36.469861000000016	7.598085000000002	4.8663749999999997
S	34.873350999999995	10.287663000000002	4.8145420000000003
S	33.180165999999998	12.945024999999993	4.6589429999999998
S	31.714726999999999	15.791681999999998	4.8541809999999996
S	29.984729000000015	18.413357999999988	4.7297079999999996
S	28.563879000000000	21.272451000000002	4.8268329999999997
S	26.862650999999996	23.901793000000014	4.6342679999999996
S	25.448886000000017	26.742567999999986	4.7960010000000004
S	23.994184000000006	29.529223000000018	4.8638079999999997
S	42.902754999999991	2.159345000000001	5.3254729999999997
S	41.186306000000019	4.854238999999997	5.0958920000000001
S	39.713123000000031	7.614828000000002	5.3279350000000001
S	38.033676999999973	10.326708999999993	5.0970430000000002
S	36.502896999999973	13.083812000000000	5.2633310000000000
S	34.834952000000012	15.743544000000000	5.0526410000000004
S	33.346882000000008	18.581763999999997	5.2944940000000003
S	31.683831000000014	21.225486000000001	5.0582130000000003
S	30.231434000000001	24.058167000000010	5.2549929999999998
S	28.570951999999983	26.648966999999990	4.9876420000000001
S	27.090184000000007	29.564153000000010	5.1863330000000003
S	46.560969999999975	2.456910999999998	4.8763329999999998
S	44.913206999999999	5.191400999999999	4.5637520000000000
S	43.380325999999966	7.913236000000004	4.8727929999999997
S	41.719152000000011	10.643995000000003	4.6052210000000002
S	40.182519999999967	13.430967000000008	4.6629959999999997
S	38.579875999999987	16.105215999999986	4.6949959999999997

S	36.957551999999997	18.788582999999991	4.5112930000000002
S	35.433362999999999	21.599271999999991	4.787589999999998
S	33.8211920000000035	24.285257999999989	4.479078999999996
S	32.272359999999990	27.129349999999987	4.7374980000000004
S	30.5999610000000004	29.8598420000000004	4.600025999999997
S	36.294176999999977	3.833639999999999	2.2980700000000001
S	34.653543999999966	6.598748999999998	2.013466999999999
S	33.153720999999973	9.2241440000000008	2.0257730000000000
S	31.584848999999984	12.051513999999992	2.2042220000000001
S	29.849989999999982	14.6687630000000002	2.014670999999999
S	28.269186999999987	17.441192999999984	2.3821520000000000
S	26.670394000000017	20.134404000000000	2.035601999999999
S	25.171085999999990	23.0046770000000009	2.2493870000000000
S	23.5715760000000003	25.806200000000005	2.0868380000000002
S	22.271637999999994	28.6897410000000015	1.8943230000000000
S	21.172263999999984	31.5831200000000010	3.922464999999999
S	39.9834170000000029	4.127661999999999	1.8241270000000001
S	38.278416000000000	6.827303999999998	1.594670999999999
S	36.908372000000000	9.610709999999992	1.810700000000000
S	35.160595999999982	12.254870999999996	1.568049000000000
S	33.6061800000000019	15.088184000000000	1.794187999999999
S	31.8998600000000003	17.6926130000000015	1.5738890000000001
S	30.412820000000000	20.5012620000000005	1.8013030000000001
S	28.776714999999994	23.1463380000000001	1.5374220000000001
S	27.3129090000000012	25.9781750000000002	1.740699000000000
S	25.7923410000000004	28.762941999999989	1.555566000000000
S	24.3153140000000008	31.879675999999999	2.0945770000000001
S	43.252246999999970	4.193553999999998	2.1855250000000002
S	41.4930390000000031	6.846582999999999	2.0649190000000002
S	40.090341999999997	9.635586999999992	2.2032090000000002
S	38.421340999999982	12.382089999999998	2.0415640000000002
S	36.7766230000000007	15.027948999999996	1.978537999999999
S	35.252944999999969	17.856042999999997	2.1305260000000001

S	33.529055999999971	20.467040999999983	2.0134020000000001
S	32.125377999999978	23.317558999999993	2.1308449999999999
S	30.439499000000014	25.920221999999990	1.9276370000000000
S	28.989208999999989	28.647311999999994	1.8817699999999999
S	27.543798999999999	31.880331999999992	2.5407310000000001
W	55.737710999999973	-26.653331000000014	3.3504330000000002
W	58.638809999999994	-26.804127999999986	3.6093359999999999
W	57.162641999999982	-24.392482999999986	3.5328620000000002
W	54.133738000000010	-23.978407000000007	3.2291580000000000
W	52.667537000000029	-21.562172000000003	3.1157800000000000
W	50.972957999999984	-18.501487000000009	3.1148099999999999
W	49.535983999999991	-16.050709000000012	3.0849850000000001
W	47.828837000000000	-13.026491000000000	3.1333440000000001
W	46.334904000000016	-10.473390999999995	3.1486719999999999
W	44.738436000000001	-7.843213999999997	3.0542539999999998
W	43.005406999999982	-4.840800999999999	3.0257520000000002
W	41.594002000000032	-2.376557000000000	3.0579040000000002
W	39.823045999999979	0.603426000000000	3.0312370000000000
W	55.480437999999995	-21.228500000000004	3.5420170000000000
W	54.172978000000005	-18.930223999999991	3.4997600000000002
W	52.403939000000012	-15.730698000000003	3.4759829999999998
W	51.035913000000007	-13.474232000000007	3.4795170000000000
W	49.207748999999997	-10.334749000000004	3.5000689999999999
W	47.811458000000018	-7.955028000000004	3.4842100000000000
W	46.017605000000032	-4.842969000000001	3.4435639999999998
W	44.702199999999977	-2.523787000000000	3.4494570000000002
W	42.811140000000017	0.613568000000000	3.4545469999999998
W	61.498783000000031	-26.966001999999996	3.7899569999999998
W	60.069091999999977	-24.357407999999995	3.8372600000000001
W	58.740586999999979	-21.684813999999994	3.9307270000000001
W	57.026465000000017	-18.611651999999994	3.9250039999999999
W	55.613360000000001	-16.157206999999997	3.8534169999999999
W	53.893653999999979	-13.144368000000001	3.8813499999999999

W	52.4355860000000007	-10.7420860000000005	3.8877359999999999
W	50.6508719999999997	-7.6968500000000004	3.9209329999999998
W	49.0486950000000022	-5.1336000000000004	3.8585910000000001
W	47.6961629999999985	-2.5595300000000001	3.8852780000000000
W	45.9137199999999979	0.4636920000000000	3.8551720000000000
S	56.7968699999999984	-28.3484049999999996	4.3717259999999998
S	55.3514709999999965	-25.1153890000000004	5.0303490000000002
S	53.9010400000000018	-22.3885189999999987	4.9842839999999997
S	52.2151289999999975	-19.7861669999999989	4.7814319999999997
S	50.8112560000000002	-16.9356059999999999	4.8990700000000000
S	49.0874489999999994	-14.3246819999999992	4.7819240000000001
S	47.5637919999999994	-11.4965229999999998	4.9341410000000003
S	45.9191629999999975	-8.8508589999999998	4.8713040000000003
S	44.2500319999999974	-6.1042500000000004	4.7098170000000001
S	42.8473559999999978	-3.3153280000000001	4.8483200000000002
S	41.0881720000000001	-0.6622190000000000	4.7279580000000001
S	60.0250839999999997	-28.3477229999999984	4.8184399999999998
S	58.5480859999999979	-25.2311119999999995	5.3572839999999999
S	57.0275639999999981	-22.4464380000000006	5.1721149999999998
S	55.5635699999999986	-19.6148549999999986	5.3753299999999999
S	53.9274619999999985	-16.9697889999999987	5.1118560000000004
S	52.4402419999999978	-14.1613640000000007	5.3393379999999997
S	50.7340390000000028	-11.5568460000000002	5.1193150000000003
S	49.1795100000000005	-8.7236279999999997	5.3453960000000000
S	47.4319649999999982	-6.0793670000000004	5.1029410000000004
S	46.0618359999999996	-3.2960330000000000	5.3188560000000003
S	44.3568989999999985	-0.5962790000000000	5.0894510000000004
S	63.1685879999999997	-28.0513869999999983	2.9914710000000002
S	62.0689490000000035	-25.1578909999999993	5.0193580000000004
S	60.7689809999999966	-22.2744190000000017	4.8264930000000001
S	59.1694650000000024	-19.4728470000000016	4.6640519999999999
S	57.6699270000000013	-16.6028200000000012	4.8784460000000003
S	56.0712299999999999	-13.9095540000000000	4.5320229999999997

S	54.4902810000000031	-11.1373250000000006	4.8997210000000004
S	52.7554939999999988	-8.5201680000000000	4.7102909999999998
S	51.1865519999999989	-5.6926360000000003	4.8886659999999997
S	49.6867859999999979	-3.0672999999999999	4.9007569999999996
S	48.0461290000000005	-0.3021450000000000	4.6159450000000000
S	53.7413170000000022	-26.3277450000000002	2.3116409999999998
S	52.0687830000000034	-23.5974229999999991	2.1740219999999999
S	50.5198239999999988	-20.7531819999999989	2.4326859999999999
S	48.9076120000000003	-18.0673959999999987	2.1240899999999998
S	47.3834390000000027	-15.2567009999999996	2.4006259999999999
S	45.7611580000000018	-12.5733800000000002	2.2170239999999999
S	44.1584050000000019	-9.8992020000000007	2.2491629999999998
S	42.6217060000000032	-7.1123849999999997	2.3073100000000002
S	40.9602569999999986	-4.3815929999999996	2.0401660000000001
S	39.4272350000000031	-1.6599379999999999	2.3496069999999998
S	37.7793449999999993	1.0745700000000000	2.0375009999999998
S	57.2510750000000002	-26.0319819999999993	1.7260510000000000
S	55.7701029999999989	-23.1167489999999987	1.9246630000000000
S	54.1098429999999979	-20.5260120000000015	1.6575130000000000
S	52.6572269999999989	-17.6934730000000009	1.8544730000000000
S	50.9941659999999999	-15.0497019999999999	1.6184400000000001
S	49.5059269999999988	-12.2116699999999998	1.8602479999999999
S	47.8382999999999967	-9.5518649999999994	1.6498999999999999
S	46.3072569999999999	-6.7949320000000002	1.8161400000000001
S	44.6277010000000018	-4.0831450000000000	1.5854740000000000
S	43.1542170000000027	-1.3226789999999999	1.8175880000000000
S	41.4376239999999996	1.3721179999999999	1.5881130000000001
S	60.3469440000000006	-25.9972549999999991	2.0493440000000001
S	58.8923739999999967	-23.2105539999999984	2.1171400000000000
S	57.4783850000000029	-20.3697069999999982	2.2789060000000001
S	55.7771490000000014	-17.7404089999999997	2.0864579999999999
S	54.3562280000000015	-14.8812780000000000	2.1837949999999999
S	52.6263920000000027	-12.2596559999999997	2.0594939999999999

S	51.160792999999982	-9.413069000000001	2.254887000000001
S	49.467666999999987	-6.755956000000003	2.099294000000000
S	47.870961999999987	-4.066368999999999	2.047442000000002
S	46.4391900000000035	-1.261563999999999	2.195044000000002
S	44.664436999999995	1.396964000000001	2.055140000000002

$W_{66}S_{132}$; $E_{tot} = -31\,314\,118.192\,179\,17\text{ eV}$; $E_{rel} = 104.481\,670\,772\,7\text{ meV/f.u.}$

W	20.015346000000010	1.466178999999999	3.405208000000000
W	18.291754999999984	4.187847999999998	3.519616000000001
W	16.785350000000011	6.827239999999998	3.586595000000000
W	15.286139000000004	9.513037000000006	3.552017999999999
W	13.858162000000001	12.304254999999995	3.525977000000001
W	23.158471999999997	1.292897000000000	3.383589999999999
W	21.522231999999989	3.619234000000001	3.487585000000002
W	19.528607999999984	6.639726999999997	3.454378000000002
W	17.938303000000012	9.471460999999997	3.470143000000002
W	16.474105000000016	12.170552000000007	3.482189000000000
W	15.349384000000006	15.151061000000003	3.434035999999999
W	26.247036999999988	1.238104000000001	3.382814000000002
W	24.644780999999983	3.510594000000002	3.455226000000001
W	23.185303000000011	7.024625999999996	3.377413000000002
W	21.775825999999986	9.707255000000000	3.487220000000002
W	20.254384000000017	12.227007000000004	3.481415999999998
W	18.046610999999986	15.367248000000000	3.505980000000001
W	16.822126999999983	17.838242000000010	3.392030999999998
W	29.334924999999984	1.293288000000000	3.385698999999998
W	27.846781000000000	3.510473999999999	3.456639000000000
W	26.245788999999985	6.892126000000002	3.336952000000001
W	24.826812000000003	9.270198999999999	3.415932999999999
W	23.015551999999996	12.537618999999994	3.462568999999998
W	21.740318999999995	14.968282000000003	3.452040999999999
W	19.579143999999994	18.141833999999993	3.505726999999998

W	18.2888720000000013	20.5444360000000010	3.6014080000000002
W	32.4774320000000003	1.4672689999999999	3.4096120000000001
W	30.9686480000000017	3.6195240000000002	3.4917579999999999
W	29.3058130000000006	7.0248629999999999	3.3804029999999998
W	27.6646910000000013	9.2702410000000004	3.4175970000000002
W	24.7376879999999986	14.9383429999999997	3.4381089999999999
W	23.1083649999999992	18.3505450000000003	3.3684189999999998
W	21.5213490000000007	20.5895949999999992	3.4940880000000001
W	19.7343739999999990	23.9295089999999995	3.3950010000000002
W	18.5956650000000003	26.2807800000000000	3.3328080000000000
W	34.2008810000000025	4.1899720000000000	3.5273330000000001
W	32.9636619999999994	6.6419779999999999	3.4615980000000000
W	30.7144809999999993	9.7079710000000006	3.4920179999999998
W	29.4741369999999989	12.5376609999999999	3.4661170000000001
W	27.7527329999999992	14.9388939999999995	3.4388310000000000
W	26.2447139999999983	18.4102519999999998	3.3346979999999999
W	24.6583410000000001	20.6353760000000008	3.4873789999999998
W	23.0413059999999987	24.0361699999999985	3.3851190000000000
W	21.5635629999999985	26.2738569999999996	3.3854899999999999
W	35.7059799999999967	6.8278900000000000	3.5961599999999998
W	34.5527820000000006	9.4759840000000004	3.4797539999999998
W	32.2343839999999986	12.2280599999999993	3.4876900000000002
W	30.7482959999999999	14.9695560000000008	3.4547759999999998
W	29.3806779999999996	18.3500580000000006	3.3675570000000001
W	27.8322840000000014	20.6357220000000012	3.4847990000000002
W	26.2454859999999996	24.0569850000000010	3.3814860000000002
W	24.6829420000000006	26.3066220000000008	3.4158960000000000
W	37.2050259999999966	9.5130420000000004	3.5638239999999999
W	36.0126509999999982	12.1754090000000001	3.4929779999999999
W	34.4464019999999991	15.3637379999999997	3.5123950000000002
W	32.9134499999999974	18.1394419999999990	3.5050669999999999
W	30.9674639999999997	20.5919220000000003	3.4858400000000000
W	29.4499969999999998	24.0366050000000016	3.3716210000000002

W	27.801390000000014	26.307023999999984	3.405317999999998
W	38.630375000000008	12.307029000000000	3.540246999999999
W	37.141202999999973	15.155227000000000	3.445882999999998
W	35.665880999999988	17.840402000000010	3.394985000000001
W	34.199184000000025	20.547436999999986	3.593437999999999
W	32.750535999999968	23.932636999999997	3.368619999999999
W	30.920532999999989	26.274089000000000	3.356317000000002
W	33.891500000000006	26.281451000000006	3.290370999999999
S	21.199946000000006	-0.220816000000000	4.258061999999998
S	19.751086999999983	3.048422000000000	5.122556000000003
S	18.110255999999997	5.774465000000002	5.265286999999998
S	16.563493000000011	8.498412000000001	5.271946999999999
S	15.009050999999995	11.230207999999993	5.255442999999996
S	13.092677999999994	14.233777999999992	4.369245000000003
S	24.593714999999995	-0.268183000000000	4.369645000000002
S	23.040043000000007	2.883741999999998	5.157452000000001
S	21.461460999999999	5.777886999999998	4.736010000000003
S	19.879789999999998	8.600726999999991	4.796059999999998
S	18.329284000000012	11.374190999999997	4.908318999999997
S	16.638068000000005	14.155162000000007	5.063418000000004
S	14.620426999999994	17.171900999999983	4.246472999999999
S	27.898514999999997	-0.268149000000000	4.370779999999999
S	26.245249999999986	2.855348000000002	5.133835000000004
S	24.643239999999987	5.662695000000003	4.762596000000003
S	23.167343999999999	8.624675999999991	5.134440999999998
S	21.712060000000010	11.420066000000003	5.198062000000002
S	19.866272999999996	14.255988000000003	4.849757999999996
S	18.190335000000010	17.087478999999983	5.189487999999999
S	16.138920999999999	20.039131000000011	4.231023000000004
S	31.292587999999985	-0.220759000000000	4.259980999999998
S	29.450265999999992	2.883675999999999	5.160337000000002
S	27.847176000000010	5.662581999999996	4.763998000000000
S	26.244734999999986	8.469364000000006	5.154538999999998

S	25.0307740000000010	11.3435690000000005	4.7081689999999998
S	23.1879010000000001	14.2332239999999999	5.1721529999999998
S	21.4683460000000004	17.0854740000000014	4.7641200000000001
S	19.8542960000000015	19.8768379999999993	5.1881399999999998
S	18.1344530000000006	22.7044040000000003	4.6768489999999998
S	32.7393029999999996	3.0487440000000001	5.1275100000000000
S	31.0292190000000012	5.7783480000000003	4.7397299999999998
S	29.3221209999999992	8.6246600000000004	5.1378300000000001
S	27.4588859999999997	11.3435220000000001	4.7097319999999998
S	26.2443740000000005	14.2419119999999992	5.0787950000000004
S	24.6802069999999993	17.1439069999999987	4.7627020000000000
S	23.0619160000000001	19.9643669999999993	5.1831079999999998
S	21.4187599999999989	22.7838719999999988	4.7530250000000001
S	34.3793640000000025	5.7750760000000003	5.2736950000000000
S	32.6098149999999976	8.6022809999999996	4.8027470000000001
S	30.7756609999999995	11.4207610000000006	5.2034349999999998
S	29.3005609999999983	14.2342300000000002	5.1747579999999997
S	27.8101309999999984	17.1447049999999983	4.7637580000000002
S	26.2461179999999992	20.0138479999999994	5.1720189999999997
S	24.6409990000000008	22.8197620000000008	4.7833959999999998
S	35.9241760000000028	8.4997520000000009	5.2820559999999999
S	34.1584199999999996	11.3769050000000007	4.9180750000000000
S	32.6230669999999989	14.2563040000000001	4.8546399999999998
S	31.0219920000000009	17.0875899999999987	4.7650249999999996
S	29.4296450000000007	19.9674839999999989	5.1787590000000003
S	27.8531370000000003	22.8217449999999999	4.7781560000000001
S	37.4756399999999985	11.2322849999999992	5.2669300000000003
S	35.8522970000000001	14.1587060000000005	5.0759509999999999
S	34.2972620000000035	17.0882110000000011	5.1923870000000001
S	32.6344629999999967	19.8808979999999984	5.1810809999999998
S	31.0740100000000012	22.7893399999999993	4.7402069999999998
S	39.3966369999999984	14.2334390000000006	4.3868349999999996
S	37.8682939999999988	17.1754449999999999	4.2560680000000000

S	36.349766999999999	20.042498999999994	4.2262259999999996
S	34.3537609999999987	22.708452999999997	4.6579360000000003
S	17.9473230000000008	1.8034220000000001	2.5922800000000001
S	16.1725439999999985	4.6304829999999999	2.7434280000000002
S	14.5868889999999993	7.4817799999999997	2.6967270000000001
S	12.9906900000000007	10.4413520000000002	2.6717290000000000
S	21.5323020000000014	1.9162680000000001	1.6852980000000000
S	19.8236449999999991	4.7923000000000000	1.9188850000000000
S	18.0929900000000004	7.6524450000000002	1.8077030000000001
S	16.5537300000000016	10.4606270000000006	1.7864059999999999
S	15.0740180000000006	13.3595520000000008	1.8068850000000001
S	24.6900140000000015	1.7689500000000000	1.6604449999999999
S	23.0570720000000016	4.8296590000000004	2.0610599999999999
S	21.3502940000000017	7.6948949999999998	2.0356730000000001
S	19.8554880000000011	10.4063920000000003	2.0573660000000000
S	18.3106240000000007	13.2615090000000002	2.2250510000000001
S	16.5846249999999991	16.1938290000000009	1.6944490000000001
S	27.8048059999999992	1.7692980000000000	1.6612460000000000
S	26.2468040000000009	4.7405660000000003	2.0424140000000000
S	24.6710260000000012	7.5514099999999997	1.6293080000000000
S	23.1966970000000003	10.5405850000000001	1.8886160000000001
S	21.4693520000000007	13.3139430000000001	1.7521089999999999
S	19.8828129999999987	16.1159959999999991	2.1037940000000002
S	18.0810800000000000	19.0112130000000015	1.7533289999999999
S	30.9619840000000011	1.9175620000000000	1.6886630000000000
S	29.4365680000000012	4.8301390000000000	2.0636540000000001
S	27.8219339999999988	7.5517390000000004	1.6308570000000000
S	26.2462720000000012	10.2386769999999991	1.7731749999999999
S	24.7328820000000000	13.3194479999999995	1.8644950000000000
S	23.1112250000000010	16.1964170000000003	2.0003289999999998
S	21.3358249999999998	18.9456759999999989	1.8289780000000000
S	19.6740899999999996	21.7799280000000017	2.0902470000000002
S	34.5459189999999978	1.8052260000000000	2.5986769999999999

S	32.6707290000000015	4.7940110000000002	1.9254240000000000
S	31.1428370000000001	7.6958659999999997	2.0410320000000000
S	29.2955180000000013	10.5407700000000002	1.8915990000000000
S	27.7574070000000006	13.3184959999999997	1.8671640000000000
S	26.2447930000000014	16.2450499999999991	2.0353539999999999
S	24.6315990000000014	19.0312920000000005	1.6490119999999999
S	22.9860070000000007	21.8705500000000015	2.0870600000000001
S	21.3815770000000001	24.6024969999999996	1.7153229999999999
S	36.3211640000000031	4.6322049999999999	2.7532630000000000
S	34.4015289999999965	7.6550380000000002	1.8169519999999999
S	32.6367169999999973	10.4072309999999995	2.0644070000000001
S	31.0212359999999983	13.3136480000000006	1.7565610000000000
S	29.3784990000000015	16.1948930000000004	1.9999199999999999
S	27.8572120000000005	19.0300289999999990	1.6478090000000001
S	26.2431939999999990	21.9057509999999986	2.0844450000000001
S	24.6311959999999992	24.6719009999999983	1.6817340000000001
S	37.9073800000000034	7.4828789999999996	2.7110370000000001
S	35.9414779999999965	10.4627379999999999	1.7986899999999999
S	34.1784460000000010	13.2603639999999992	2.2297490000000000
S	32.6080970000000008	16.1131920000000015	2.1090740000000001
S	31.1530729999999991	18.9423950000000012	1.8277550000000000
S	29.5001139999999999	21.8677120000000009	2.0778349999999999
S	27.8507549999999995	24.6695090000000015	1.6737080000000000
S	39.5010490000000019	10.4440740000000005	2.6891219999999998
S	37.4181439999999981	13.3621739999999996	1.8195349999999999
S	35.9075789999999984	16.1927100000000017	1.7011510000000001
S	34.4088870000000000	19.0089560000000013	1.7511939999999999
S	32.8120580000000004	21.7751170000000016	2.0764770000000001
S	31.1008950000000013	24.5963390000000004	1.6918219999999999
S	17.9350829999999988	24.7390439999999998	1.8980079999999999
S	19.9084280000000007	25.7448480000000011	5.1415199999999999
S	19.8338129999999992	27.7886080000000000	2.3003499999999999
S	23.1027699999999996	25.7892110000000017	5.1325960000000004

S	23.0221100000000014	27.8481209999999990	2.5142869999999999
S	26.2474139999999991	25.8131689999999985	5.1414629999999999
S	26.2407070000000004	27.8757440000000010	2.5145270000000002
S	29.3901819999999994	25.7951410000000010	5.1148780000000000
S	32.5838820000000027	25.7584109999999988	5.1072199999999999
S	32.6469359999999966	27.7761209999999998	2.2458119999999999
S	34.5577290000000019	24.7278139999999986	1.8716140000000001
S	29.4588490000000007	27.8444530000000015	2.4857309999999999

$W_{66}S_{132}$; $E_{tot} = -31\,314\,118.862\,763\,70$ eV; $E_{rel} = 94.321\,299\,106\,0$ meV/f.u.

W	-0.5862410000000000	57.2439200000000028	10.3564629999999998
W	0.5876970000000000	59.6187269999999998	10.4675379999999993
W	-2.2913999999999999	59.8804810000000032	10.3190519999999992
W	-3.8954040000000001	62.5846650000000011	10.3199769999999997
W	-5.4569710000000002	65.3103739999999959	10.3660890000000006
W	-7.0256239999999996	68.0258039999999937	10.3864560000000008
W	-8.6067040000000006	70.7423639999999949	10.3672590000000007
W	-10.1960200000000007	73.4633610000000061	10.3305910000000001
W	-11.7812699999999992	76.1919270000000068	10.3115389999999998
W	-13.3490380000000002	78.9302100000000024	10.3310370000000002
W	-14.9097050000000007	81.6675110000000046	10.3654849999999996
W	-16.4706849999999996	84.3948910000000012	10.3800200000000000
W	-18.0374119999999998	87.1111669999999947	10.3551029999999997
W	2.5535519999999998	57.1505989999999997	10.6133159999999993
W	-0.9604350000000000	62.1884579999999971	10.4408399999999997
W	-2.5848040000000001	64.9267499999999984	10.4218550000000008
W	-4.2246759999999997	67.7337210000000027	10.4236290000000000
W	-5.8420090000000000	70.5259460000000047	10.4257380000000008
W	-7.4392009999999997	73.2862580000000037	10.4125960000000006
W	-9.0074310000000004	75.9999159999999989	10.3982220000000005
W	-10.5584690000000005	78.6887260000000026	10.3982290000000006
W	-12.1235400000000002	81.4067730000000012	10.4122269999999997

W	-13.7152270000000005	84.1719089999999994	10.4236360000000001
W	-15.3243880000000008	86.9679770000000048	10.4190369999999994
W	5.3817990000000000	57.0365779999999987	10.8905010000000004
W	4.2682039999999999	59.5724960000000010	10.7936390000000006
W	2.6554160000000002	62.7142570000000035	10.8055909999999997
W	1.0970970000000000	65.4050500000000028	10.7412949999999991
W	-0.4784020000000000	68.0893059999999934	10.6741720000000004
W	-2.0780110000000001	70.8277740000000051	10.6394889999999993
W	-3.6886369999999999	73.6031169999999975	10.6328910000000008
W	-5.2768590000000000	76.3505059999999958	10.6411519999999999
W	-6.8327130000000000	79.0466480000000047	10.6466180000000001
W	-8.3886109999999992	81.7440179999999970	10.6400819999999996
W	-9.9737109999999998	84.4959360000000004	10.6316129999999998
W	-11.5715000000000003	87.2798910000000063	10.6388289999999994
W	8.3818380000000001	56.9013249999999999	11.0195679999999996
W	6.9077209999999996	59.6407609999999977	11.1285120000000006
W	5.3795159999999997	62.5152590000000004	10.9829939999999997
W	3.8285809999999998	65.2325529999999958	10.8800019999999993
W	2.2688000000000001	67.9255310000000065	10.8302300000000002
W	0.6846260000000000	70.6372870000000006	10.7517639999999997
W	-0.9065680000000000	73.3615240000000028	10.6974169999999997
W	-2.4846889999999999	76.0957410000000039	10.6977030000000006
W	-4.0512980000000001	78.8330770000000030	10.7221930000000008
W	-5.6271899999999997	81.5641949999999980	10.7209129999999995
W	-7.2132730000000000	84.2907560000000018	10.6954270000000005
W	-8.7911350000000006	87.0256679999999960	10.6968189999999996
S	0.6339360000000001	55.6058609999999973	11.3098069999999993
S	-1.0641430000000001	58.7283419999999978	12.0938580000000009
S	-2.6732779999999998	61.4344669999999979	12.0613390000000003
S	-4.2499240000000000	64.1451059999999984	12.0812740000000005
S	-5.8270590000000002	66.8871160000000060	12.1178030000000003
S	-7.4192920000000004	69.6227370000000008	12.1211369999999992
S	-9.0127050000000004	72.3496350000000064	12.0957749999999997

S	-10.5946850000000001	75.0667080000000055	12.0701079999999994
S	-12.1608839999999994	77.7822019999999981	12.0704250000000002
S	-13.7218610000000005	80.5125579999999985	12.0953370000000007
S	-15.2872050000000002	83.2566020000000009	12.1176410000000008
S	-16.8612690000000001	86.0024980000000028	12.1101010000000002
S	3.8008080000000000	55.4558400000000020	11.6039440000000003
S	2.3097620000000001	58.7881720000000030	12.1434549999999994
S	0.7410730000000000	61.5285840000000022	12.0093599999999991
S	-0.8250210000000000	64.2457969999999960	11.8946360000000002
S	-2.4077350000000002	66.9870760000000018	11.8321780000000008
S	-3.9994440000000000	69.7479260000000068	11.8333030000000008
S	-5.5935969999999999	72.5074649999999963	11.8475839999999994
S	-7.1738470000000003	75.2427540000000050	11.8622449999999997
S	-8.7369190000000003	77.9479209999999938	11.8696610000000007
S	-10.2965859999999996	80.6560769999999962	11.8611000000000004
S	-11.8751890000000007	83.3942720000000008	11.8459190000000003
S	-13.4680830000000000	86.1553550000000001	11.8310849999999999
S	6.9428250000000000	55.4534170000000017	11.9578109999999995
S	5.4800690000000003	58.5554119999999969	12.6534180000000003
S	3.9384589999999999	61.4682310000000030	12.4442579999999996
S	2.3556979999999998	64.3469410000000011	12.5331270000000004
S	0.7626430000000000	67.0622549999999933	12.4596440000000008
S	-0.8020060000000000	69.7861199999999968	12.3878930000000000
S	-2.3750589999999998	72.5292460000000005	12.3503179999999997
S	-3.9499800000000000	75.2738939999999985	12.3598330000000001
S	-5.5132979999999998	78.0012339999999966	12.3861100000000004
S	-7.0780709999999996	80.7138259999999974	12.3850560000000005
S	-8.6570669999999996	83.4330750000000023	12.3578550000000007
S	-10.2463890000000006	86.1702140000000014	12.3491400000000002
S	10.1175359999999994	55.9080409999999972	10.2665629999999997
S	8.8974689999999992	58.6364879999999999	12.3224129999999992
S	7.4627660000000002	61.6145039999999966	12.1068780000000000
S	6.0281099999999999	64.5369309999999956	11.8077210000000008

S	4.3566180000000001	67.2897980000000047	11.8896069999999998
S	2.7909470000000001	70.0503580000000028	11.7456420000000001
S	1.2130080000000001	72.7766129999999976	11.6417210000000004
S	-0.3596270000000000	75.4997450000000043	11.6006689999999999
S	-1.9396510000000000	78.2247080000000068	11.6380280000000003
S	-3.5075099999999999	80.9667579999999987	11.6399629999999998
S	-5.0964720000000003	83.6966639999999984	11.6352089999999997
S	-6.6652950000000004	86.4287499999999937	11.5980220000000003
S	-2.5653380000000001	57.4134669999999971	9.3805510000000005
S	-4.3215009999999996	60.2761300000000020	9.3772549999999999
S	-5.9517270000000000	63.0721750000000014	9.4171560000000003
S	-7.5448810000000002	65.8362690000000015	9.4587100000000000
S	-9.1334250000000008	68.5854479999999995	9.4560309999999994
S	-10.7268709999999992	71.3217810000000014	9.4299459999999993
S	-12.3227949999999993	74.0533060000000063	9.4121059999999996
S	-13.9034809999999993	76.7938599999999951	9.4123280000000005
S	-15.4689960000000006	79.5417149999999964	9.4296469999999992
S	-17.0401319999999998	82.2896180000000044	9.4511540000000007
S	-18.6242990000000006	85.0407689999999974	9.4454849999999997
S	-20.2196490000000004	87.8042070000000052	9.3973969999999998
S	1.0523039999999999	57.8484660000000019	8.8064330000000002
S	-0.7250090000000000	60.5697619999999972	8.6854940000000003
S	-2.3328240000000000	63.3011189999999999	8.7051850000000002
S	-3.9429390000000000	66.0726850000000070	8.7232249999999993
S	-5.5568819999999999	68.8434950000000043	8.7213150000000006
S	-7.1565219999999998	71.5949530000000038	8.7030949999999994
S	-8.7461629999999992	74.3226949999999960	8.6698269999999997
S	-10.3194809999999997	77.0349899999999934	8.6522269999999999
S	-11.8794360000000001	79.7553939999999955	8.6703799999999998
S	-13.4451859999999996	82.4973719999999986	8.7019730000000006
S	-15.0265160000000009	85.2590789999999998	8.7171269999999996
S	-16.6171599999999984	88.0431700000000035	8.7158689999999996
S	4.1281189999999999	57.9190139999999971	9.0297029999999996

S	2.545210000000000	60.700133000000010	9.401961999999993
S	0.918578000000000	63.411566999999980	9.275854000000007
S	-0.688625000000000	66.115163999999929	9.229117999999997
S	-2.312424000000000	68.858538999999933	9.213903000000002
S	-3.928008000000002	71.618556999999956	9.213324000000001
S	-5.525737000000003	74.370186000000039	9.197438999999993
S	-7.097109999999998	77.092984000000013	9.176510000000004
S	-8.656853999999992	79.796570000000027	9.176577999999992
S	-10.227921000000003	82.521159999999947	9.197374999999992
S	-11.811173999999994	85.282577000000034	9.212369999999999
S	-13.392374999999995	88.062460999999990	9.212213000000002
S	7.198539000000002	57.920034000000011	9.343719999999994
S	5.844216000000003	60.832822999999976	9.331246000000002
S	4.272236999999996	63.605623000000014	9.170769999999992
S	2.724619000000001	66.342039999999972	9.097246000000002
S	1.141502999999999	69.040493999999954	9.030160999999997
S	-0.480121000000000	71.754551000000064	8.971562999999997
S	-2.094380999999998	74.495996000000052	8.949089000000007
S	-3.672474999999999	77.242594999999943	8.962044999999998
S	-5.238825000000003	79.967416999999975	8.971792999999999
S	-6.814899999999997	82.687568999999963	8.960373000000006
S	-8.403644999999991	85.429861000000025	8.947765999999997
S	-9.969101000000002	88.200704000000018	8.972094999999995
W	-19.616339000000000	89.826052000000042	10.306627999999999
W	-18.493230000000005	92.565924999999929	10.435563999999994
W	-21.157157000000015	92.567193000000032	10.308764000000000
W	-22.589632999999992	95.361406999999998	10.353609999999998
W	-16.934315000000016	89.790465999999950	10.415760000000006
W	-19.946393000000005	95.191306999999948	10.465975999999995
W	-21.101863999999991	98.126459999999945	10.620112000000007
W	-13.142417000000000	90.033936999999946	10.674739999999999
W	-14.679237000000005	92.740561999999971	10.741908000000005
W	-16.230657000000008	95.434749999999940	10.807017999999993

W	-18.146274999999993	98.4035690000000045	10.7990919999999999
W	-19.787570999999998	100.633960000000019	10.902200000000006
W	-10.3548010000000001	89.766734999999971	10.753850999999992
W	-11.911075999999996	92.495116999999934	10.833740000000006
W	-13.463903999999994	95.1930490000000020	10.884232000000008
W	-15.0426330000000004	97.895065999999999	10.988260999999996
W	-16.7689440000000012	100.6551070000000010	11.136540000000001
W	-18.406017999999995	103.3005730000000000	11.032724999999992
S	-18.447676999999988	88.7373900000000049	12.070344999999997
S	-20.006198999999987	91.4564050000000037	12.050485999999994
S	-21.544029999999993	94.201268999999964	12.088210999999994
S	-23.398990999999988	97.2342060000000004	11.313200999999994
S	-15.063195999999996	88.913071999999997	11.829433999999991
S	-16.645831999999986	91.6535800000000052	11.891130999999997
S	-18.2158680000000004	94.3670740000000023	12.007293000000007
S	-19.803864999999983	97.094381999999960	12.146613999999996
S	-21.944770999999994	100.0511630000000025	11.618249000000005
S	-11.835922999999993	88.9039060000000063	12.388408999999993
S	-13.4132250000000006	91.620688999999987	12.461048999999992
S	-14.968327999999996	94.357850999999966	12.534805000000004
S	-16.669495999999988	97.1672350000000051	12.447540000000000
S	-18.420325999999993	99.958067999999973	12.662005000000006
S	-20.3777590000000011	102.7758270000000067	11.972975999999992
S	-8.2378180000000008	89.152951999999991	11.643280000000007
S	-9.810133999999997	91.883607999999953	11.749409000000000
S	-11.4181620000000006	94.620622999999948	11.893677999999995
S	-12.9666200000000007	97.4455430000000007	11.811382999999993
S	-14.7811140000000005	100.148493999999995	12.112954000000002
S	-16.6430840000000018	102.8791520000000048	12.332321999999996
S	-18.401033999999992	105.300921999999999	10.281247000000005
S	-21.8260380000000005	90.614565999999964	9.357830999999991
S	-23.4316430000000011	93.5652460000000019	9.372645000000003
S	-18.211470999999995	90.8246500000000054	8.697312999999994

S	-19.774682999999996	93.5835380000000043	8.6805310000000002
S	-21.2464610000000000	96.4825569999999999	8.8079040000000006
S	-14.9552580000000006	90.8404299999999978	9.2273139999999998
S	-16.4932419999999986	93.5843430000000041	9.2747600000000006
S	-18.0302270000000000	96.3491630000000043	9.4045369999999995
S	-19.6510420000000003	99.1110099999999932	9.0379989999999992
S	-11.5078980000000008	90.9629319999999950	9.0325199999999999
S	-13.0528309999999994	93.6836930000000052	9.1003349999999994
S	-14.6497279999999996	96.3923489999999958	9.1748349999999999
S	-16.2677590000000016	99.1399289999999951	9.3375400000000006
S	-18.1167650000000009	101.7687180000000069	9.3543939999999992

$W_{66}S_{132}$; $E_{tot} = -31\,314\,121.174\,633\,24$ eV; $E_{rel} = 59.292\,972\,742\,4$ meV / **f.u.**

W	32.8930039999999977	1.6631760000000000	3.2837320000000001
W	31.2260419999999996	4.4211809999999998	3.2909679999999999
W	34.4525009999999980	3.7983630000000002	3.4332199999999999
W	29.7106099999999991	7.0215339999999999	3.3612120000000001
W	28.1345050000000008	9.7052189999999996	3.3794000000000000
W	26.4924159999999986	12.4084470000000007	3.1497869999999999
W	24.7281270000000006	15.4823819999999994	3.1410849999999999
W	23.2749510000000015	18.0642050000000012	3.1664690000000002
W	21.6799129999999991	20.7361429999999984	3.0086330000000001
W	19.9543539999999986	23.8331039999999987	3.0943730000000000
W	18.4450930000000000	26.5105250000000012	3.2282600000000001
W	16.9373509999999996	29.2246260000000007	3.3319960000000002
W	15.3830989999999996	31.9288869999999996	3.2795250000000000
W	35.9817129999999992	1.5032300000000001	3.3293379999999999
W	32.6341869999999972	7.0244000000000000	3.4031590000000000
W	31.1589190000000009	9.3461189999999998	3.4806870000000001
W	29.2251879999999993	12.5801929999999995	3.4001239999999999
W	28.1026969999999992	15.1144590000000001	3.2810609999999998
W	26.0044940000000011	17.9152039999999992	3.2809539999999999

W	24.5862510000000007	21.0053069999999984	3.3143950000000002
W	23.2615960000000008	23.3287380000000013	3.3580320000000001
W	21.4562859999999986	26.5915549999999996	3.3637800000000002
W	20.0123080000000009	29.0039049999999996	3.3837630000000001
W	17.9451859999999996	31.9797210000000014	3.4187609999999999
W	38.9680999999999997	1.4987610000000000	3.4450490000000000
W	37.5412510000000026	3.7438199999999999	3.5177019999999999
W	36.1249729999999971	7.1440690000000000	3.4369820000000000
W	34.2990589999999997	9.3322319999999994	3.5821220000000000
W	32.9246369999999970	12.7822720000000007	3.4789020000000002
W	30.8413329999999988	15.2078840000000000	3.4788260000000002
W	29.7925900000000006	17.8967440000000018	3.3349259999999998
W	27.8341670000000008	21.1457559999999987	3.4303100000000000
W	26.3023869999999995	23.3880470000000003	3.4967050000000000
W	24.4650590000000001	26.6756910000000005	3.5156749999999999
W	22.8767309999999995	29.0918939999999999	3.4676640000000001
W	21.4776769999999999	31.5980290000000004	3.5108020000000000
W	42.0680350000000018	1.6344879999999999	3.4995310000000002
W	40.8209060000000008	3.8751720000000001	3.6062259999999999
W	39.1584489999999974	7.1586819999999998	3.5204900000000001
W	37.5871640000000014	9.4271060000000002	3.6209190000000002
W	35.9755680000000027	12.7960530000000006	3.5367820000000001
W	34.4841240000000013	15.0826290000000007	3.6114769999999998
W	32.5855180000000004	18.2261249999999997	3.5807090000000001
W	31.3193340000000013	20.5460339999999988	3.5145339999999998
W	29.2872720000000015	23.6993100000000005	3.5914920000000001
W	28.2103180000000009	26.5707020000000007	3.5883090000000002
W	26.6548279999999984	29.1419080000000008	3.5208550000000001
W	24.7907679999999999	32.3460439999999991	3.5356709999999998
W	44.0052599999999998	3.8767670000000001	4.0242519999999997
W	42.1104759999999985	6.9149550000000000	3.7003149999999998
W	40.6388529999999975	9.4375630000000008	3.6939579999999999
W	39.1178170000000023	12.2441870000000002	3.7464909999999998

W	37.410753999999972	15.121117999999992	3.6935780000000000
W	35.890064999999999	17.777635000000001	3.7922419999999999
W	34.1410610000000005	20.855738999999998	3.8097560000000001
W	32.6946020000000033	23.3190780000000011	3.8117529999999999
W	30.9148710000000015	26.4744750000000018	3.7429579999999998
W	29.3387220000000006	29.1554089999999988	3.4765419999999998
W	27.7350360000000009	31.8868490000000016	3.4282620000000001
S	34.0756650000000008	-0.0351400000000000	4.1390079999999996
S	32.614668999999992	3.2493979999999998	4.9785100000000000
S	31.0692720000000016	5.9786130000000002	5.0599259999999999
S	29.3968050000000005	8.7083600000000008	5.0992709999999999
S	27.7457439999999984	11.4285700000000006	4.9998509999999996
S	26.1266280000000002	14.2191139999999994	4.7138850000000003
S	24.4737439999999999	17.0140279999999997	4.9486090000000003
S	22.9679660000000005	19.8272270000000006	4.7976000000000001
S	21.2960990000000017	22.5412430000000015	4.6788470000000002
S	19.7992349999999995	25.4026059999999987	4.8641490000000003
S	18.2519029999999987	28.1476450000000007	4.9684559999999998
S	16.4830030000000001	30.8805550000000011	5.0703069999999997
S	37.4856819999999971	-0.0897800000000000	4.3195980000000000
S	35.9147419999999968	3.0363880000000001	5.1600149999999996
S	34.3794189999999986	5.9051989999999996	4.7325749999999998
S	32.6973500000000001	8.6918039999999994	5.2117220000000000
S	31.0976379999999999	11.5343070000000001	4.6968139999999998
S	29.3979029999999995	14.2291580000000000	5.1283370000000001
S	27.8460299999999989	17.0400050000000007	4.7001359999999996
S	26.2453189999999985	19.8439189999999996	4.7884289999999998
S	24.6764030000000005	22.6158730000000006	5.1097060000000001
S	23.0230369999999986	25.3535819999999994	4.8122090000000002
S	21.4608929999999987	28.2097599999999993	5.1707400000000003
S	19.7212420000000002	30.9418140000000008	4.8899229999999996
S	40.8442870000000013	-0.0482240000000000	4.3594600000000003
S	39.1488489999999985	3.0695120000000000	5.1901940000000000

S	37.550832999999972	5.874175000000001	4.9087430000000003
S	35.9473150000000032	8.7138589999999994	5.2469409999999996
S	34.346049999999982	11.5035380000000007	4.9015469999999999
S	32.689951999999981	14.3811060000000008	5.1203799999999999
S	31.1055680000000017	17.049444999999986	5.1201920000000003
S	29.4544350000000001	19.821578999999998	4.8599930000000002
S	27.845742999999988	22.7355480000000014	5.2391430000000003
S	26.2745660000000001	25.532980999999995	4.7659580000000004
S	24.7156650000000013	28.3652580000000007	5.0322519999999997
S	23.146354999999998	31.046963999999991	5.0158240000000003
S	42.3560200000000009	3.0480320000000001	5.4185369999999997
S	40.667965999999998	5.9259870000000001	5.1293170000000003
S	39.1522340000000000	8.8042010000000008	5.3559140000000003
S	37.4905860000000004	11.4893640000000001	5.1207859999999998
S	35.9947050000000033	14.373023999999991	5.3929220000000004
S	34.272066999999998	17.0682480000000005	5.1765200000000000
S	32.768684999999978	19.8811590000000002	5.3728899999999999
S	31.0622250000000015	22.528681999999999	5.1289610000000003
S	29.5158340000000017	25.4532230000000013	5.2982449999999996
S	28.050229999999991	28.310815999999991	5.2779610000000003
S	26.3379690000000011	31.0949010000000001	5.0509630000000003
S	45.9479690000000005	3.3102790000000000	4.7371220000000003
S	44.256346999999981	6.1275300000000001	4.5358530000000004
S	42.729475999999982	8.8995970000000000	4.7039439999999999
S	41.1991020000000034	11.6802220000000005	4.5286039999999996
S	39.605590999999969	14.4652440000000002	4.3977240000000002
S	37.970770999999992	17.2675680000000007	4.6240040000000002
S	36.321761999999997	20.0333630000000014	4.4363849999999996
S	34.8063900000000004	22.9052340000000001	4.6936739999999997
S	32.9127310000000008	25.4913740000000004	4.7232300000000000
S	31.569065999999994	28.539853999999983	4.4084260000000004
S	29.8933250000000008	31.3389710000000008	4.2667349999999997
S	30.851842999999988	2.0437050000000001	2.3982290000000002

S	29.1349790000000013	4.8258089999999996	2.4917630000000002
S	27.5393919999999994	7.5906979999999997	2.5549019999999998
S	25.8922789999999985	10.2449469999999998	2.6433570000000000
S	24.4879479999999994	13.2551349999999992	2.2109610000000002
S	22.6186809999999987	15.9510810000000003	2.3110070000000000
S	21.0823609999999988	18.7221179999999983	2.1774149999999999
S	19.5320080000000011	21.6128639999999983	2.3876970000000002
S	17.8349949999999993	24.3579870000000014	2.3608590000000000
S	16.2840360000000004	27.1535019999999996	2.4477359999999999
S	14.6862860000000008	29.9539009999999983	2.4282490000000001
S	34.4187989999999999	2.1394299999999999	1.5919630000000000
S	32.8327839999999966	5.0644619999999998	1.8594240000000000
S	31.1273519999999984	7.7461349999999998	1.6412480000000000
S	29.6188479999999998	10.5837400000000006	1.9104989999999999
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S	26.3491220000000013	16.1581480000000006	1.6654030000000000
S	24.6878519999999995	19.0330170000000010	1.6320580000000000
S	23.0957310000000007	21.7370400000000004	1.5115000000000001
S	21.6042260000000006	24.6008579999999988	1.7800890000000000
S	19.8803260000000002	27.2970450000000007	1.6237260000000000
S	18.3697710000000001	30.1663730000000001	1.8371610000000000
S	16.6323700000000017	33.0711370000000002	1.6418010000000001
S	37.5272599999999983	2.1126999999999998	1.6646230000000000
S	36.0183910000000012	5.0255869999999998	2.0424899999999999
S	34.3902440000000027	7.7564289999999998	1.8255720000000000
S	32.8041880000000035	10.5932980000000008	2.1292819999999999
S	31.1239020000000011	13.3709129999999998	1.9356840000000000
S	29.5475689999999993	16.1518809999999995	1.6801919999999999
S	27.9178490000000004	19.0163760000000011	2.0948579999999999
S	26.2946290000000005	21.7633860000000006	1.7152099999999999
S	24.7307629999999996	24.5625280000000004	1.9798640000000001
S	23.0984209999999983	27.4148439999999987	1.7348220000000001
S	21.5015390000000011	30.0709540000000004	1.7359070000000001

S	19.884999000000005	32.985235000000030	2.184972999999998
S	40.611654000000015	2.201445999999998	1.792334000000001
S	39.189903999999985	5.044114000000004	2.198951000000001
S	37.647142000000023	7.852549999999999	1.766861999999999
S	35.981194999999996	10.645554999999999	2.260911000000001
S	34.468936999999968	13.460718999999992	1.791382999999999
S	32.771965999999990	16.178224000000002	2.231145999999999
S	31.211676000000006	18.945695000000006	1.732939999999999
S	29.645831999999986	21.819666000000016	2.078279000000002
S	27.893141000000000	24.639119999999984	2.014171999999999
S	26.372659999999998	27.334955000000008	2.026481000000000
S	24.770506000000010	30.189872000000012	2.296514000000002
S	23.046838000000010	32.939613999999988	2.048922999999998
S	44.049394999999970	1.953314999999999	2.456262000000002
S	42.592637000000034	5.017764999999998	2.243603999999999
S	40.879438999999979	7.810350999999998	1.913195999999999
S	39.255634999999981	10.577410999999997	2.044929000000002
S	37.840887000000022	13.407154000000002	2.026219999999999
S	36.076382000000024	16.194977999999990	2.015632999999998
S	34.511158999999993	19.018910000000018	2.186572000000000
S	32.841591000000011	21.764011000000000	2.004928000000000
S	31.288191000000012	24.605245000000000	2.232095000000002
S	29.746869000000002	27.442468999999991	1.860123000000000
S	28.017065999999998	30.200980000000013	1.775466999999999
S	26.389081999999984	32.967171000000004	1.782885000000001
W	16.924206000000016	34.724097999999979	3.412353000000000
W	19.961938000000000	35.052461000000010	3.566597999999999
W	18.385404000000012	37.494681999999974	3.885999000000000
W	23.138932000000005	34.898640000000003	3.579819999999998
W	21.283418999999985	37.342616999999971	3.629116999999999
W	26.192202999999992	34.604720000000004	3.521878000000001
W	24.414336999999997	37.210017000000006	3.611340999999999
S	14.519980000000003	33.841831999999966	4.045253999999999

S	18.264399999999984	33.8081370000000021	5.0174779999999997
S	16.0297960000000010	36.5997470000000007	4.2626390000000001
S	21.4650180000000006	33.7117959999999997	4.9244579999999996
S	19.8487089999999995	36.6280410000000032	5.4331139999999998
S	17.4897780000000012	39.1146310000000028	5.0359389999999999
S	24.7519160000000014	33.9890439999999998	5.2418449999999996
S	22.9263690000000011	36.6772429999999972	5.3260240000000003
S	28.3489080000000016	34.1403990000000022	4.1863109999999999
S	26.4861100000000000	37.0183820000000026	4.4389880000000002
S	18.2839589999999994	35.8789620000000014	1.9068879999999999
S	21.5461069999999992	35.7687499999999972	1.9298759999999999
S	19.8372339999999987	38.8076200000000000	2.5679289999999999
S	24.7903589999999987	35.6815799999999967	1.8703500000000000
S	23.1987160000000010	38.8348549999999975	2.6747519999999998

$W_{66}S_{132}$; $E_{tot} = -31\,314\,122.544\,605\,02$ eV; $E_{rel} = 38.535\,824\,560\,6$ meV / **f.u.**

W	20.0725330000000000	2.3954670000000000	4.1983020000000000
W	18.0263120000000008	4.4087470000000000	3.1423169999999998
W	16.4897250000000000	7.0959019999999997	3.2070680000000000
W	14.9345400000000001	9.8481269999999999	3.3568970000000000
W	13.3793860000000002	12.5396800000000006	3.4057539999999999
W	11.8516700000000004	15.2225780000000004	3.3704030000000000
W	10.3431169999999995	17.9474790000000013	3.1983150000000000
W	8.5372620000000001	20.9319969999999991	2.8455800000000000
W	6.9385599999999998	24.0069270000000010	3.0419700000000001
W	5.5325810000000004	26.5025319999999986	3.0899860000000001
W	3.9944809999999999	29.0029719999999998	3.2514379999999998
W	21.0766479999999987	4.3570620000000000	2.9343680000000001
W	19.4545309999999994	6.7486639999999998	3.1585930000000002
W	17.8985869999999991	9.3546750000000003	3.2640120000000001
W	16.1371900000000004	12.2834160000000008	3.3258320000000001
W	14.5583650000000002	14.9978180000000005	3.3367550000000001

W	13.064493999999998	17.721429000000005	3.2959010000000002
W	11.6103240000000003	21.0728319999999982	3.1871689999999999
W	10.1909519999999993	23.3391470000000005	3.2814610000000002
W	8.4226440000000000	26.6620249999999999	3.2302990000000000
W	7.0817629999999996	28.9691289999999988	3.1949320000000001
W	22.5380600000000015	6.7890670000000002	2.9714680000000002
W	21.3916630000000012	9.9009640000000001	3.2976269999999999
W	19.9450789999999998	12.5663219999999995	3.4664920000000001
W	18.3967920000000014	15.2166250000000005	3.4308060000000000
W	16.8721649999999990	17.9534200000000013	3.3273609999999998
W	14.8183609999999994	21.0993059999999986	3.2828560000000002
W	13.3153159999999993	23.3379230000000000	3.3936720000000000
W	11.6215639999999993	26.7761350000000000	3.2761019999999998
W	10.2561499999999999	29.1072960000000016	3.2859910000000001
W	24.4789479999999990	9.7946390000000001	2.9524430000000002
W	22.8551469999999988	12.1411949999999997	3.3395269999999999
W	21.0999160000000003	15.3562689999999993	3.4608140000000001
W	19.8199310000000004	17.7894480000000001	3.3780180000000000
W	17.9330679999999987	21.0446160000000013	3.3723879999999999
W	16.4323559999999986	23.3416740000000011	3.4430559999999999
W	14.8347169999999995	26.7602739999999990	3.3412959999999998
W	13.3719040000000007	29.0512319999999988	3.4138419999999998
W	26.0953909999999993	12.6640580000000007	3.3249119999999999
W	24.8940389999999994	15.0878709999999998	3.3943279999999998
W	22.6797819999999994	18.1485319999999994	3.5162719999999998
W	21.6329799999999999	20.9046039999999991	3.4029479999999999
W	19.5050209999999993	23.3790240000000011	3.4153620000000000
W	18.4276130000000009	26.6417670000000015	3.4225110000000001
W	16.4657090000000004	29.0565689999999996	3.4044900000000000
W	27.6311120000000017	15.3233449999999998	3.4630100000000001
W	26.4630259999999993	17.8078010000000013	3.4018540000000002
W	24.3470359999999992	20.9613650000000007	3.4670740000000002
W	23.2265960000000007	23.4672190000000001	3.3982440000000000

W	21.365128999999996	26.652779999999999	3.391343000000000
W	19.670643999999994	29.097683000000000	3.290832000000000
W	29.166992000000005	17.987396000000004	3.353200000000002
W	28.0107290000000013	21.040943999999996	3.354734000000001
W	26.2218240000000016	23.379528000000005	3.436326999999999
W	24.187333999999999	26.562107000000010	3.344895999999999
W	22.859548000000002	29.073336000000012	3.244285999999998
W	30.835893999999997	20.817617999999995	3.020248000000000
W	29.190137000000000	23.441572000000007	3.330738000000002
W	27.914253999999997	26.752147000000008	3.285490999999999
W	26.0642670000000010	29.061439000000000	3.338515000000001
W	32.475175999999976	24.017835000000016	3.074770000000000
W	30.979652999999990	26.712074000000012	3.237296999999999
W	29.203317999999994	29.102000000000003	3.310562000000000
W	33.871830000000028	26.523015999999984	3.088010999999998
W	32.308146000000007	29.010975999999994	3.176925000000002
W	35.391021000000021	29.040247000000008	3.205801000000001
S	20.739499999999996	2.501062999999998	6.227929999999997
S	17.849713000000013	5.960496000000000	4.871042000000001
S	16.280326999999998	8.685762000000004	4.991489999999998
S	14.659034999999994	11.436064999999993	5.102605999999998
S	13.044197999999997	14.156121000000006	5.122594999999996
S	11.484132999999999	16.938126000000005	5.033446999999998
S	9.874361000000004	19.866410999999994	4.620270999999998
S	8.248260999999994	22.638192000000001	4.611112000000003
S	6.915949999999996	25.551391999999999	4.821778000000001
S	5.434205000000004	28.288706999999987	4.890676000000000
S	21.180047999999993	5.881053999999998	4.697409999999996
S	19.702487999999989	8.692311999999994	4.685528999999998
S	18.044464000000014	11.443754999999995	4.620495000000000
S	16.460919000000005	14.258715999999997	4.750847000000003
S	14.874484000000007	17.021157999999998	4.729250999999996
S	13.175846999999992	19.835111999999987	4.626521999999996

S	11.641909999999993	22.672128000000007	5.013722999999997
S	10.106427000000000	25.473687000000017	4.623146000000002
S	8.630617000000009	28.462457000000006	4.937254000000003
S	23.050173999999984	8.558417999999996	4.590595999999997
S	21.354333000000005	11.446274000000007	5.087461000000002
S	19.784794000000015	14.242898999999995	5.163806000000001
S	18.184391000000015	17.067350999999986	5.077360999999998
S	16.421227999999993	19.850172000000006	4.820780000000001
S	14.847538000000001	22.712914000000014	5.118337999999996
S	13.282463999999992	25.528880999999984	4.663700000000004
S	11.741303000000003	28.465116999999993	5.061277999999997
S	24.692001000000012	11.344127999999995	4.825643999999996
S	22.992999000000011	14.234776999999993	4.691765000000002
S	21.345969000000002	17.065546000000012	5.158146999999996
S	19.725294000000017	19.907315000000005	4.663522999999996
S	18.044684000000002	22.694382999999984	5.143610999999999
S	16.536224000000007	25.565225000000016	4.646825999999999
S	14.922459999999992	28.467490999999990	5.119788999999999
S	26.366710000000012	14.182639999999992	5.144872999999996
S	24.607410000000016	17.067933000000000	4.801893999999999
S	22.981732999999984	19.883981999999996	5.145048000000001
S	21.358902000000005	22.711307000000015	4.927304000000004
S	19.781880000000010	25.510574999999993	4.923588999999998
S	18.126325000000014	28.474896000000011	5.040352999999996
S	27.976313000000011	16.979876000000009	5.157157999999999
S	26.261416000000005	19.878236999999986	4.702367999999999
S	24.654652999999997	22.657084000000011	5.151990999999998
S	22.891500000000006	25.481086999999987	4.940684000000001
S	21.302315000000001	28.560417000000011	5.009723000000001
S	29.584510000000016	19.852993000000014	4.873617999999996
S	27.818909999999989	22.679318999999996	5.103663000000001
S	26.132038000000014	25.588878000000011	4.555120999999998
S	24.471692000000009	28.416720999999990	4.967337999999998

S	31.1680780000000013	22.6779760000000010	4.6608970000000003
S	29.3451799999999992	25.5339920000000014	4.7258089999999999
S	27.6489919999999998	28.4648980000000016	5.0292440000000003
S	32.4907820000000029	25.5965990000000012	4.8328769999999999
S	30.7965270000000011	28.4932300000000005	4.9656989999999999
S	17.7562700000000007	2.3003540000000000	4.0752720000000000
S	16.1409440000000011	4.7979740000000000	2.0288210000000002
S	14.3459249999999994	7.5126010000000001	2.5829360000000001
S	12.8228270000000002	10.3231040000000007	2.5260270000000000
S	11.2622520000000002	13.1373309999999996	2.4219860000000000
S	9.6376729999999995	15.9225119999999993	2.4814550000000000
S	8.2054089999999995	18.8102829999999983	2.1462340000000002
S	6.4641209999999996	21.7273929999999993	2.2568299999999999
S	4.9153900000000004	24.4476230000000001	2.0680710000000002
S	3.4199290000000002	27.1699739999999998	2.0738430000000001
S	2.2826919999999999	29.9644130000000004	4.1049860000000002
S	21.6202359999999985	1.9684830000000000	2.6051989999999998
S	19.4977100000000014	5.0059199999999997	1.3907609999999999
S	17.9226169999999989	7.7536920000000000	1.4998549999999999
S	16.4073239999999991	10.5377279999999995	1.6781170000000001
S	14.7773079999999997	13.3004440000000006	1.6293979999999999
S	13.2290779999999994	16.0462540000000011	1.5969840000000000
S	11.7261749999999996	18.9498539999999984	1.6720340000000000
S	10.0804200000000002	21.7758600000000015	1.3847210000000001
S	8.5852260000000005	24.6762310000000014	1.6792030000000000
S	6.9109369999999997	27.3859339999999989	1.4541409999999999
S	5.2772690000000004	30.3912019999999998	2.0832570000000001
S	23.1620230000000014	4.8602850000000002	1.8818589999999999
S	21.1174290000000013	7.8932650000000004	1.6309849999999999
S	19.6496910000000007	10.6316340000000000	1.8903710000000000
S	18.0608070000000005	13.3029890000000002	2.0120360000000002
S	16.4487200000000016	16.0406860000000009	2.0451999999999999
S	14.9203670000000006	18.8884219999999985	2.0752560000000000

S	13.2573050000000006	21.7267590000000013	1.5692560000000000
S	11.6978519999999993	24.6116069999999993	1.9254110000000000
S	10.1001989999999999	27.5139659999999999	1.5949460000000000
S	8.4767779999999995	30.6084439999999987	2.3881850000000000
S	24.7409700000000008	7.5651549999999999	2.2968310000000001
S	22.9095189999999995	10.5730470000000008	1.4682839999999999
S	21.3845090000000013	13.4345560000000006	1.8306519999999999
S	19.7215400000000010	16.1400310000000005	1.6385170000000000
S	18.2274610000000017	18.9799679999999995	1.8162750000000001
S	16.4447000000000010	21.6994499999999988	1.6182650000000001
S	14.8834339999999994	24.6203450000000004	2.0009229999999998
S	13.3047409999999999	27.4867789999999985	1.6390950000000000
S	11.7340610000000005	30.7277020000000007	2.6238350000000001
S	26.5327720000000014	10.3947839999999996	2.2846069999999998
S	24.5529989999999998	13.3378560000000004	1.7705580000000001
S	23.0113759999999985	16.1708299999999987	2.1002120000000000
S	21.3216690000000000	19.0077129999999990	1.8241600000000000
S	19.7356429999999996	21.7025720000000000	1.8483520000000000
S	18.0975119999999983	24.6031580000000005	1.9989470000000000
S	16.6001410000000007	27.4146779999999985	1.8027230000000001
S	14.9402670000000004	30.6542439999999985	2.5954310000000000
S	28.2017589999999991	13.1340509999999995	2.5458590000000001
S	26.2535629999999998	16.1233910000000016	1.6772590000000001
S	24.5945029999999996	18.9174340000000001	2.1119349999999999
S	22.9791200000000018	21.8208790000000015	1.6701760000000001
S	21.3277189999999983	24.5260870000000004	2.1444399999999999
S	19.7896760000000000	27.4411130000000014	1.6506010000000000
S	18.1097630000000009	30.6570819999999991	2.5745439999999999
S	29.8224410000000013	15.9332279999999997	2.5701749999999999
S	27.8241399999999999	18.9834640000000014	1.7867640000000000
S	26.1754759999999997	21.6781879999999987	1.8248340000000001
S	24.6029130000000009	24.5997810000000001	1.8812210000000000
S	22.8373099999999987	27.4276699999999991	1.5851020000000000

S	21.3320140000000009	30.6493059999999993	2.4454639999999999
S	31.3693309999999990	18.7551209999999990	2.3380580000000002
S	29.4200760000000017	21.8007629999999999	1.5056430000000001
S	27.7190079999999988	24.5946040000000004	1.8794340000000000
S	26.0476059999999983	27.3960739999999987	1.7860640000000001
S	24.5265459999999997	30.6533580000000008	2.5643919999999998
S	32.9033870000000022	21.7513019999999990	2.3638020000000002
S	30.8295640000000013	24.6876290000000012	1.7087079999999999
S	29.3373619999999988	27.5507230000000014	1.5601840000000000
S	27.6648099999999992	30.7580880000000008	2.7364799999999998
S	30.9016950000000001	30.6275879999999994	2.3365109999999998
S	33.9765960000000007	28.3296419999999998	4.8677720000000004
S	32.4954350000000005	27.4060610000000011	1.4590760000000000
S	34.5154420000000002	24.4458599999999997	2.1274999999999999
S	35.9723720000000000	27.1902900000000010	2.0548820000000001
S	34.0963800000000035	30.4150489999999998	2.0313859999999999
S	37.1031639999999996	30.0211809999999986	4.0340230000000004

$W_{66}S_{132}$; $E_{tot} = -31\,314\,123.133\,764\,21$ eV; $E_{rel} = 29.609\,170\,166\,6$ meV/f.u.

W	23.0067950000000003	1.7052719999999999	3.2311519999999998
W	21.3747909999999983	4.4340640000000002	3.2246500000000000
W	17.8603370000000012	15.0495560000000008	3.3841960000000002
W	19.8834480000000013	7.1850310000000004	3.3363470000000000
W	18.3131890000000013	9.8614750000000004	3.3832360000000001
W	16.7179630000000010	12.5298590000000001	3.4032239999999998
W	15.1352930000000008	15.2116019999999992	3.4344809999999999
W	13.5423200000000001	17.9055089999999986	3.4022239999999999
W	12.0823950000000000	20.8251899999999992	3.3382149999999999
W	26.1368699999999983	1.4100690000000000	3.7358380000000002
W	24.3694719999999982	4.0091089999999996	3.3312270000000002
W	22.8297680000000014	6.6750389999999999	3.2904160000000000
W	21.1150009999999995	9.5783699999999996	3.3283190000000000

W	19.481902999999991	12.327704999999999	3.370289999999998
W	16.2475340000000017	17.809208999999992	3.3890400000000001
W	14.7193410000000000	20.9943370000000016	3.4496859999999998
W	13.5205380000000002	23.6107480000000010	3.3778709999999998
W	27.1846409999999992	4.0505250000000004	3.5923370000000001
W	26.4071159999999985	7.2415640000000003	3.3159920000000001
W	24.9000249999999994	9.8852039999999999	3.4056199999999999
W	23.3107849999999992	12.6000049999999995	3.4543080000000002
W	21.6815360000000013	15.4073879999999992	3.4826899999999998
W	20.0306309999999996	18.1500720000000015	3.4821119999999999
W	18.4448140000000009	20.7941310000000001	3.4357370000000000
W	16.1782770000000014	23.7273700000000005	3.4873580000000000
W	15.0317290000000003	26.2740890000000000	3.4259970000000002
W	27.6589099999999988	9.7485400000000002	3.2212900000000002
W	26.0608289999999982	12.3812080000000009	3.3149389999999999
W	24.4401399999999995	15.1189199999999992	3.3076219999999998
W	22.7852849999999982	17.9775910000000003	3.3340770000000002
W	21.1328439999999986	20.6997180000000007	3.3906109999999998
W	20.0473940000000006	23.5263039999999997	3.3948849999999999
W	17.7567270000000015	26.4573630000000009	3.5521300000000000
W	16.5890479999999982	28.9349780000000010	3.6080199999999998
W	29.3785479999999986	12.6379470000000005	3.3617580000000000
W	28.2713369999999991	15.3802219999999998	3.3988499999999999
W	26.0262160000000016	18.3313999999999986	3.4275129999999998
W	24.8877050000000004	20.8727559999999990	3.4117109999999999
W	22.8884569999999989	23.8426730000000013	3.5089340000000000
W	21.5794509999999988	26.2685549999999992	3.4935179999999999
W	19.8200569999999985	29.4686190000000003	3.6378100000000000
W	18.1972610000000010	31.8421939999999992	4.0047009999999998
W	30.9646100000000004	15.3945959999999999	3.5155500000000002
W	29.8578119999999991	18.0583579999999984	3.4215480000000000
W	27.5681650000000005	21.0024680000000004	3.4424730000000001
W	25.9036420000000014	23.5940149999999988	3.4071400000000001

W	24.300959999999999	26.408118999999992	3.5024160000000002
W	22.713112999999999	29.078756999999995	3.4868950000000001
W	21.236737999999990	31.7293580000000013	3.6575790000000001
W	20.0906060000000011	34.846865999999986	3.9128069999999999
W	32.5064970000000031	18.079460999999984	3.4814340000000001
W	31.255193999999995	20.8687490000000011	3.4421130000000000
W	29.773044999999998	23.7243980000000008	3.4695779999999998
W	28.116483999999998	26.663913999999983	3.5220340000000001
W	26.5190100000000015	29.409456999999997	3.6070739999999999
W	24.886476999999993	32.1828020000000024	3.6949230000000002
W	23.117281999999994	34.9469210000000032	3.7505690000000000
W	21.498287999999987	37.3208640000000003	3.9096449999999998
W	33.9040400000000020	20.917245999999987	3.4878719999999999
W	32.453440999999980	23.787791999999996	3.4665309999999998
W	30.8351690000000005	26.493597999999986	3.4254370000000001
W	29.2654570000000014	29.170359999999987	3.4842800000000000
W	27.7122390000000003	31.8405340000000017	3.5767760000000002
W	26.1564900000000016	34.5687110000000004	3.7246389999999998
W	24.4212570000000007	37.256968999999980	3.8426550000000002
W	22.863368999999987	39.927506999999985	3.8034089999999998
S	24.0440790000000000	-0.1140730000000000	3.9515509999999998
S	22.607352999999998	3.2657729999999998	4.9399230000000003
S	21.186527999999991	6.0204820000000003	5.0022180000000001
S	19.5921890000000012	8.7619530000000001	5.0890599999999999
S	17.952134999999984	11.4427280000000007	5.1260500000000002
S	16.363859999999990	14.1359800000000000	5.1485930000000000
S	14.778378999999993	16.8788890000000009	5.1468080000000000
S	13.2750690000000002	19.7310680000000005	5.0352550000000003
S	11.216668999999996	22.6868510000000008	4.1970499999999999
S	27.1692870000000006	-0.0408730000000000	4.9471650000000000
S	25.7442840000000004	3.1661359999999998	5.1919110000000002
S	24.635214999999988	6.0495469999999996	4.7494740000000002
S	23.014323999999984	8.7784659999999999	4.6334150000000003

S	21.382540999999998	11.558045999999992	4.729339999999997
S	19.755504999999994	14.325355000000001	4.762349000000004
S	18.115514999999985	17.077794999999983	4.756429999999999
S	16.500316999999990	19.863378999999983	4.747850999999998
S	14.786467999999993	22.656787999999988	5.149976999999998
S	12.865945000000000	25.624953999999989	4.351434000000002
S	28.257909000000015	5.743584000000002	4.577315999999997
S	26.371355000000012	8.809098000000005	5.044840999999999
S	24.651458000000016	11.550636000000008	5.122817000000004
S	23.036581999999992	14.317622000000001	5.127183999999997
S	21.377061000000012	17.127841000000001	5.146926999999998
S	19.718106999999998	19.849388999999986	5.186379999999998
S	18.074248999999982	22.713132999999991	4.790004999999998
S	16.362149999999997	25.433115999999983	5.218575000000004
S	14.455745000000003	28.462848999999985	4.332710999999998
S	27.907519000000006	11.551318999999994	4.891538999999999
S	26.341156999999990	14.375825000000007	4.688653999999997
S	24.598362999999991	17.106221999999989	4.847217999999998
S	23.018177000000014	19.900227000000010	4.790027000000003
S	21.414546000000014	22.593295999999987	5.034307000000001
S	19.666207000000000	25.420058000000009	4.857955999999997
S	18.110182999999993	28.240752000000005	5.168527000000001
S	16.140896999999989	31.185832000000013	4.642389999999998
S	29.621379999999985	14.255143999999996	5.134299999999996
S	27.935016999999984	17.209735999999995	4.827671999999997
S	26.275131999999993	19.959243000000007	5.170833000000000
S	24.547408000000008	22.699749000000006	5.066492000000002
S	22.995115999999994	25.468710999999990	5.290898000000003
S	21.295932000000005	28.183099999999996	5.133230000000002
S	19.741455999999994	31.050093000000004	5.508109000000001
S	31.216470999999985	17.053052000000010	5.214788000000004
S	29.458438000000010	19.991595000000002	4.843526999999999
S	27.879761999999995	22.824037000000006	4.875834000000002

S	26.2650560000000013	25.5350180000000009	4.8226779999999998
S	24.6288820000000008	28.3239550000000015	4.9155030000000002
S	23.0355890000000016	31.0026870000000017	5.0335109999999998
S	32.7181229999999985	19.8140679999999989	5.1775419999999999
S	31.1961289999999991	22.7372300000000003	5.1124029999999996
S	29.5397050000000014	25.5441490000000009	5.1295630000000001
S	27.9111830000000012	28.3261170000000000	5.2566259999999998
S	26.2994669999999999	31.0857150000000004	5.3291570000000004
S	34.7056729999999973	22.7875480000000010	4.3913029999999997
S	33.1576680000000010	25.7998319999999985	4.1834470000000001
S	31.4840209999999985	28.5460740000000008	4.3000069999999999
S	29.8351019999999991	31.3029989999999998	4.4532030000000002
S	21.0935890000000015	2.0244650000000002	2.1646860000000001
S	19.2764549999999986	4.8380970000000003	2.5447440000000001
S	17.7726320000000015	7.6310969999999996	2.5081490000000000
S	16.1808990000000001	10.3932850000000006	2.4696310000000001
S	14.5306929999999994	13.1426730000000003	2.5218759999999998
S	12.8479109999999999	15.9105349999999994	2.6311770000000001
S	11.3149870000000004	18.9191159999999989	2.4607320000000001
S	24.7400020000000005	2.1575460000000000	1.7281550000000001
S	22.9146280000000004	4.9969130000000002	1.5742400000000001
S	21.3971319999999992	7.8442379999999998	1.6605900000000000
S	19.7507890000000010	10.6398329999999994	1.6499290000000000
S	18.1251509999999989	13.3751780000000000	1.6705900000000000
S	16.477669999999998	16.1075729999999986	1.6902779999999999
S	14.8303490000000000	18.9765629999999987	1.8274999999999999
S	13.2696609999999993	21.9243309999999987	1.6503159999999999
S	28.0149669999999986	2.2290800000000002	2.5393040000000000
S	26.1185879999999990	5.1130319999999996	1.8999010000000001
S	24.6589600000000004	7.8830840000000002	1.9236810000000000
S	23.0067920000000008	10.6329220000000007	2.0092279999999998
S	21.3703070000000004	13.4102119999999996	2.1006900000000002
S	19.7407129999999995	16.1608139999999985	2.0910820000000001

S	18.0864030000000007	18.8954340000000016	2.0452669999999999
S	16.5320450000000001	21.7674899999999987	2.0369100000000002
S	14.7635570000000005	24.6889539999999990	1.6795700000000000
S	28.1976970000000016	7.8364289999999999	1.9819880000000001
S	26.3398369999999993	10.7006990000000002	1.5879799999999999
S	24.6981450000000002	13.4331090000000000	1.6365050000000001
S	23.0731450000000002	16.2242330000000017	1.6762450000000000
S	21.3732550000000003	19.0013590000000008	1.6800250000000001
S	19.7595489999999998	21.7986860000000000	1.7078679999999999
S	18.0859379999999987	24.5595849999999984	2.1125560000000001
S	16.3347060000000006	27.4336850000000005	1.7852500000000000
S	29.8780099999999997	10.5035790000000002	2.5375610000000002
S	27.8929219999999987	13.4740850000000005	1.8574860000000000
S	26.3407330000000002	16.2801019999999994	2.0595930000000000
S	24.5708009999999994	19.0799260000000004	1.7839400000000001
S	22.9776479999999985	21.8159929999999989	2.1249549999999999
S	21.3535010000000014	24.6042249999999996	1.7537220000000000
S	19.6764040000000016	27.3872140000000002	2.2941669999999998
S	17.9854309999999984	30.2608400000000017	2.1337630000000001
S	31.6002159999999996	13.2099279999999997	2.8150070000000000
S	29.6955139999999993	16.2630669999999995	1.7187460000000001
S	27.9611260000000001	19.0115289999999995	2.1163490000000000
S	26.2411940000000001	21.9005410000000005	1.6833419999999999
S	24.5133319999999983	24.6130759999999995	1.8025169999999999
S	22.8917110000000008	27.3911790000000011	1.7964160000000000
S	21.2899589999999996	30.1722600000000014	1.8707689999999999
S	19.5944390000000013	33.0446749999999980	2.3250519999999999
S	33.2209440000000029	16.0590870000000017	2.6994220000000002
S	31.2628279999999990	19.0764339999999990	1.7683770000000001
S	29.4685309999999987	21.8260129999999997	2.0180169999999999
S	27.8464409999999987	24.6427160000000001	2.1859810000000000
S	26.1912079999999996	27.4217779999999998	2.1816469999999999
S	24.6087619999999987	30.1786929999999991	2.2823540000000002

S	22.9869340000000015	32.8981899999999996	2.3351630000000001
S	34.7813060000000007	19.0721130000000016	2.6174879999999998
S	32.7313059999999965	22.0329349999999984	1.7919490000000000
S	31.1616159999999986	24.7939509999999999	1.7337600000000000
S	29.5615179999999995	27.5604049999999994	1.7328669999999999
S	27.9828550000000007	30.2763559999999998	1.8118749999999999
S	26.3833950000000002	32.9870289999999997	1.9329120000000000
S	17.8986419999999988	34.0522139999999993	4.6523529999999997
S	21.4974880000000006	33.7599560000000025	5.2829030000000001
S	19.3964169999999996	36.8021699999999967	4.8825900000000004
S	24.6784290000000013	33.8719910000000013	5.3788970000000003
S	22.9514670000000010	36.5826360000000008	5.5571640000000002
S	20.9812159999999999	39.4679039999999972	4.9502620000000004
S	28.2986049999999985	34.1273789999999977	4.3749289999999998
S	26.5138069999999999	36.8551939999999973	4.6937100000000003
S	24.6994840000000018	39.5206889999999973	4.9871569999999998
S	22.8218479999999992	41.9039059999999992	2.9818169999999999
S	21.4141240000000010	35.6706920000000025	2.1448119999999999
S	24.8062289999999983	35.6886289999999988	2.0785049999999998
S	23.0067829999999987	38.3475090000000023	2.1437059999999999

$W_{66}S_{132}$; $E_{tot} = -31\,314\,123.421\,927\,97$ eV; $E_{rel} = 25.243\,052\,590\,9$ meV/f.u.

W	27.3541629999999998	-0.3702500000000000	3.2217850000000001
W	25.7398009999999999	2.3491040000000001	3.2485290000000000
W	24.2797429999999999	5.0961410000000003	3.3244660000000001
W	22.7540550000000010	7.8123800000000001	3.3587220000000002
W	21.1870529999999988	10.5237820000000006	3.3647030000000000
W	19.6014340000000011	13.2272619999999996	3.3736069999999998
W	18.0225860000000004	15.9312299999999993	3.3972509999999998
W	16.4653479999999988	18.6385919999999992	3.3656500000000000
W	15.0030110000000008	21.5270329999999994	3.3566870000000000
W	28.7978120000000004	1.8788830000000001	3.3733339999999998

W	30.500607999999997	-0.612323000000000	3.602780000000001
W	27.137805000000002	4.625623000000000	3.321623999999999
W	25.586719999999997	7.447377999999996	3.356368999999999
W	23.977971000000001	10.234453000000002	3.360837000000001
W	22.368890000000004	13.031281999999991	3.366096000000002
W	20.720057000000006	15.763263999999995	3.341956999999998
W	19.159459999999993	18.535937000000006	3.341505000000002
W	17.642278999999985	21.689858999999984	3.445053000000001
W	16.425616999999990	24.321086999999986	3.436189000000002
W	31.806794000000000	1.952450000000000	3.452767999999998
W	30.810721999999984	5.010093999999996	3.535906999999999
W	29.411538000000002	7.725965000000004	3.517428000000002
W	27.877162999999995	10.494391000000002	3.522908999999998
W	26.209614999999994	13.185745000000007	3.380253999999999
W	24.415016000000014	16.261283999999998	3.382988999999998
W	22.961486000000007	18.880881999999997	3.454791999999999
W	21.402174999999997	21.500779999999989	3.373062000000000
W	19.087091999999984	24.415756999999993	3.503461999999999
W	17.926338000000012	27.044653000000003	3.501736000000002
W	33.433117000000029	4.540411999999999	3.526708999999999
W	32.144232999999998	7.427386000000003	3.401092999999999
W	30.647838000000001	10.163251000000007	3.397854999999998
W	28.923311999999992	13.255527000000007	3.389383000000000
W	27.525126000000002	16.019275000000004	3.371221999999999
W	25.946497999999983	18.621545999999986	3.408773000000001
W	24.129625999999982	21.793296000000016	3.483480999999998
W	22.918086999999999	24.254899999999992	3.396409999999999
W	20.627718000000016	27.171008000000005	3.571000000000002
W	19.475056999999996	29.741824000000011	3.531334000000002
W	33.969881999999984	10.599731000000002	3.310681000000002
W	32.690855999999966	13.412259999999998	3.427547999999998
W	30.370764000000012	15.997885999999994	3.365826999999999
W	28.856415999999994	18.647428000000014	3.350626000000001

W	27.3890770000000003	21.2330809999999985	3.4774090000000002
W	25.6521320000000017	24.5242129999999996	3.5691290000000002
W	24.4704200000000007	26.9778640000000003	3.4933000000000001
W	22.2131650000000000	29.9317460000000004	3.6684429999999999
W	35.3530969999999982	13.2150820000000007	3.4325709999999998
W	34.1436289999999971	15.9408499999999993	3.4106310000000000
W	32.6404959999999988	19.0019770000000001	3.4571589999999999
W	31.0916959999999989	21.7656080000000003	3.4968750000000002
W	29.4672839999999994	24.4351979999999998	3.5722510000000001
W	27.2642530000000001	27.3437550000000016	3.7232170000000000
W	25.9831070000000004	29.7086590000000008	3.6777310000000001
W	36.7756529999999984	15.9725889999999993	3.4367920000000001
W	35.3241670000000028	18.8594009999999983	3.4243769999999998
W	33.7868810000000011	21.5678920000000005	3.4055080000000002
W	32.2325719999999976	24.2346000000000004	3.4818030000000002
W	30.6297020000000018	26.8992240000000002	3.7055899999999999
W	28.8864170000000016	29.9820449999999994	4.1096729999999999
W	21.0323050000000009	32.4488569999999967	3.6452920000000000
W	24.0633680000000005	32.9449759999999969	3.7541380000000002
W	22.6429809999999989	35.1684139999999985	3.8175750000000002
W	27.0464179999999992	32.8683729999999983	3.9307639999999999
W	25.5982100000000017	35.3006570000000011	3.9424760000000001
W	24.1188220000000015	37.8734120000000019	3.7981020000000001
S	28.2697029999999998	-2.1829170000000002	4.0461950000000000
S	27.0181520000000006	1.1710980000000000	4.9558470000000003
S	25.5026739999999990	3.9085869999999998	5.0323279999999997
S	23.9820869999999999	6.6768280000000004	5.0784950000000002
S	22.4096229999999998	9.4150790000000004	5.0959310000000002
S	20.8229620000000004	12.1266739999999995	5.1010809999999998
S	19.2524830000000016	14.8443330000000007	5.1118699999999997
S	17.7074099999999994	17.6067299999999989	5.1054300000000001
S	16.2120280000000001	20.4223339999999993	5.0360800000000001
S	14.1110319999999998	23.3523360000000011	4.2449769999999996

S	31.389472999999988	-2.270316999999999	4.665657000000004
S	30.337309999999987	1.095453999999999	5.135110000000001
S	28.906237000000008	3.926807000000002	4.788087000000000
S	27.422549000000001	6.681693000000001	4.717085000000000
S	25.859580999999986	9.468716000000006	4.725316000000003
S	24.249255000000016	12.242649000000001	4.728569000000002
S	22.602850000000001	15.065042999999993	4.722739999999999
S	21.029804999999996	17.797764000000008	4.709831999999996
S	19.466816999999989	20.567986999999987	4.703007000000004
S	17.708823999999999	23.345503000000008	5.170668000000000
S	15.699085999999994	26.295766000000004	4.351951999999998
S	32.050297000000005	3.679600000000002	5.190995000000000
S	30.718422000000003	6.662215999999999	5.231671000000004
S	29.185666999999987	9.449839000000008	5.201746000000000
S	27.540870000000017	12.245846000000002	5.134725000000004
S	25.821189000000004	15.015449000000003	4.915702999999997
S	24.344940000000011	17.844048000000008	5.132566999999999
S	22.745502999999994	20.633666000000016	5.131927000000001
S	20.991793000000013	23.396755999999999	4.786656999999999
S	19.264341000000017	26.125333999999987	5.232799000000000
S	17.306514000000000	29.108463000000004	4.428581000000003
S	34.360681999999971	6.287300000000001	4.502900000000003
S	32.533709000000018	9.389106000000000	4.879675999999999
S	30.823266000000003	12.286222000000004	4.660931999999999
S	29.041563000000000	15.033991000000003	5.045251000000004
S	27.493807000000003	17.798190000000017	5.077918000000004
S	25.832947999999982	20.571553999999990	5.001462000000001
S	24.331739999999999	23.426052999999996	5.220925000000003
S	22.553426999999992	26.172458999999999	4.867102000000000
S	20.813258000000011	28.909568000000002	5.304333999999999
S	33.962307000000027	12.187592999999997	5.107478000000004
S	32.331119999999985	15.160702999999998	4.910057000000001
S	30.765226999999994	17.902532999999983	4.769599000000004

S	29.2386780000000002	20.6264049999999983	4.7966249999999997
S	27.5402549999999984	23.3661129999999986	4.7737319999999999
S	25.8868900000000011	26.1946319999999986	5.3052720000000004
S	24.1353499999999990	28.9301719999999989	5.0214590000000001
S	35.5887150000000005	14.9108059999999991	5.1572139999999997
S	34.0304780000000022	17.8444140000000004	5.0502240000000000
S	32.4572909999999979	20.6849390000000000	5.1736899999999997
S	30.8419589999999992	23.4191159999999989	5.2518640000000003
S	29.0702779999999983	26.1778569999999995	5.2198789999999997
S	27.4067809999999987	29.0007289999999998	5.5547500000000003
S	37.5726659999999981	17.8439039999999984	4.3572179999999996
S	36.0508030000000019	20.8601099999999988	4.2105040000000002
S	34.3566670000000016	23.6513799999999996	4.4107390000000004
S	32.7361670000000018	26.4744020000000013	4.4233490000000000
S	30.8922840000000001	29.1544559999999997	4.7891420000000000
S	25.4156790000000008	-0.0445060000000000	2.1987800000000002
S	23.6672499999999992	2.7754059999999998	2.4926800000000000
S	22.2054250000000017	5.5965270000000000	2.4319829999999998
S	20.6324269999999999	8.3503539999999994	2.4752879999999999
S	19.0339060000000018	11.0969909999999992	2.4836909999999999
S	17.4073630000000001	13.8562250000000002	2.5081709999999999
S	15.7481930000000006	16.6467489999999998	2.5942110000000000
S	14.2356160000000003	19.6403910000000010	2.4376030000000002
S	29.0706319999999998	0.0537100000000000	1.6886509999999999
S	27.3232210000000002	2.9232220000000000	1.6437500000000000
S	25.7986469999999990	5.7797020000000003	1.6354040000000001
S	24.2307099999999984	8.5533579999999994	1.6573560000000001
S	22.6373299999999986	11.3383620000000001	1.6667230000000000
S	21.0182429999999982	14.0760349999999992	1.6490400000000001
S	19.3512519999999988	16.8273049999999991	1.6435560000000000
S	17.7523240000000015	19.7169460000000001	1.7881940000000001
S	16.1790979999999998	22.6542600000000007	1.6813950000000000
S	32.3144559999999998	0.0001400000000000	2.3036170000000000

S	30.495705999999984	2.991012000000000	1.952760000000000
S	29.043092999999989	5.745076000000000	2.048988000000000
S	27.499947999999998	8.538945999999993	2.109464000000000
S	25.889566999999996	11.266332000000002	2.068963999999998
S	24.280156000000016	14.122913000000005	2.101433000000000
S	22.585771999999986	16.893450999999989	2.017895999999999
S	21.041036999999993	19.594046999999998	2.001237999999999
S	19.457059999999985	22.485634000000010	2.035369999999999
S	17.647283000000016	25.430098999999985	1.744250000000000
S	34.118361000000002	2.553335000000000	2.685066000000000
S	32.410975999999980	5.663463000000000	1.762899999999999
S	30.891978999999992	8.485205999999998	1.700294000000000
S	29.253146000000010	11.346182999999999	1.807229999999999
S	27.516483999999984	14.156943000000000	1.676881000000000
S	25.879737999999997	16.921859000000013	1.688506000000000
S	24.367470999999983	19.825818999999992	1.885488000000000
S	22.682949000000007	22.540471000000000	1.686473000000000
S	20.979396000000013	25.282924000000013	2.125757999999998
S	19.182249999999998	28.142772999999983	1.802208000000000
S	34.196491999999992	8.510275000000000	2.359767000000000
S	32.399079999999979	11.374624000000007	1.894779000000000
S	30.808484000000000	14.145111000000000	1.953024000000000
S	29.050356000000007	16.929037000000010	1.655696000000000
S	27.448104000000007	19.677789000000006	1.703203999999999
S	25.952885999999995	22.610067000000008	2.027413000000000
S	24.246344000000006	25.357544000000008	1.744297999999999
S	22.551335999999992	28.059654999999993	2.235768000000000
S	20.793247999999984	30.848479999999986	1.881284000000000
S	36.155009999999972	11.125002000000003	2.680385999999999
S	34.125599999999986	14.191736000000006	1.699650000000000
S	32.318742000000003	16.982146000000002	2.102288999999999
S	30.754110000000007	19.774546000000008	2.088064000000000
S	29.179238999999990	22.528390999999992	2.109878000000000

S	27.583073999999999	25.406791999999994	2.265191999999999
S	25.866351000000016	28.148119999999987	1.908757000000000
S	24.150202000000002	30.857700999999987	2.415979000000001
S	37.634022999999991	14.103002000000000	2.577621000000002
S	35.596592999999986	17.106680000000008	1.749042999999999
S	34.085695999999987	19.910968000000004	1.684500000000001
S	32.544724999999997	22.680676999999993	1.712266000000001
S	30.924725999999997	25.430873999999993	1.845352000000001
S	29.179995999999992	28.292757000000017	2.321870999999998
S	27.558067999999987	31.057455000000009	2.343649999999998
S	18.857811999999991	31.942629000000002	4.323602000000002
S	22.491779000000011	31.735835000000016	5.281164999999997
S	20.567121000000002	34.643408999999983	4.687243999999997
S	25.656107999999997	31.753744000000011	5.297006999999998
S	24.108959999999997	34.579580999999975	5.570183000000001
S	22.264693999999987	37.406427999999982	4.941937000000002
S	29.277322000000016	32.145502999999979	4.718469999999999
S	27.665648999999984	34.826113999999969	4.968515000000000
S	25.999635000000014	37.486063999999989	4.972889000000003
S	24.081627999999985	39.850138000000012	2.979422000000000
S	22.365808999999987	33.581350000000005	2.038775999999999
S	25.740103999999988	33.674230000000014	2.146320999999999
S	24.063728000000011	36.287439999999966	2.142157999999998

$\mathbf{W}_{66}\mathbf{S}_{132}$; $E_{tot}=-31\ 314\ 123.602\ 578\ 85\ \text{eV}$; $E_{rel}=22.505\ 918\ 045\ 4\ \text{meV/f.u.}$

W	28.068673000000004	4.477609000000002	3.318518000000001
W	26.297979000000015	7.110547000000004	3.281880000000001
W	24.647401999999996	9.849610999999994	3.277485000000000
W	23.074645000000003	12.608463000000004	3.319608999999998
W	21.509284999999984	15.331820000000004	3.325181000000002
W	19.930071999999991	18.042553999999991	3.285448999999998
W	18.356587999999986	20.765207000000002	3.244019999999999

W	16.824145999999989	23.505410999999987	3.244629999999999
W	15.319390999999995	26.274564000000016	3.180035000000002
W	13.805621000000004	29.103434000000000	3.008184000000000
W	12.315778999999991	31.816404999999996	3.049688000000002
W	31.187547999999996	4.448304000000003	3.522232999999999
W	29.175183000000005	6.883308000000004	3.338838000000000
W	27.623508000000011	9.445059000000005	3.342404000000002
W	26.001559000000003	12.180704000000004	3.337842000000002
W	24.335920000000016	15.010545999999997	3.333502999999999
W	22.715113999999998	17.799070000000004	3.324828999999998
W	21.131318000000003	20.539775999999998	3.304495999999999
W	19.577694999999985	23.250057999999992	3.269820999999999
W	18.059529999999988	25.995490000000002	3.211929000000000
W	16.439073000000005	29.168590999999993	3.170583999999998
W	15.296341999999992	31.706261999999988	3.019674999999999
W	34.090505000000003	4.351011999999999	3.685763000000001
W	32.885720999999966	7.073870000000003	3.544284999999999
W	31.302797000000018	9.919503999999999	3.548004000000002
W	29.689544000000015	12.666650000000006	3.526651000000002
W	28.088502999999993	15.399589000000006	3.502527000000002
W	26.503599999999987	18.137947000000005	3.493513000000001
W	24.915489000000009	20.883299999999984	3.487719999999999
W	23.313511999999993	23.634779000000018	3.481672000000001
W	21.724080000000007	26.371855000000000	3.460957000000001
W	20.188749000000014	29.096212999999988	3.365066999999998
W	18.136393999999992	31.702435999999987	3.143765999999998
W	37.624287000000025	4.349353999999999	3.769426999999999
W	35.571731999999972	6.955315999999998	3.548036999999999
W	34.036189999999977	9.679477999999996	3.452345000000002
W	32.446787999999980	12.416655000000004	3.431547999999998
W	30.844470999999986	15.168326999999997	3.425517999999998
W	29.256396999999998	17.913624999999997	3.419705000000000
W	27.671614999999992	20.652110000000004	3.410552000000000

W	26.0704850000000015	23.3848720000000014	3.3864600000000000
W	24.4574829999999999	26.1319780000000002	3.3648950000000002
W	22.8747110000000013	28.9779039999999988	3.3686410000000002
W	21.6699939999999991	31.7006279999999983	3.2272930000000000
W	40.4641629999999992	4.3455579999999996	3.8933599999999999
W	39.3215470000000025	6.8832269999999998	3.7425519999999999
W	37.7012229999999988	10.0560589999999994	3.7011289999999999
W	36.1828450000000004	12.8015620000000006	3.6434289999999998
W	34.6290369999999967	15.5119199999999999	3.6087530000000001
W	33.0451880000000031	18.2525429999999993	3.5884790000000000
W	31.4246119999999998	21.0410860000000000	3.5795400000000002
W	29.7589639999999989	23.8707920000000016	3.5751559999999998
W	28.1368690000000008	26.6070069999999994	3.5707019999999998
W	26.5862149999999993	29.1693719999999992	3.5740280000000002
W	24.5730800000000009	31.6035819999999994	3.3908459999999998
W	43.4443249999999992	4.2356930000000004	3.8633620000000000
W	41.9551000000000016	6.9484060000000003	3.9047459999999998
W	40.4414760000000015	9.7767520000000001	3.7331819999999998
W	38.9363889999999984	12.5460399999999996	3.6686559999999999
W	37.4036899999999974	15.2864170000000001	3.6693929999999999
W	35.8302189999999996	18.0090789999999998	3.6278450000000002
W	34.2509560000000022	20.7197139999999997	3.5878739999999998
W	32.6856140000000011	23.4428289999999997	3.5933419999999998
W	31.1131239999999991	26.2018169999999984	3.6353920000000000
W	29.4624249999999996	28.9409419999999997	3.6313140000000002
W	27.6914270000000009	31.5737600000000000	3.5947870000000002
S	29.3618109999999994	2.8852009999999999	4.2852610000000002
S	27.5912830000000007	5.9881970000000004	5.0348499999999996
S	25.9484500000000011	8.6992779999999996	4.9984510000000002
S	24.3430409999999995	11.4348360000000007	5.0171720000000004
S	22.7399960000000014	14.1993630000000000	5.0552659999999996
S	21.1314589999999995	16.9364719999999984	5.0446299999999997
S	19.5356379999999987	19.6492140000000006	5.0083159999999998

S	17.9875250000000015	22.3736320000000006	4.9808919999999999
S	16.5099720000000012	25.1752180000000010	4.9425150000000002
S	14.9734940000000005	27.9951669999999986	4.8008569999999997
S	13.5889640000000007	30.8928720000000006	4.7217830000000003
S	32.5551680000000019	2.7580190000000000	4.4206000000000003
S	30.9884160000000008	6.1383369999999999	4.9737260000000001
S	29.3878430000000002	8.8056629999999991	4.8441609999999997
S	27.7822050000000011	11.5169339999999991	4.7658100000000001
S	26.1765730000000012	14.2737520000000000	4.7043499999999998
S	24.5812160000000013	17.0474040000000002	4.7095370000000001
S	22.9846070000000005	19.8031860000000002	4.7241010000000001
S	21.3841849999999987	22.5421000000000014	4.7257540000000002
S	19.8016649999999998	25.2794559999999997	4.6925819999999998
S	18.2263969999999986	28.0906930000000017	4.5321049999999996
S	16.6966870000000007	30.9228820000000013	4.8382560000000003
S	35.8135899999999978	2.8203939999999998	4.2903640000000003
S	34.1596550000000008	5.9738319999999998	5.3150100000000000
S	32.6402240000000035	8.8253959999999996	5.2137840000000004
S	31.0147240000000011	11.5974290000000000	5.2269170000000003
S	29.4080949999999994	14.3390640000000005	5.2131360000000004
S	27.8188209999999998	17.0782010000000000	5.2005619999999997
S	26.2292440000000013	19.8274369999999998	5.1909869999999998
S	24.6327819999999988	22.5782729999999994	5.1755500000000003
S	23.0342179999999992	25.3319359999999989	5.1653380000000002
S	21.4208269999999992	28.0971259999999994	5.1116140000000003
S	19.8534959999999998	31.0900789999999994	4.7764819999999997
S	38.9544830000000033	2.7734660000000000	4.7970660000000001
S	37.4060750000000013	6.0757789999999998	5.1897690000000001
S	35.8471890000000002	8.8718339999999998	4.9805080000000004
S	34.3266789999999986	11.6651439999999997	4.8777010000000001
S	32.7412449999999993	14.4196410000000004	4.8471640000000003
S	31.1476180000000014	17.1675579999999997	4.8412499999999996
S	29.5459509999999987	19.9239919999999984	4.8396499999999998

S	27.933189999999997	22.6857770000000016	4.8280409999999998
S	26.328269999999998	25.4132490000000004	4.8024380000000004
S	24.7099930000000008	28.1212640000000000	4.7942400000000003
S	23.0048169999999992	30.8676600000000008	5.0072289999999997
S	42.0812629999999999	2.8299409999999998	4.9635350000000003
S	40.6267530000000008	5.9481010000000003	5.5738550000000000
S	39.0571819999999974	8.8209549999999997	5.3109159999999997
S	37.5218109999999996	11.7260519999999993	5.3971159999999996
S	35.9436809999999980	14.4610660000000006	5.3567380000000000
S	34.3686179999999979	17.1949819999999995	5.3150969999999997
S	32.7819220000000016	19.9481259999999985	5.2795829999999997
S	31.1808149999999991	22.7323480000000018	5.2570119999999996
S	29.5787769999999988	25.5171250000000001	5.2821619999999996
S	27.9644489999999983	28.2478900000000017	5.3188420000000001
S	26.1071770000000001	30.9669139999999992	5.1967930000000004
S	45.1516039999999990	3.2126209999999999	3.0775679999999999
S	44.0110609999999980	6.0314129999999997	5.0572489999999997
S	42.5625270000000029	8.9694140000000004	4.7903279999999997
S	41.142096999999997	11.8456170000000007	4.4774110000000000
S	39.5182390000000012	14.6417330000000003	4.6207099999999999
S	37.9440579999999983	17.4405019999999986	4.5674580000000002
S	36.3516789999999972	20.1999549999999992	4.5119829999999999
S	34.7682239999999965	22.9593190000000007	4.4660299999999999
S	33.1695769999999968	25.7390100000000004	4.4880149999999999
S	31.5189519999999987	28.5683770000000017	4.5001300000000004
S	29.6982910000000011	31.4553970000000014	4.5189469999999998
S	26.0625089999999986	4.5969350000000002	2.3937550000000001
S	24.2416640000000001	7.4834079999999998	2.4126059999999998
S	22.5909890000000004	10.3123260000000005	2.4248120000000002
S	20.9921940000000014	13.0921120000000002	2.4469430000000001
S	19.4085169999999998	15.8515479999999993	2.4012730000000002
S	17.8161589999999990	18.6110520000000008	2.3459319999999999
S	16.2421030000000002	21.4098660000000010	2.2926329999999999

S	14.618332999999998	24.205966000000001	2.435696999999998
S	13.197907000000007	27.082346999999986	2.122630000000000
S	11.749295999999993	30.020555999999991	1.855666000000000
S	10.608587999999992	32.839421000000015	3.835192999999999
S	29.653532999999995	5.085706000000001	1.716299999999999
S	27.796227999999993	7.804128999999996	1.594352999999999
S	26.181681000000011	10.534487999999996	1.630737000000001
S	24.579602999999988	13.319176000000006	1.656180000000000
S	22.978342999999989	16.103452000000008	1.633670000000000
S	21.391605999999995	18.856617000000000	1.598163000000000
S	19.816652999999987	21.590467000000003	1.556530000000000
S	18.238683999999992	24.325492000000006	1.516086000000000
S	16.703451999999986	27.230743000000004	1.602163999999999
S	15.133767999999999	30.103711000000006	1.339086000000000
S	13.679116000000005	33.222087999999994	1.949457999999999
S	32.755876000000007	5.184174999999998	1.905721999999999
S	31.050903000000017	7.930625000000000	2.118503000000000
S	29.432331999999988	10.638460999999995	2.110396999999999
S	27.827291999999999	13.365857000000001	2.085073000000000
S	26.214477999999997	16.127615999999997	2.073589999999998
S	24.612712999999994	18.884108000000012	2.071969000000002
S	23.019003999999989	21.631923000000005	2.066087000000000
S	21.433655000000017	24.386341000000016	2.035485000000000
S	19.913260000000011	27.179701999999989	1.932576000000001
S	18.354469999999992	29.975974000000008	1.723306999999999
S	16.805994999999994	33.278424000000011	2.116000000000001
S	35.906981999999993	4.961595000000000	2.136595999999999
S	34.339475999999977	7.954402000000000	1.801469000000000
S	32.726112999999980	10.719509000000004	1.747834000000001
S	31.127507000000014	13.473295000000002	1.737703000000000
S	29.531102000000006	16.224177000000010	1.722213999999999
S	27.941514000000015	18.973489000000007	1.712582000000000
S	26.352181999999991	21.712495000000005	1.699997999999999

S	24.745637999999996	24.454091999999993	1.6861830000000000
S	23.1201790000000003	27.226221999999999	1.6993689999999999
S	21.6007180000000005	30.0778129999999990	1.5980710000000000
S	19.9469710000000013	33.2314349999999976	2.6227900000000002
S	39.0637320000000017	5.1289650000000000	2.0747749999999998
S	37.534055999999996	7.9609090000000000	2.3809990000000001
S	35.9587879999999984	10.7721689999999999	2.2205879999999998
S	34.3762339999999966	13.5094499999999993	2.1873790000000000
S	32.775705999999996	16.2483569999999986	2.1890250000000000
S	31.1790440000000011	19.0041070000000012	2.2035170000000002
S	29.5837879999999984	21.7776899999999998	2.2086820000000000
S	27.9781540000000000	24.5347429999999989	2.1474150000000001
S	26.3722439999999985	27.2463629999999988	2.0694849999999998
S	24.7720109999999991	29.9134780000000013	1.9395420000000001
S	23.2053769999999986	33.2939560000000014	2.4924350000000000
S	42.1713749999999976	5.1590049999999996	2.1912240000000001
S	40.7869799999999998	8.0566030000000008	2.1121240000000001
S	39.2505459999999999	10.8764140000000005	1.9707100000000000
S	37.7729220000000012	13.6779030000000006	1.9324770000000000
S	36.2246700000000033	16.4023420000000009	1.9049799999999999
S	34.6287980000000033	19.1150100000000016	1.8685050000000001
S	33.0203509999999980	21.8520159999999990	1.8576130000000000
S	31.4174840000000017	24.6167119999999997	1.8957299999999999
S	29.8122800000000012	27.3527979999999999	1.9145000000000001
S	28.1695899999999995	30.0645850000000010	1.8781420000000000
S	26.3992980000000017	33.1675219999999982	2.6281620000000001

W₆₆S₁₃₂; $E_{tot} = -31\,314\,125.087\,969\,44$ eV; $E_{rel} = 0$ meV/f.u.

W	20.0034220000000005	1.5415700000000001	3.4421640000000000
W	18.2505459999999999	4.2487839999999997	3.5271610000000000
W	16.7336050000000007	6.9069529999999997	3.6294360000000001
W	15.2060420000000001	9.5524719999999999	3.5674739999999998

W	13.731773999999997	12.446123000000000	3.468486000000000
W	23.125470000000000	1.386303000000001	3.357400999999999
W	21.373364999999997	3.776241000000002	3.469328000000000
W	19.495473000000005	6.620998000000002	3.488901999999999
W	17.912527000000008	9.392830000000000	3.507165000000001
W	16.355563000000001	12.639079000000006	3.539045000000002
W	15.158485999999999	15.249829000000001	3.436563000000000
W	26.232231999999998	1.391218000000001	3.284462000000000
W	24.350045000000015	3.730097000000002	3.434158000000000
W	23.261420000000011	6.992602999999999	3.456894000000001
W	21.721063000000009	9.731840999999993	3.560210000000001
W	20.098150000000004	12.454449000000003	3.439992000000002
W	17.809128000000012	15.327643000000001	3.509303000000001
W	16.690932000000001	17.945785000000008	3.385200000000002
W	29.359311000000017	1.383450000000001	3.346738999999999
W	28.096416000000014	3.704279999999998	3.434734000000002
W	26.235302000000008	7.023311999999998	3.371376999999998
W	24.507543999999993	9.389811999999992	3.426483999999999
W	22.831799000000002	12.540625000000004	3.448083000000000
W	21.626657999999990	15.152587000000005	3.387343000000000
W	19.391726999999995	18.043375999999985	3.495346000000001
W	18.311178000000017	20.625070999999984	3.384440999999998
W	32.471079000000031	1.519797000000001	3.443954000000002
W	31.089570999999994	3.730786999999999	3.474626000000002
W	29.253648999999993	7.019529000000004	3.488478999999999
W	28.174990000000011	9.525176999999993	3.368815999999998
W	25.800924999999994	12.386252000000007	3.445189000000001
W	24.362080999999999	15.062402999999998	3.411840000000002
W	23.213110000000004	17.781821999999982	3.387582000000001
W	21.356998999999983	21.109124999999988	3.499530000000000
W	19.938887000000011	23.354637000000003	3.521885000000002
W	34.217937999999966	4.236985999999999	3.545468000000001
W	33.035122000000012	6.670461000000004	3.485189999999998

W	30.862791999999989	9.721814999999994	3.549418999999999
W	29.676420000000002	12.276614000000004	3.416970000000001
W	28.167801999999982	15.208320999999998	3.462429000000002
W	26.249013999999990	18.230509999999989	3.419337000000001
W	24.660159000000002	20.445706000000013	3.516419000000000
W	22.909981999999994	23.753280000000002	3.514072000000001
W	21.621311999999996	26.113417999999994	3.450626000000002
W	35.789312999999999	6.894263999999997	3.607880999999999
W	34.657513000000016	9.432221000000002	3.472045000000000
W	32.389893000000007	12.412373000000005	3.495470000000001
W	30.881025999999985	15.142243000000006	3.391017999999999
W	29.345082999999989	17.752155999999994	3.353898000000000
W	27.783356999999987	20.485475999999985	3.485167000000001
W	26.176694000000012	23.913638999999999	3.487235000000001
W	24.790161999999987	26.191935000000009	3.523407999999999
W	37.317627000000017	9.538586000000005	3.577649000000001
W	36.152059999999988	12.158569000000000	3.458947999999999
W	34.653914999999978	15.358290999999995	3.475757999999999
W	33.112861999999998	18.156625999999993	3.460812999999999
W	31.528577999999995	20.934906999999990	3.449317999999999
W	29.400462999999985	23.917376000000009	3.473049000000001
W	27.859787000000007	26.175229999999991	3.566606999999999
W	38.783462000000001	12.296158999999994	3.559813000000001
W	37.356710999999971	15.203207000000008	3.469043000000001
W	35.837994999999994	17.910827999999986	3.404348000000002
W	34.299419000000003	20.582893999999996	3.412526999999999
W	32.990926999999992	23.359660999999991	3.459916000000002
W	30.841055999999982	26.227900000000018	3.401545000000000
W	33.951576000000029	26.305364999999983	3.172445000000002
S	21.230601000000001	-0.143000000000000	4.247681000000000
S	19.668283999999999	3.105999999999999	5.158951000000001
S	18.043316999999983	5.820136999999999	5.301943999999998
S	16.475463999999988	8.573456999999994	5.318705999999997

S	14.958069999999993	11.395118999999993	5.175597999999999
S	12.860424000000001	14.318030999999995	4.297686999999998
S	24.633344999999985	-0.238303000000000	4.089234000000003
S	22.923767000000016	2.908262999999998	5.141642000000000
S	21.422588000000011	5.862301999999997	4.794380000000003
S	19.800436000000013	8.660562000000005	4.853005999999997
S	18.174084000000006	11.496230999999999	4.781600000000001
S	16.436709000000005	14.329556999999994	5.216673000000001
S	14.510120999999998	17.286408999999990	4.341822999999998
S	27.835354999999998	-0.238682000000000	4.078832000000002
S	26.226030000000015	2.989736000000002	4.922424999999996
S	24.658428000000007	5.778070999999997	4.902427999999996
S	23.041461999999992	8.587892000000001	5.210829000000004
S	21.382438000000005	11.481688000000001	5.171444000000002
S	19.706669999999990	14.326273999999997	4.832282000000002
S	18.000398000000006	17.107195000000008	5.186492000000003
S	16.133365000000013	20.150128999999997	4.160591000000002
S	31.236065000000000	-0.156794000000000	4.252564999999997
S	29.528960999999989	2.904154999999998	5.149964999999999
S	27.832561999999994	5.778640000000002	4.881666000000001
S	26.296875000000000	8.720465000000008	4.986336999999998
S	24.458777000000013	11.406992999999999	5.016390000000003
S	22.974344999999996	14.239171999999999	5.183539999999998
S	21.322821999999986	17.059426999999995	4.826525000000002
S	19.748578999999994	19.911436999999994	5.038923999999997
S	17.786100999999986	22.899796999999995	4.196729999999996
S	32.798662000000002	3.090482000000002	5.165821000000002
S	31.090140999999991	5.852051999999996	4.765178999999998
S	29.512001999999990	8.632068999999995	5.209901000000003
S	27.773225000000001	11.470143000000002	4.791290000000000
S	26.260881000000013	14.248283000000007	4.819016000000004
S	24.701411000000002	16.975289000000001	4.988221000000002
S	22.961358000000006	19.782488000000007	4.961970000000000

S	21.4459930000000014	22.7489929999999987	5.2242240000000004
S	34.4868349999999992	5.8128620000000000	5.2966759999999997
S	32.7417420000000021	8.6555710000000001	4.8580139999999998
S	31.0845309999999984	11.4288840000000000	5.2268220000000003
S	29.5397530000000010	14.1903150000000000	5.1083379999999998
S	27.8630169999999993	17.0516150000000017	5.0251640000000002
S	26.2750860000000017	19.8691239999999993	5.2100700000000000
S	24.6629719999999999	22.6088670000000000	4.8497779999999997
S	36.0699809999999985	8.5233179999999997	5.3064720000000003
S	34.3118989999999968	11.4288080000000001	4.8771279999999999
S	32.7864799999999974	14.3311050000000009	4.8421599999999998
S	31.2140430000000002	17.1063170000000007	4.7802780000000000
S	29.6468510000000016	19.8431940000000004	4.7899180000000001
S	27.8903290000000013	22.6450640000000014	4.8359649999999998
S	37.5854870000000005	11.2548259999999996	5.2733449999999999
S	36.0411959999999993	14.1860909999999993	5.0592160000000002
S	34.4611590000000021	17.0834089999999996	5.1652790000000000
S	32.8440810000000027	19.8697799999999987	5.1553820000000004
S	31.2163259999999987	22.7578640000000014	4.9296590000000000
S	39.5770949999999999	14.2047249999999998	4.4163759999999996
S	38.0881720000000001	17.2071250000000013	4.2250310000000004
S	36.4371769999999984	19.9915209999999988	4.3511980000000001
S	34.7554429999999996	22.6807639999999999	4.6652969999999998
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S	12.9742909999999991	10.5074839999999998	2.6335180000000000
S	21.4881869999999999	2.0331229999999998	1.6928170000000000
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S	18.0719099999999990	7.6698500000000003	1.8157700000000001
S	16.4848199999999991	10.5799260000000004	1.9627859999999999
S	14.8821449999999995	13.5247349999999997	1.7426770000000000
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S	26.2347609999999989	4.8507680000000004	2.2181320000000002
S	24.6288090000000004	7.7411599999999998	1.6733300000000000
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S	21.3458399999999990	13.3812010000000008	1.6944770000000000
S	19.7082850000000001	16.1555910000000011	2.0730439999999999
S	18.0030479999999997	18.9923830000000002	1.6896960000000001
S	30.9991209999999988	2.0098180000000001	1.6828339999999999
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S	26.2933899999999987	10.4997050000000005	2.0458150000000002
S	24.5040529999999990	13.3375430000000001	1.7342670000000000
S	23.0198360000000015	16.1251779999999982	1.6843379999999999
S	21.3381830000000008	18.9644370000000002	2.2525960000000000
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S	34.5229050000000015	1.8158540000000001	2.5911170000000001
S	32.7161529999999985	4.8605980000000004	1.9082429999999999
S	31.1869130000000006	7.7146260000000000	2.1310750000000001
S	29.5309160000000013	10.5657660000000000	1.7148049999999999
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S	24.6277790000000003	18.8688479999999998	1.7350800000000000
S	23.0720729999999996	21.7487050000000011	2.0271040000000000
S	21.2271399999999986	24.4825200000000009	1.8232250000000001
S	36.3315920000000006	4.6358850000000000	2.7624540000000000
S	34.4394220000000004	7.6738580000000001	1.8059700000000001
S	32.7915130000000019	10.4803339999999992	2.1287729999999998
S	31.0832450000000016	13.3432949999999995	1.7439739999999999

S	29.5083780000000004	16.0818820000000002	1.6577040000000001
S	27.8847529999999999	18.8803589999999986	1.7354080000000001
S	26.2600720000000010	21.7872260000000004	2.1423220000000001
S	24.5610299999999988	24.5874090000000010	1.8482700000000001
S	37.9419710000000023	7.4876990000000001	2.6445310000000002
S	36.0445029999999988	10.4579640000000005	1.7881000000000000
S	34.3518419999999978	13.3060700000000001	2.1623340000000000
S	32.8086569999999966	16.1540660000000003	2.0753810000000001
S	31.2195670000000014	18.9300290000000011	2.0761599999999998
S	29.5673649999999988	21.7472589999999997	2.1757529999999998
S	27.8182340000000003	24.5744019999999992	1.8033210000000000
S	39.6261549999999971	10.4097120000000007	2.7294809999999998
S	37.5950500000000005	13.3749000000000002	1.8453599999999999
S	36.1427380000000014	16.2259700000000002	1.7094890000000000
S	34.6288089999999968	18.9806440000000016	1.6750490000000000
S	33.0599789999999985	21.7132180000000012	1.7125140000000001
S	31.1045440000000006	24.5200040000000001	1.8947840000000000
S	19.7618499999999990	25.4827419999999982	4.8920529999999998
S	23.1384989999999995	25.5802720000000008	5.1856400000000002
S	22.9054690000000001	27.6934460000000016	2.5480680000000002
S	26.2818980000000018	25.6000650000000007	5.2824169999999997
S	26.1879890000000017	27.8169100000000000	2.7486850000000000
S	29.4497479999999996	25.6359610000000018	5.2420910000000003
S	32.7144019999999998	25.4760549999999988	4.9120569999999999
S	32.4933660000000017	27.7231839999999998	2.2587440000000001
S	34.4137109999999993	24.6155940000000015	1.7821929999999999
S	29.3574829999999984	27.7635910000000017	2.5576949999999998
S	35.7011740000000017	27.3433449999999993	3.8139310000000002
S	19.3627770000000012	26.8963959999999993	3.3747490000000000

$W_{105}S_{210}$; $E_{tot} = -49\,817\,926.235\,627\,72$ eV; $E_{rel} = 38.315\,311\,533\,3$ meV/f.u.

W	20.9761239999999987	-0.2025830000000000	3.3007640000000000
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W	19.201937999999984	2.431084999999999	3.250257000000000
W	17.557977000000011	5.173409000000004	3.243764000000001
W	15.993206000000007	7.921655999999996	3.281251999999998
W	14.423104999999996	10.631830000000008	3.286067000000001
W	12.845174999999993	13.339871000000005	3.275907000000001
W	11.276149999999995	16.069849000000014	3.314738000000002
W	9.691221000000005	18.857113999999993	3.360431999999999
W	8.072406000000009	21.624507000000013	3.306495000000000
W	6.495936999999996	24.349524999999999	3.261312999999999
W	4.941770000000000	27.078039999999990	3.272702000000002
W	3.380662000000001	29.785568999999989	3.276362999999999
W	1.783088000000000	32.513716999999998	3.250414999999998
W	0.228668000000000	35.308031999999972	3.267415000000002
W	-1.164191000000000	38.161490000000006	3.320476999999999
W	24.088384000000014	-0.230090000000000	3.538485000000001
W	22.090097000000001	2.196704000000000	3.328421000000001
W	20.542238999999986	4.752349999999999	3.308713000000000
W	18.893101999999990	7.515936000000000	3.283218000000002
W	17.227962999999990	10.351905000000004	3.279719000000001
W	15.634273999999996	13.117271999999998	3.287836000000000
W	14.119944000000003	15.795030000000006	3.301286999999999
W	12.627084999999992	18.466992000000012	3.328848999999999
W	10.822993999999996	21.592832000000014	3.326055999999999
W	9.258114000000008	24.225315999999994	3.297291000000000
W	7.698944000000000	26.877597000000015	3.285413000000001
W	6.102468000000000	29.639265000000017	3.281460000000000
W	2.910749000000000	35.306558000000026	3.319345000000002
W	4.479486999999998	32.496667000000022	3.290575000000000
W	1.471189000000001	37.926606999999971	3.334849999999999
W	0.369622000000000	40.871277999999967	3.528335000000002
W	26.991333000000009	-0.324666000000000	3.732302999999999
W	28.476673999999992	2.281069000000000	3.578831000000001
W	25.794478000000016	2.391770999999999	3.563909999999999

W	24.2013740000000013	5.2469460000000003	3.5418470000000002
W	22.5969400000000000	7.9817359999999997	3.4931939999999999
W	21.0011979999999987	10.7007329999999996	3.4514770000000001
W	19.4232820000000004	13.4309110000000000	3.4464690000000000
W	17.8489849999999990	16.1766350000000010	3.4656690000000001
W	16.2537899999999986	18.9431690000000010	3.4797430000000000
W	14.6312920000000002	21.7088399999999986	3.4611179999999999
W	13.0502950000000002	24.4975619999999985	3.4853350000000001
W	11.4548220000000001	27.2629069999999984	3.4747110000000001
W	9.8661410000000007	30.0005130000000015	3.4587729999999999
W	8.2918319999999994	32.7320160000000016	3.4643389999999998
W	6.7352449999999999	35.4730220000000003	3.5000610000000001
W	5.1694459999999998	38.2299700000000016	3.5364339999999999
W	3.4936850000000002	41.0398750000000021	3.5375619999999999
W	1.7381059999999999	43.4351539999999972	3.6877279999999999
W	30.5359830000000017	-0.3135590000000000	3.8049719999999998
W	26.9346570000000014	5.0047550000000003	3.4688539999999999
W	25.3500249999999987	7.7399360000000001	3.4287869999999998
W	23.7529670000000017	10.4790790000000005	3.3974980000000001
W	22.1678280000000001	13.2067110000000003	3.3704299999999998
W	20.5878650000000007	15.9369029999999992	3.3587680000000000
W	18.9964699999999986	18.6866899999999987	3.3591380000000002
W	17.3914299999999997	21.4525940000000013	3.3622269999999999
W	15.7918780000000005	24.2270569999999985	3.3668170000000002
W	14.2020689999999998	27.0012609999999995	3.3724170000000000
W	12.6180009999999996	29.7562409999999993	3.3762520000000000
W	9.4751609999999999	35.2270770000000013	3.4073940000000000
W	11.0442859999999996	32.4898689999999988	3.3869189999999998
W	7.9023399999999997	37.9792890000000014	3.4233180000000001
W	6.3264120000000004	40.7187130000000010	3.4394030000000000
W	4.7391990000000002	43.4168710000000004	3.5225439999999999
W	3.5187990000000000	46.5019100000000023	3.7131599999999998
W	33.3780369999999991	-0.3142050000000000	3.8871039999999999

W	34.8643860000000032	2.2855080000000001	3.8857260000000000
W	32.2277529999999999	2.2288239999999999	3.7573420000000000
W	30.6139459999999985	5.3729659999999999	3.7337720000000001
W	29.0811610000000016	8.1329089999999997	3.6780930000000001
W	27.5184040000000003	10.8548469999999995	3.6448589999999998
W	25.9367090000000005	13.5800439999999991	3.6174759999999999
W	24.3589610000000008	16.2895310000000002	3.5909580000000001
W	22.7848490000000012	18.9811060000000005	3.5625920000000000
W	21.1892570000000013	21.7131739999999986	3.5407869999999999
W	19.5496879999999997	24.5461780000000012	3.5386289999999998
W	17.9176099999999998	27.3854399999999991	3.5561029999999998
W	16.3511589999999991	30.1350510000000007	3.5869030000000000
W	14.8095680000000005	32.8439679999999967	3.6152139999999999
W	13.2533349999999999	35.5658379999999994	3.6307570000000000
W	11.6840309999999992	38.2992860000000022	3.6375860000000002
W	10.1082870000000007	41.0161999999999978	3.6420780000000001
W	8.4836139999999993	43.7243039999999965	3.6649680000000000
W	6.5664520000000000	46.6944159999999968	3.6543660000000000
W	4.9385279999999998	48.9629419999999982	3.7602359999999999
W	36.3548210000000012	-0.4267240000000000	3.7932579999999998
W	33.3469089999999966	5.1228899999999999	3.7569010000000000
W	31.8230229999999992	7.8850879999999997	3.7104729999999999
W	30.2891580000000005	10.6256780000000006	3.7293820000000002
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W	22.3482459999999996	24.3166629999999984	3.5402269999999998
W	20.7523499999999999	27.0842640000000010	3.5501920000000000
W	19.1709110000000003	29.8527689999999986	3.6105489999999998
W	16.0274169999999998	35.3523100000000028	3.7018719999999998
W	17.5997130000000013	32.6080919999999992	3.6692380000000000
W	14.4523720000000004	38.0902979999999971	3.7099340000000001

W	12.870169999999999	40.818899000000018	3.6946949999999998
W	11.2630370000000006	43.5181889999999996	3.6416450000000000
W	9.6314639999999994	46.2187359999999998	3.6530730000000000
W	7.9329239999999999	48.9514250000000004	3.7484600000000001
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S	17.2501330000000017	6.7605199999999996	4.9816549999999999
S	15.6550589999999996	9.5107649999999992	5.0146790000000001
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S	12.5218679999999996	14.9492999999999991	5.0264319999999998
S	10.9805379999999992	17.7397029999999987	5.0378319999999999
S	9.3660969999999999	20.5342820000000010	5.0341909999999999
S	7.7207819999999998	23.2627120000000005	5.0165480000000002
S	6.1337120000000001	25.9573479999999996	5.0064810000000000
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S	22.2824559999999998	4.1284919999999996	4.8298319999999997
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S	19.0804510000000001	9.5978379999999994	4.6471450000000001
S	17.4956640000000014	12.3640360000000005	4.6831160000000001
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S	14.3509709999999995	17.8161260000000006	4.7770530000000004
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S	11.1200799999999997	23.4109949999999998	4.7756010000000000
S	9.5572070000000000	26.1297269999999990	4.7430009999999996
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S	14.2668630000000007	14.1577149999999996	1.5629759999999999
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S	6.3740040000000002	31.6170709999999993	4.6554029999999997
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S	1.7411639999999999	39.8562969999999979	4.9743300000000001
S	-0.4005280000000000	42.9048510000000007	4.4412490000000000
S	-0.4671070000000000	33.3440099999999973	2.3825910000000001
S	-2.0620870000000000	36.3622480000000010	2.3932739999999999
S	3.1352500000000001	33.5100169999999977	1.6061700000000001
S	1.5676319999999999	36.2760689999999997	1.5821940000000001

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S	27.0628479999999989	1.3073290000000000	5.3507709999999999
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S	23.9034469999999999	6.9237510000000002	5.2149060000000000
S	22.3027400000000000	9.6547610000000006	5.1765330000000001
S	20.7278309999999983	12.3819110000000006	5.1523139999999996
S	19.1598989999999993	15.1218240000000002	5.1522690000000004
S	17.5764110000000002	17.8739689999999989	5.1570689999999999
S	15.9445610000000002	20.6318820000000009	5.1518670000000002
S	14.3575409999999994	23.3802500000000002	5.1553110000000002
S	12.7853060000000003	26.1731109999999987	5.1664849999999998
S	11.1945940000000004	28.9225679999999983	5.1648690000000004
S	31.8810590000000005	-1.8818619999999999	4.8226870000000002
S	30.3210569999999997	1.4165970000000001	5.2203480000000004
S	28.7481930000000006	4.1995649999999998	5.0051350000000001
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S	22.4619269999999993	15.2119509999999991	4.8037340000000004
S	20.8866470000000000	17.9458109999999991	4.7895310000000002
S	19.2917279999999991	20.6973009999999995	4.7848160000000002
S	17.6832099999999990	23.4665010000000009	4.7860040000000001
S	16.0892039999999987	26.2459880000000005	4.7966389999999999
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S	17.5185010000000005	14.1928940000000008	2.0361560000000001
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S	12.734000999999992	22.500555999999996	2.0389320000000000
S	11.1514550000000003	25.2404060000000001	2.0584009999999999
S	9.5761930000000000	27.9735900000000015	2.0423680000000002
S	7.9952690000000004	30.7338869999999993	2.0282950000000000
S	28.8087860000000013	0.2777820000000000	2.1806440000000000
S	27.2506440000000012	3.2733010000000000	1.8256010000000000
S	25.6415030000000002	6.0406969999999998	1.7507459999999999
S	24.0492160000000013	8.7918599999999998	1.7137410000000000
S	22.4517330000000008	11.5334070000000004	1.6759219999999999
S	20.8548350000000013	14.2718299999999996	1.6601349999999999
S	19.2644160000000007	17.0160829999999983	1.6671849999999999
S	17.6721620000000001	19.7724769999999985	1.6777620000000000
S	16.0780320000000003	22.5464440000000010	1.6794549999999999
S	14.4785830000000004	25.3160449999999990	1.6862140000000001
S	12.8921740000000007	28.0737300000000012	1.6811460000000000
S	11.3127750000000002	30.8220969999999994	1.6764410000000001
S	9.6072220000000002	31.6537040000000012	5.1662710000000001
S	8.0348699999999997	34.3855199999999996	5.1875400000000003
S	6.4731199999999998	37.1433889999999991	5.2149010000000002
S	4.8916490000000001	39.9441229999999976	5.2010839999999998
S	3.1937760000000002	42.7003869999999992	5.3078820000000002
S	1.2957330000000000	45.7025849999999991	4.2764309999999996
S	12.9250860000000003	31.7403660000000016	4.8239890000000001
S	11.3509910000000005	34.4733450000000019	4.8381400000000001
S	9.7756609999999995	37.2219550000000012	4.8502340000000004
S	8.1868490000000005	39.9815660000000008	4.8715299999999999
S	6.5381039999999997	42.7096080000000029	4.9533040000000002
S	6.4115110000000000	33.5170349999999999	2.0428299999999999
S	4.8515879999999996	36.2715409999999991	2.0816490000000001
S	3.3164340000000001	39.0232910000000004	2.1160380000000001
S	1.7843100000000001	41.8632369999999980	1.9071060000000000
S	9.7391810000000003	33.5702420000000004	1.6897880000000001
S	8.1620819999999998	36.3178649999999976	1.7174590000000001

S	6.5737290000000002	39.0663330000000002	1.7366619999999999
S	4.9800870000000002	41.8402460000000005	1.7869290000000000
S	3.1642709999999998	44.6888409999999965	2.1152860000000002
S	35.0115580000000008	-1.8387990000000001	4.9124410000000003
S	33.5571079999999995	1.2842389999999999	5.5695649999999999
S	31.9786549999999998	4.1561500000000002	5.3447089999999999
S	30.4057490000000001	7.0451610000000002	5.4285329999999998
S	28.8124199999999995	9.7861700000000003	5.3952780000000002
S	27.2304449999999996	12.5223700000000004	5.3639080000000003
S	25.6581750000000000	15.2571480000000008	5.3397300000000003
S	24.0944049999999983	17.9900659999999988	5.3120479999999999
S	22.5272380000000005	20.7263960000000012	5.2668970000000002
S	20.9402320000000017	23.4891530000000017	5.2176559999999998
S	19.3330149999999996	26.2723750000000003	5.2254459999999998
S	17.7323820000000012	29.0318089999999991	5.2885879999999998
S	38.0414730000000034	-1.4440050000000000	2.9584589999999999
S	36.9445679999999967	1.3602810000000001	4.9898100000000003
S	35.4914040000000028	4.3020189999999996	4.7646800000000002
S	34.0432369999999977	7.1825070000000002	4.5099749999999998
S	32.3977369999999993	9.9565870000000007	4.6991529999999999
S	30.8306390000000015	12.7475900000000006	4.6657070000000003
S	29.2482609999999994	15.4931180000000008	4.6326809999999998
S	27.6712980000000002	18.2300849999999990	4.5775920000000001
S	26.0728949999999990	20.9634870000000006	4.5303170000000001
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S	22.8910020000000003	26.4713610000000017	4.4023930000000000
S	21.2949620000000017	29.2255609999999990	4.4710840000000003
S	31.9519829999999985	0.4725040000000000	2.0935959999999998
S	30.4292979999999993	3.2959209999999999	2.4019930000000000
S	28.8624960000000002	6.1068579999999999	2.2598859999999998
S	27.2823940000000000	8.8525139999999993	2.2144240000000002
S	25.6875490000000006	11.5898769999999995	2.1911160000000001
S	24.0976019999999984	14.3246300000000009	2.1567110000000000

S	22.513685999999999	17.054187999999999	2.1229770000000001
S	20.927600999999999	19.7951580000000007	2.1209989999999999
S	19.330605999999995	22.5663950000000000	2.1600500000000000
S	17.7240329999999986	25.3544079999999994	2.1670490000000000
S	16.1271710000000006	28.1240880000000004	2.1385869999999998
S	14.550200999999995	30.8666750000000008	2.1449639999999999
S	35.0509819999999976	0.5090020000000000	2.1558860000000002
S	33.6766310000000004	3.4082979999999998	2.1184859999999999
S	32.145963999999993	6.2228320000000004	2.0028869999999999
S	30.6756719999999987	9.0333909999999999	1.9794050000000001
S	29.1385429999999985	11.7709119999999992	1.9705870000000001
S	27.562865999999996	14.4941429999999993	1.9464630000000001
S	25.967442999999994	17.2122929999999990	1.9108560000000001
S	24.356636999999992	19.9314229999999988	1.8702690000000000
S	22.7267459999999986	22.6708320000000008	1.8343719999999999
S	21.1038369999999986	25.4484749999999984	1.8234900000000001
S	19.5154110000000003	28.2443890000000017	1.8525830000000001
S	17.9636290000000010	31.0244390000000010	1.8995599999999999
S	16.1448679999999989	31.7632529999999988	5.3391010000000003
S	14.5610510000000009	34.4917370000000005	5.3599839999999999
S	12.9810490000000005	37.2295110000000022	5.3658020000000004
S	11.4057320000000004	39.9751679999999965	5.3701350000000003
S	9.8300540000000005	42.7300830000000005	5.3713179999999996
S	19.7101679999999995	31.9849829999999997	4.5659219999999996
S	18.1417840000000012	34.7418880000000030	4.6102449999999999
S	16.5629349999999995	37.4840540000000004	4.6407259999999999
S	14.9788150000000009	40.2332570000000018	4.6393019999999998
S	13.3481480000000001	42.9912520000000029	4.6318229999999998
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S	11.4059369999999998	36.3389340000000018	2.1972980000000000
S	9.8314369999999993	39.0851589999999973	2.1990150000000002
S	8.2419840000000004	41.8233170000000030	2.2156920000000002
S	6.5895149999999996	44.5869580000000028	2.3265430000000000

S	16.4174180000000014	33.7746580000000023	1.9385589999999999
S	14.8602039999999995	36.5091759999999965	1.9579190000000000
S	13.2866990000000005	39.2300479999999965	1.9552000000000000
S	11.6820409999999999	41.9270509999999987	1.9317740000000001
S	9.9819259999999996	44.6048219999999986	1.9209190000000000
S	8.3070339999999998	47.3391140000000021	2.0018600000000002
S	6.4824979999999996	49.9814689999999970	2.0130640000000000
S	4.9032030000000004	47.3129390000000001	1.9873449999999999
S	11.7647990000000000	45.8008779999999973	4.4105610000000004
S	9.9974819999999998	48.4997510000000034	4.6249079999999996
S	8.1752420000000008	51.2286909999999978	4.8281489999999998
S	8.1144020000000001	45.5369200000000021	5.2527130000000000
S	6.4178249999999997	48.3405739999999966	5.4459410000000004
S	4.4373160000000000	51.1513610000000014	4.7647100000000000
S	4.9139499999999998	45.4682370000000020	5.1378469999999998
S	2.8347639999999998	48.4626069999999984	4.7073000000000000
S	6.2855970000000001	53.5566699999999969	2.7790580000000000

$W_{105}S_{210}$; $E_{tot} = -49\,817\,926.665\,503\,42\text{ eV}$; $E_{rel} = 34.221\,257\,247\,6\text{ meV/f.u.}$

W	22.8492619999999995	-3.4375570000000000	3.4946030000000001
W	21.3071739999999998	-1.1996840000000000	3.2416160000000001
W	19.7491440000000011	1.5651530000000000	3.2911980000000001
W	18.1804799999999993	4.2681940000000003	3.3718100000000000
W	16.6049590000000009	6.9689420000000002	3.3546170000000002
W	15.0431139999999992	9.6869800000000009	3.3329979999999999
W	13.5155110000000001	12.4049230000000001	3.3029180000000000
W	11.9194859999999991	15.0883249999999993	3.1236429999999999
W	10.0603850000000001	18.2167780000000015	2.9591870000000000
W	8.5217010000000002	21.0283189999999998	3.1593070000000001
W	7.0190530000000004	23.7672500000000007	3.2951880000000000
W	5.4219710000000001	26.5517670000000017	3.2861929999999999
W	3.8684370000000001	29.1329479999999990	3.2084920000000001

W	2.2765670000000000	31.5466760000000015	3.4546660000000000
W	22.8658880000000018	1.0208759999999999	3.3222100000000001
W	24.4881250000000001	-1.2392479999999999	3.3002840000000000
W	20.9954949999999982	3.9398909999999998	3.3309090000000001
W	19.3793119999999988	6.7046479999999997	3.3601839999999998
W	17.7865019999999987	9.4537999999999993	3.3614009999999999
W	16.2235019999999999	12.2127619999999997	3.3396170000000001
W	14.6454719999999998	14.9769939999999995	3.2725300000000002
W	13.0441839999999996	18.3141700000000007	3.3547630000000002
W	11.4642750000000007	20.7037359999999993	3.2397100000000001
W	9.9160109999999992	23.3431469999999983	3.2245040000000000
W	8.3671860000000002	26.0973609999999994	3.2499080000000000
W	6.8009899999999996	29.3789580000000008	3.2898559999999999
W	5.3267910000000001	31.5826600000000006	3.3743159999999999
W	25.9405970000000003	1.4441729999999999	3.2458000000000000
W	24.7511590000000012	4.2341319999999998	3.3819539999999999
W	23.2186100000000017	7.0050359999999996	3.4642590000000002
W	21.6020520000000005	9.7608549999999994	3.4688829999999999
W	20.0452650000000006	12.4570270000000001	3.4601389999999999
W	18.3455690000000011	15.4131409999999995	3.4517440000000001
W	16.7369780000000006	18.1406199999999984	3.4516909999999998
W	15.1565680000000000	20.8732520000000008	3.4275400000000000
W	13.5448920000000008	23.8819419999999987	3.4163039999999998
W	11.9764610000000005	26.6210220000000000	3.3596870000000001
W	10.4637449999999994	29.3039459999999998	3.2714620000000001
W	8.3265580000000003	31.7290059999999983	3.2603830000000000
W	27.4878280000000004	3.9632800000000001	3.2313800000000001
W	26.0777549999999998	6.5569139999999999	3.3181210000000001
W	24.3371379999999995	9.6732309999999995	3.3572700000000002
W	22.8890090000000015	12.1893360000000008	3.3993159999999998
W	21.1232630000000015	15.4261350000000004	3.4501249999999999
W	19.5391709999999996	17.8975930000000005	3.4017990000000000
W	17.9167810000000003	20.6330330000000011	3.3730899999999999

W	16.291375999999996	23.609539999999991	3.319545999999999
W	14.688596000000004	26.385750999999991	3.261756999999998
W	13.152927000000000	29.149560000000010	3.188311000000001
W	11.617739999999995	31.886109999999986	2.949182000000000
W	29.146957000000004	6.599267000000002	3.122262999999998
W	27.990383999999988	9.803433000000001	3.375589999999999
W	25.965869999999989	12.236243999999992	3.443347999999999
W	24.937473000000007	15.068175999999993	3.388482999999999
W	22.718772999999988	18.163123999999998	3.517049999999998
W	21.708636999999995	20.744716000000004	3.419791000000000
W	19.895426000000005	23.918607999999990	3.375646999999998
W	18.379733999999991	26.199889999999999	3.374919999999999
W	16.747789999999984	29.596503999999995	3.287372000000000
W	15.207910999999993	31.865096000000012	3.193171000000000
W	31.055458000000016	9.729590000000000	3.186719000000001
W	29.544547999999989	12.012738000000006	3.424459999999998
W	27.689295000000013	15.370903999999995	3.540649000000002
W	26.446072999999984	17.857336000000001	3.461211000000000
W	24.695651000000016	20.431246000000016	3.577467000000000
W	23.008677999999997	23.897161000000005	3.444363000000001
W	21.479787999999992	26.169530999999992	3.525211000000001
W	19.900700000000005	29.645673999999996	3.384547000000000
W	18.353649000000008	31.885359000000011	3.386954999999999
W	32.604148999999996	12.599119000000000	3.415086000000001
W	31.383922999999993	15.029481000000005	3.417060000000002
W	29.174492999999982	18.090467000000003	3.562336999999999
W	27.803029999999997	20.494122999999983	3.534326000000001
W	26.183438999999999	23.932171000000003	3.458308999999999
W	24.606352999999986	26.168207999999999	3.586129999999998
W	23.062635000000002	29.632007000000015	3.430747999999999
W	21.487601000000015	31.915442999999998	3.418819000000001
W	34.156619999999967	15.315485000000007	3.457510999999998
W	32.979506999999981	17.774748999999999	3.389390000000001

W	30.6824420000000018	20.7453590000000005	3.4580869999999999
W	29.4646620000000006	23.8741249999999994	3.4536840000000000
W	27.8015949999999989	26.1448460000000011	3.6105170000000002
W	26.2272919999999985	29.6043379999999985	3.4574039999999999
W	24.6396489999999986	31.9106230000000011	3.4103970000000001
W	35.6800160000000020	18.0140899999999995	3.3945029999999998
W	34.4669680000000014	20.5173839999999998	3.3272590000000002
W	32.6863900000000029	23.9027169999999991	3.3655870000000001
W	31.0310139999999990	26.1327239999999996	3.5647869999999999
W	29.3678430000000006	29.5771329999999999	3.4433500000000001
W	27.7992850000000011	31.8923419999999993	3.4011230000000001
W	37.1814370000000025	20.7449650000000005	3.1933400000000001
W	35.8786410000000018	23.8859409999999990	3.2236050000000001
W	34.2130289999999988	26.1488429999999994	3.4608330000000000
W	32.4957720000000023	29.5685089999999988	3.3992270000000002
W	30.9552939999999985	31.8758470000000003	3.3997880000000000
W	38.9787400000000019	23.7904960000000010	2.8709549999999999
W	37.3213310000000007	26.1648020000000017	3.2944710000000001
W	35.6440509999999975	29.5557410000000012	3.3180719999999999
W	34.0909970000000015	31.8505719999999997	3.4346480000000001
W	40.5694670000000031	26.7722589999999983	3.0945360000000002
W	39.2025580000000033	29.4322589999999984	3.2806190000000002
W	37.2340349999999987	31.8265899999999995	3.3903870000000000
W	41.9822950000000006	29.2365369999999984	3.1423000000000001
W	40.4253629999999973	31.7753049999999995	3.2646839999999999
W	43.5074609999999993	31.7926310000000001	3.3594879999999998
S	21.1139849999999996	0.4125950000000000	4.9601910000000000
S	19.4546160000000015	3.1311160000000000	5.0746490000000000
S	17.8139679999999991	5.8566500000000001	5.0974069999999996
S	16.2186529999999998	8.5678730000000005	5.0850989999999996
S	14.6705609999999993	11.3077629999999996	5.0614980000000003
S	13.0795259999999995	14.1023949999999996	4.9666889999999997
S	11.4066430000000008	16.9896950000000011	4.6142810000000001

S	9.784247999999998	19.790039000000002	4.837510000000000
S	8.301484000000003	22.611598999999982	4.948114999999996
S	6.764636999999996	25.442828999999997	4.983366000000002
S	5.339488000000002	28.227080000000008	4.945050000000002
S	3.735748000000001	30.834030999999995	5.072871000000001
S	24.572880999999989	0.377441000000000	4.974742000000000
S	22.883679999999982	3.140556000000001	4.655561999999998
S	21.274985000000009	5.922822000000000	4.715615999999998
S	19.672316999999996	8.693196000000004	4.752430000000004
S	18.060611999999990	11.461413999999995	4.757092000000001
S	16.447048999999998	14.277984999999993	4.723232999999996
S	14.738948999999999	17.077524000000004	4.617905999999996
S	13.154493000000004	19.995480000000006	4.889345999999997
S	11.664607000000002	22.713637999999996	4.710166000000001
S	10.119704000000005	25.454589999999996	4.649500999999999
S	8.561524000000004	28.257297999999987	4.538050000000001
S	6.937763000000003	31.111609999999989	5.057437000000002
S	26.126298999999995	3.032452999999998	5.002500999999996
S	24.558803000000010	5.889115999999996	5.101847000000002
S	22.968859999999994	8.678675000000001	5.132026999999999
S	21.346948999999986	11.458498000000005	5.163851000000002
S	19.745288999999996	14.258245999999998	5.076384000000000
S	18.017769999999987	17.077452000000010	5.147935000000004
S	16.424348999999994	19.816192000000009	5.149282999999996
S	14.900147999999997	22.688922000000016	5.029821000000001
S	13.291119000000001	25.553408000000010	5.086393000000002
S	11.748060999999999	28.337330999999989	5.012927000000004
S	10.130093999999997	31.223900000000004	4.797576000000003
S	27.820401000000004	5.744704999999997	4.910851000000001
S	26.225331000000006	8.650529999999998	4.655793000000001
S	24.508359999999997	11.390895000000004	5.104161000000004
S	22.970306000000008	14.281342999999997	4.707114999999999
S	21.233133999999997	17.133023000000014	5.103080000000003

S	19.7257789999999993	19.9211999999999989	4.8108190000000004
S	18.1265229999999988	22.7248079999999995	4.6935630000000002
S	16.5116930000000011	25.5734139999999996	4.7812609999999998
S	14.9769190000000005	28.4358080000000015	4.6277460000000001
S	13.3221209999999992	31.2686549999999990	4.6300840000000001
S	29.5675290000000004	8.4533249999999995	4.7112550000000004
S	27.8373430000000006	11.4270879999999995	5.0271509999999999
S	26.2616370000000003	14.1273129999999991	5.0871100000000000
S	24.5547390000000014	16.9985530000000011	4.7875470000000000
S	23.0145669999999996	19.8638539999999999	5.2185910000000000
S	21.4015050000000002	22.6997050000000016	4.9037350000000002
S	19.8024920000000009	25.5555729999999990	5.1691479999999999
S	18.2335400000000014	28.3971620000000016	4.7443080000000002
S	16.6620279999999994	31.3555080000000004	5.0277989999999999
S	31.2786270000000002	11.3118200000000009	5.0258459999999996
S	29.5376089999999998	14.1546079999999996	4.7541599999999997
S	27.8850720000000010	16.9685570000000006	5.2661439999999997
S	26.2547700000000006	19.6719580000000001	5.1984009999999996
S	24.6263730000000010	22.6378939999999993	4.8256240000000004
S	23.0059719999999999	25.5334770000000013	5.2542749999999998
S	21.4317850000000014	28.3790489999999984	4.8004140000000000
S	19.8871530000000014	31.4189709999999991	5.1371390000000003
S	32.8991830000000007	14.1804729999999992	5.1679240000000002
S	31.1121960000000009	17.0169919999999983	4.8165410000000000
S	29.4440109999999997	19.8331060000000008	5.2445360000000001
S	27.8125880000000016	22.6459730000000015	4.8143710000000004
S	26.1985360000000007	25.5501399999999990	5.2874379999999999
S	24.6175409999999992	28.3772459999999995	4.8489370000000003
S	23.0599489999999996	31.4429289999999995	5.1547479999999997
S	34.5008470000000003	16.9420859999999998	5.1597999999999997
S	32.6954110000000000	19.8025079999999996	4.7993480000000002
S	31.0948010000000004	22.6814609999999988	4.8735949999999999
S	29.4339329999999997	25.5066039999999994	5.2512970000000001

S	27.8165100000000010	28.3598059999999990	4.8729610000000001
S	26.2195450000000001	31.4463459999999984	5.1510520000000000
S	36.0625789999999995	19.7321750000000016	5.0448250000000003
S	34.3595309999999969	22.6319690000000016	4.6770090000000000
S	32.6877660000000034	25.5110670000000006	5.1945449999999997
S	31.0096600000000002	28.3371959999999987	4.8405100000000001
S	29.3752560000000003	31.4092270000000013	5.1443690000000002
S	17.6302610000000008	1.9615199999999999	2.5781749999999999
S	16.0908799999999985	4.7807800000000000	2.4295149999999999
S	14.4785830000000004	7.5504889999999998	2.4265450000000000
S	12.9090900000000008	10.3297319999999999	2.3804390000000000
S	11.2995500000000000	13.0758109999999999	2.3409559999999998
S	9.9123929999999998	16.0755389999999991	2.0587320000000000
S	7.9527409999999996	18.7446230000000007	2.3513989999999998
S	6.4339820000000003	21.5640760000000000	2.3615450000000000
S	4.8009100000000000	24.3016070000000006	2.7285550000000001
S	3.2718419999999999	26.9989530000000002	2.4383040000000000
S	1.7931870000000001	29.7698900000000002	2.1452879999999999
S	0.5276970000000000	32.4255799999999965	4.3258669999999997
S	21.2997100000000010	2.1846350000000001	1.6998020000000000
S	19.6430569999999989	5.0081910000000001	1.6428760000000000
S	18.0659570000000009	7.7741129999999998	1.6489650000000000
S	16.4919480000000007	10.5369650000000004	1.6354320000000000
S	14.9152170000000002	13.2925070000000005	1.5887940000000000
S	13.2823410000000006	16.1909250000000000	1.6707259999999999
S	11.6432000000000002	19.0387689999999985	1.4817450000000001
S	10.0179659999999995	21.7122330000000012	1.4948159999999999
S	8.4262029999999992	24.4634800000000006	1.5379620000000001
S	6.8812749999999996	27.3805860000000010	1.7384189999999999
S	5.2044930000000003	30.0416130000000017	1.5567720000000000
S	3.5451769999999998	33.0202910000000003	2.3417690000000002
S	24.4258239999999986	2.2698849999999999	1.8000710000000000
S	22.8797110000000004	5.0100210000000001	2.0195230000000000

S	21.2997970000000016	7.7523720000000003	2.0827040000000001
S	19.6855849999999997	10.5299429999999994	2.0788929999999999
S	18.1341670000000015	13.3419740000000004	2.1250510000000000
S	16.4926229999999983	16.1447250000000011	2.0081690000000001
S	14.8805270000000007	18.9772199999999991	1.9253030000000000
S	13.3117040000000006	21.8089419999999983	2.0550850000000001
S	11.7148330000000005	24.5484499999999990	1.9672609999999999
S	10.1431629999999995	27.3116720000000015	1.8697830000000000
S	8.5279100000000003	30.0687390000000008	1.7236149999999999
S	6.7753370000000004	33.2064319999999995	2.3562110000000001
S	28.0708810000000000	1.8495040000000000	2.3586170000000002
S	26.1920940000000009	4.9093520000000002	1.5411980000000001
S	24.6328330000000015	7.7952990000000000	1.7708299999999999
S	22.9336909999999996	10.5528580000000005	1.6164040000000000
S	21.4066229999999997	13.4100450000000002	1.8624890000000001
S	19.7709879999999991	16.2184379999999990	1.6688600000000000
S	18.1515440000000012	18.9608649999999983	1.6925969999999999
S	16.5571790000000014	21.8082269999999987	1.7259329999999999
S	14.9774519999999995	24.6706639999999986	1.6114440000000001
S	13.3879789999999996	27.4394530000000003	1.5399090000000000
S	11.7818889999999996	30.1919480000000000	1.4143370000000000
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S	29.7380490000000002	4.5301760000000000	2.4178009999999999
S	27.7488290000000006	7.6862899999999996	1.7564759999999999
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S	21.2919109999999989	18.9817590000000003	1.8514980000000001
S	19.8163909999999994	21.7444719999999982	2.1348660000000002
S	18.2023529999999987	24.5274329999999985	1.7649360000000001
S	16.6470480000000016	27.4161879999999982	2.0389370000000002
S	15.0235869999999991	30.1666430000000005	1.6708799999999999
S	13.3675840000000008	33.1832879999999975	2.1782539999999999

S	31.207830999999988	7.452119999999999	2.345621000000000
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S	27.839489000000004	13.279170000000006	2.182208999999998
S	26.274743000000008	16.127579000000008	1.739824000000000
S	24.605094999999986	18.778638000000008	1.966674000000000
S	23.158031000000011	21.762986000000015	1.979298999999999
S	21.466090999999987	24.535430000000016	1.698252000000001
S	19.899647000000016	27.486954999999983	2.089881999999998
S	18.323019999999996	30.266840999999994	1.627693000000001
S	16.639551999999983	33.469611999999979	2.499750000000001
S	33.121279999999987	10.260913000000004	2.511667000000001
S	31.075343000000002	13.236122999999992	1.800561000000001
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S	27.764469999999993	18.917764999999993	1.748369000000001
S	26.193524000000000	21.766905000000013	2.165133000000000
S	24.618407000000013	24.572282999999988	1.767962000000000
S	23.056806000000017	27.457146000000016	2.144166999999999
S	21.492907999999999	30.269846000000011	1.699206000000000
S	19.856270999999996	33.443913000000020	2.465333000000002
S	34.693345000000008	13.070926999999993	2.591680999999999
S	32.735353000000035	16.056497000000002	1.696854000000001
S	31.064961000000003	18.845245999999995	2.115940999999998
S	29.290699000000000	21.754964999999986	1.947060000000000
S	27.828192000000014	24.551939999999983	1.806829999999999
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S	23.051701999999988	33.469180000000015	2.515921000000001
S	36.252898000000018	15.906729999999996	2.454911000000001
S	34.281500999999987	18.833508999999994	1.634379000000000
S	32.590015000000011	21.688290999999995	2.139413999999999
S	31.029795000000000	24.507546000000014	1.743538999999999
S	29.401250999999985	27.411750999999989	2.196673000000001
S	27.806093000000006	30.209351000000016	1.724244000000001

S	26.221955999999987	33.445309999999992	2.4963709999999999
S	24.880480999999996	-3.1388829999999999	4.5843109999999996
S	19.471410999999998	-0.7237490000000000	2.0883750000000001
S	26.321640999999996	-0.7320470000000000	2.0987930000000001
S	22.9302300000000017	-0.6963890000000000	1.5786950000000000
S	22.7819520000000004	-4.2507429999999999	1.5156210000000001
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S	29.382667999999989	33.438352999999993	2.5083240000000000
S	32.518855999999995	31.353650999999993	5.1441699999999999
S	30.948589999999994	30.218448999999997	1.6997190000000000
S	34.190713999999998	28.329522999999982	4.7556279999999997
S	32.5690250000000034	27.4214960000000012	2.1165389999999999
S	35.9026110000000003	25.479655999999985	5.0523809999999996
S	34.217815999999991	24.5380670000000016	1.6267520000000000
S	37.648930999999975	22.6717350000000017	4.6179079999999999
S	35.7773740000000018	21.7584540000000004	1.6952309999999999
S	37.8721680000000021	18.7153600000000004	2.4646659999999998
S	39.2431640000000002	25.4418280000000010	4.6685299999999996
S	39.260064999999973	21.653698999999996	2.1256290000000000
S	37.404511999999969	24.5926520000000011	1.4113750000000000
S	37.3950650000000024	28.3213480000000004	4.5705900000000002
S	35.685468999999977	31.238562999999992	5.1185929999999997
S	35.743712999999996	27.4139020000000002	1.9460150000000001
S	34.098013999999992	30.2729700000000008	1.6589400000000001
S	32.557988999999992	33.412903999999975	2.5023140000000001
S	40.609108999999966	28.2860900000000015	4.8991150000000001
S	41.071691999999988	24.499245999999994	2.2837649999999998
S	38.8669930000000008	31.1962750000000000	5.0045580000000003
S	38.947426999999976	27.477949999999999	1.7114750000000001
S	35.7598660000000024	33.4786300000000026	2.7181600000000001
S	37.3859700000000004	30.2257730000000002	1.7418730000000000
S	42.5941550000000007	27.2281930000000010	2.0857549999999998
S	42.0596340000000026	31.0312920000000005	4.9662220000000001

S	40.6718109999999982	30.2341370000000005	1.5002400000000000
S	38.9591080000000005	33.3362520000000018	2.4253840000000002
S	45.1998099999999994	32.7638540000000020	4.2364470000000001
S	42.2222450000000009	33.2103219999999979	2.2150069999999999
S	44.1103450000000024	29.9804349999999999	2.1706420000000000

$W_{105}S_{210}$; $E_{tot} = -49817926.82131956$ eV; $E_{rel} = 32.7372940095$ meV/f.u.

W	21.2029660000000000	-0.4694080000000000	3.3579650000000001
W	19.4603099999999998	2.2783120000000001	3.3590599999999999
W	17.8622329999999998	5.0071469999999998	3.3925559999999999
W	16.2364959999999998	7.6749340000000004	3.3572340000000001
W	14.6361790000000003	10.3685589999999994	3.3366009999999999
W	13.0744120000000006	13.0747619999999998	3.3202389999999999
W	11.4733809999999998	15.7939620000000005	3.1660080000000002
W	9.6280190000000001	18.8959340000000005	3.0626159999999998
W	8.0931540000000002	21.7900330000000011	3.3056909999999999
W	6.6065360000000002	24.5073189999999990	3.4165139999999998
W	5.0906310000000001	27.1923579999999987	3.3988980000000000
W	3.5793409999999999	30.0310260000000007	3.4168669999999999
W	24.3448290000000007	-0.6227780000000001	3.4639590000000000
W	22.6818339999999985	1.6984930000000000	3.4554950000000000
W	20.6957470000000008	4.8120000000000003	3.3970609999999999
W	19.0287819999999996	7.4558099999999996	3.3898310000000000
W	17.3969820000000013	10.1586029999999994	3.3511760000000002
W	15.7829300000000003	12.8783069999999995	3.3072080000000001
W	14.2256429999999998	15.6013050000000000	3.2592449999999999
W	12.7452340000000000	18.9342170000000003	3.2348960000000000
W	11.2179319999999993	21.1842819999999996	3.3484120000000002
W	9.3652160000000002	24.4067000000000007	3.3767619999999998
W	7.9280720000000002	26.9347090000000016	3.3995389999999999
W	6.1778829999999996	30.1321559999999984	3.4401000000000002
W	5.0355160000000003	32.7938029999999969	3.4097780000000002

W	27.478128999999991	-0.6553470000000000	3.5625220000000000
W	28.8685420000000015	1.6637430000000000	3.5919850000000002
W	25.7613640000000004	1.6420920000000001	3.5241799999999999
W	24.3210520000000017	5.0518989999999997	3.3668160000000000
W	22.6690800000000010	7.2505050000000004	3.4897640000000001
W	21.1193939999999998	10.7151250000000005	3.4656490000000000
W	19.5765090000000015	13.3305389999999999	3.4685419999999998
W	18.0570890000000013	15.9200599999999994	3.3272819999999999
W	15.9008570000000002	19.0178420000000017	3.3049879999999998
W	14.2491579999999995	21.2182870000000001	3.4071440000000002
W	12.9972549999999991	24.5872090000000014	3.3814540000000002
W	10.9414269999999991	26.9940409999999993	3.4098860000000002
W	9.9207289999999997	30.0212660000000007	3.4188010000000002
W	7.7000330000000003	32.6411810000000031	3.4258700000000002
W	6.5485410000000002	35.4981810000000024	3.4718049999999998
W	30.6200909999999986	-0.6193950000000000	3.5860550000000000
W	27.4454230000000017	5.0980309999999998	3.4048470000000002
W	25.8587939999999996	7.3359509999999997	3.5167750000000000
W	24.1958090000000006	10.6739409999999992	3.4537130000000000
W	22.4594880000000003	13.2746849999999998	3.4649410000000000
W	21.0513970000000015	15.8695339999999998	3.4290240000000001
W	19.4008919999999989	18.9412260000000003	3.4149780000000001
W	17.8854380000000006	21.5193469999999998	3.4300259999999998
W	16.0537990000000015	24.6008740000000010	3.4106209999999999
W	14.4807009999999998	26.8642609999999991	3.5206029999999999
W	12.6316170000000003	30.1592139999999986	3.5110610000000002
W	9.5903770000000002	35.8796460000000010	3.5378620000000001
W	11.4914539999999992	32.6196600000000032	3.4247200000000002
W	8.1366680000000002	38.2261519999999990	3.5855030000000001
W	33.8367199999999997	-0.6102050000000000	3.7127170000000000
W	35.5890899999999988	1.9974000000000001	3.7295870000000000
W	31.9748799999999989	1.7161569999999999	3.6583549999999998
W	30.5826250000000002	5.1247179999999997	3.4990779999999999

W	29.0215080000000007	7.3594520000000001	3.5794809999999999
W	27.0543909999999990	10.5145700000000009	3.5090620000000001
W	25.6470950000000002	12.9657450000000001	3.4812880000000002
W	23.8272310000000012	15.9390699999999992	3.4589289999999999
W	22.1806790000000014	18.6514920000000011	3.3384170000000002
W	20.6358630000000005	21.3804410000000011	3.3493719999999998
W	19.0597490000000001	24.0647780000000004	3.3865520000000000
W	17.5601599999999998	26.8559780000000003	3.5111439999999998
W	16.3075240000000008	30.2533339999999988	3.5397900000000000
W	14.2208469999999991	32.7634159999999994	3.5875819999999998
W	13.1271020000000007	35.3450539999999975	3.4408919999999998
W	10.9222950000000001	38.2495219999999989	3.6149800000000001
W	9.7867610000000003	40.8866889999999970	3.6943109999999999
W	36.8248180000000005	-0.6722260000000000	3.8839109999999999
W	33.6896389999999997	5.1390710000000004	3.6655370000000000
W	32.2231560000000030	7.3964939999999997	3.7208070000000002
W	30.8199590000000008	10.7474080000000001	3.6153800000000000
W	29.3094509999999993	13.4921539999999993	3.5587700000000000
W	27.6723210000000002	16.1988640000000004	3.5157560000000001
W	26.0375830000000015	18.9812319999999985	3.5023040000000001
W	24.4353639999999999	21.7284049999999986	3.4900370000000001
W	22.8592540000000000	24.4652409999999989	3.5102470000000001
W	21.2607479999999995	27.2089180000000006	3.5404209999999998
W	19.3415740000000014	30.2670369999999984	3.5632370000000000
W	15.9565909999999995	35.7619100000000003	3.6762100000000002
W	17.8511179999999996	32.5399340000000024	3.6470430000000000
W	14.7064699999999995	38.1277830000000009	3.6237900000000001
W	12.8807630000000000	41.3376549999999980	3.7529420000000000
W	11.4229959999999995	43.5835369999999998	3.9107379999999998
W	39.7136179999999968	-0.8614230000000000	3.7187399999999999
W	38.2379669999999976	1.8129150000000001	3.7316760000000002
W	36.8834659999999985	4.4874939999999999	3.7889230000000000
W	35.3581620000000001	7.4441189999999997	4.0622080000000000

W	33.541108000000013	10.551942999999996	3.7437900000000002
W	32.001731999999970	13.300112999999996	3.5556690000000000
W	30.433060999999986	16.027810999999998	3.5409009999999999
W	28.819967999999994	18.755441999999986	3.555146999999998
W	27.214707000000006	21.492484999999985	3.5534210000000002
W	25.624438999999989	24.214051000000013	3.5375860000000001
W	24.047225999999984	26.922283000000002	3.4994260000000001
W	22.487926999999991	29.646588999999987	3.5663380000000000
W	20.931380000000008	32.537177999999973	3.8325849999999999
W	19.081745999999990	35.647320999999980	3.9006959999999999
W	17.447378000000005	38.348348000000014	3.8170199999999999
W	15.921443999999993	40.907677999999971	3.7907250000000001
W	14.325571999999993	43.608930000000009	3.9041299999999999
W	12.849301999999998	46.277825999999975	3.8768470000000002
S	18.038185999999996	40.436272000000024	4.7133390000000004
S	14.586403000000007	42.042681999999992	2.1151970000000002
S	12.850576999999995	44.730165999999970	2.1815340000000001
S	22.323046000000015	-2.1341540000000001	4.2932759999999996
S	20.848872000000001	1.1445609999999999	5.0335200000000002
S	19.175031000000006	3.8730690000000001	5.0864250000000002
S	17.439023999999999	6.5771790000000001	5.1150029999999997
S	15.825005000000009	9.265530999999993	5.086097999999998
S	14.252535999999992	11.987593999999996	5.062662999999997
S	12.663923999999997	14.777753000000006	4.9848220000000003
S	11.032864000000000	17.686388000000009	4.679033999999997
S	9.421646000000009	20.528358999999982	4.9012560000000001
S	7.889405000000000	23.344815000000005	5.0725199999999999
S	6.327013000000000	26.158853000000006	5.125131999999998
S	4.791169000000000	28.916754000000010	5.0961520000000000
S	25.691825000000015	-2.2230430000000001	4.390203999999998
S	24.146865999999993	0.9856620000000000	5.1998800000000003
S	22.560856999999986	3.8461210000000001	4.6788730000000003
S	20.851061000000014	6.6376059999999999	4.958224999999997

S	19.2883190000000013	9.4678050000000002	4.7602580000000003
S	17.6646779999999985	12.1974940000000007	4.7139870000000004
S	16.0507409999999986	14.9247479999999992	4.6859900000000003
S	14.3162730000000007	17.6909610000000015	4.6211490000000000
S	12.7138320000000000	20.5106290000000016	5.0920560000000004
S	11.1827640000000006	23.3584439999999987	4.6288330000000002
S	9.5089120000000005	26.1351480000000009	5.0987760000000000
S	8.0155110000000001	29.0189279999999989	4.6994059999999998
S	19.1517990000000005	-0.1266750000000000	2.4892020000000001
S	17.3835909999999991	2.6827359999999998	2.5750139999999999
S	15.7881040000000006	5.4706619999999999	2.4135840000000002
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S	12.5177650000000007	10.9926530000000007	2.3501699999999999
S	10.8422140000000002	13.7483500000000003	2.4371600000000000
S	9.4180829999999993	16.7313310000000008	2.1995079999999998
S	7.5134800000000004	19.5398919999999983	2.4934880000000001
S	5.9967969999999999	22.3460579999999993	2.5013660000000000
S	4.4014040000000003	25.1743409999999983	2.5574599999999998
S	2.8338830000000002	28.0805480000000003	2.5481609999999999
S	22.7750430000000001	-0.0532840000000000	1.6856810000000000
S	21.0452489999999983	2.9158249999999999	1.8670730000000000
S	19.3246590000000005	5.7598039999999999	1.6711950000000000
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S	16.0715259999999986	11.1919649999999997	1.6195860000000000
S	14.4575720000000008	13.9368610000000004	1.5651420000000000
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S	11.1446729999999992	19.6006390000000010	1.4899309999999999
S	9.6412139999999997	22.4926929999999992	1.8185680000000000
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S	4.7190610000000000	31.1139870000000016	1.6792549999999999
S	2.7521260000000001	31.9018459999999990	4.3006940000000000
S	6.2774299999999998	31.8280600000000007	5.1671290000000001

S	4.373929999999997	34.871583999999986	4.269226999999999
S	28.940397999999983	-2.196203999999998	4.4806020000000002
S	27.3239410000000014	0.9760720000000001	5.2748379999999999
S	25.791451999999996	3.8121060000000000	4.8087229999999996
S	24.2304540000000017	6.6336870000000001	5.1874940000000000
S	22.549465999999989	9.4140650000000008	4.8575359999999996
S	20.9523510000000002	12.3174560000000000	5.1848809999999999
S	19.348365999999986	15.060330999999997	5.1093659999999996
S	17.5577080000000016	17.8295120000000011	4.7401429999999998
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S	14.387985999999997	23.3377680000000005	4.8071320000000002
S	12.752879999999993	26.216166999999987	5.0612440000000003
S	11.221591999999993	28.9399020000000000	5.0495130000000001
S	32.172289999999967	-2.2570370000000000	4.2584540000000004
S	30.4897300000000016	0.9547490000000000	5.3404860000000003
S	28.9414030000000011	3.8300649999999998	4.8604539999999998
S	27.418594999999998	6.7334620000000003	5.2300969999999998
S	25.6670410000000011	9.4530720000000006	5.0157879999999997
S	24.1079590000000010	12.3399680000000007	5.1516840000000004
S	22.519494999999992	15.068308999999993	5.1785180000000004
S	20.7860960000000006	17.7865320000000011	5.0151700000000003
S	19.252273999999999	20.5553050000000006	5.1657039999999999
S	17.565131999999984	23.3466020000000007	5.0275109999999996
S	16.046185999999987	26.2329210000000010	5.2368069999999998
S	14.4892590000000006	29.0456840000000014	4.7812500000000000
S	25.9344730000000006	-0.1352340000000000	1.7810900000000001
S	24.265809999999983	2.8840599999999998	2.0357170000000000
S	22.5396830000000001	5.6374180000000003	1.8112459999999999
S	20.9511350000000007	8.5252189999999999	2.1843669999999999
S	19.276205999999984	11.2811400000000006	2.0566789999999999
S	17.670953999999983	13.981583999999998	2.0234040000000002
S	16.0897490000000012	16.809620999999999	2.0646239999999998
S	14.3413400000000006	19.6194680000000012	1.5782879999999999

S	12.7955430000000003	22.4468959999999988	1.9207939999999999
S	11.1695259999999994	25.2286040000000007	1.8582860000000001
S	9.5463889999999996	28.1047750000000001	1.8862909999999999
S	7.9861240000000002	30.9115509999999993	1.9037750000000000
S	29.0656019999999984	-0.0905100000000000	1.8559580000000000
S	27.4228629999999995	2.8910149999999999	2.1305220000000000
S	25.8478600000000007	5.7179799999999998	1.6856380000000000
S	24.1658189999999991	8.5444750000000003	2.1462960000000000
S	22.5764649999999989	11.4257399999999993	1.7853010000000000
S	20.9663460000000015	14.1339389999999998	1.7328450000000000
S	19.4296049999999987	16.9336729999999989	1.8094809999999999
S	17.6487620000000014	19.6830940000000005	1.7920929999999999
S	16.0181329999999988	22.4507550000000009	2.1367560000000001
S	14.5060509999999994	25.2917899999999989	1.6814119999999999
S	12.8068120000000008	28.0782330000000009	2.1624370000000002
S	11.2405899999999992	30.9668330000000012	1.6860800000000000
S	9.5775400000000008	31.8470540000000000	4.8776270000000004
S	7.9675919999999998	34.6050919999999991	4.9982639999999998
S	5.9332260000000003	37.6579869999999985	4.2582279999999999
S	12.8548700000000000	31.7663580000000003	5.2747430000000000
S	11.2321869999999997	34.6373010000000008	4.8760659999999998
S	9.4445789999999992	37.4357869999999977	5.3699529999999998
S	6.3651390000000001	33.8678820000000016	1.7475190000000000
S	9.5953700000000008	33.7531699999999972	2.2261500000000001
S	7.9176789999999997	36.5814069999999987	1.8314779999999999
S	35.2565719999999985	-2.2405629999999999	4.6414090000000003
S	33.7751400000000004	1.0831679999999999	5.2410660000000000
S	32.1002689999999973	3.8705360000000000	5.0135030000000000
S	30.5789140000000010	6.7494889999999996	5.3190410000000004
S	28.9611219999999996	9.5627259999999996	4.8177149999999997
S	27.4580349999999989	12.3913639999999994	4.9280609999999996
S	25.7579279999999997	15.1149950000000004	4.7749290000000002
S	24.1288340000000012	17.9126049999999992	4.7815640000000004

S	22.5392040000000016	20.6197279999999985	4.7409090000000003
S	20.9363540000000015	23.3939449999999987	4.7779550000000004
S	19.3836370000000002	26.1271020000000007	4.8472860000000004
S	17.7540340000000008	28.9655489999999993	4.9401679999999999
S	38.3760919999999999	-2.1420189999999999	5.0115530000000001
S	36.9073869999999999	0.9580660000000000	5.5174669999999999
S	35.2894470000000027	3.8513099999999998	5.2718200000000000
S	33.7621249999999975	6.7178279999999999	5.5341659999999999
S	32.1437689999999989	9.5209089999999996	5.2399339999999999
S	30.6216700000000017	12.4244640000000004	5.3033440000000001
S	29.0025639999999996	15.1767029999999998	5.2496640000000001
S	27.3566730000000007	17.8914830000000009	5.2165359999999996
S	25.7427190000000010	20.6499260000000007	5.2182459999999997
S	24.1519119999999994	23.3867280000000015	5.2248390000000002
S	22.6067420000000006	26.1647420000000004	5.2380829999999996
S	20.9454139999999995	29.0104350000000011	5.1429760000000000
S	32.2577020000000019	-0.0129450000000000	1.9522690000000000
S	30.5835019999999993	2.9195650000000000	2.2111459999999998
S	29.0538570000000007	5.7194820000000002	1.7521869999999999
S	27.4475470000000001	8.5589239999999993	2.0693480000000002
S	25.7367169999999987	11.3251790000000003	1.7130860000000001
S	24.2167040000000000	14.1633770000000005	1.9016970000000000
S	22.5375329999999998	16.9082960000000000	1.7176600000000000
S	20.8901269999999997	19.7272469999999984	1.6391080000000000
S	19.2841200000000015	22.4613019999999999	1.6687220000000000
S	17.7177340000000001	25.2503379999999993	1.7516980000000000
S	16.1161810000000010	28.1421509999999984	2.1233379999999999
S	14.5100770000000008	30.9191630000000011	2.0145629999999999
S	35.3694119999999970	0.1413690000000000	2.0881959999999999
S	33.7842550000000017	2.9619689999999999	2.4118070000000000
S	32.2534390000000002	5.7738430000000003	1.8975409999999999
S	30.7163779999999988	8.6385459999999998	2.2707799999999998
S	29.0473730000000003	11.4499420000000001	2.1508389999999999

S	27.452798000000014	14.176572000000002	2.1365210000000001
S	25.779257999999987	16.962219999999985	2.1514190000000002
S	24.159939999999989	19.732168999999990	2.1068650000000000
S	22.559045999999986	22.501948999999998	2.0936940000000002
S	20.9640740000000001	25.259720999999990	2.1371750000000000
S	19.370235000000010	28.110807999999987	2.254026999999998
S	17.828534999999987	30.965137999999996	1.836376999999999
S	16.112020000000011	31.872686000000016	5.185317999999996
S	14.492846999999994	34.570835999999999	5.209521999999998
S	12.801287999999996	37.322718000000018	4.950052999999996
S	19.4079160000000002	31.861357999999992	5.4219600000000003
S	17.627368000000006	34.599682999999989	5.2434260000000004
S	16.131094999999984	37.389876999999985	5.468030999999999
S	12.8935300000000002	33.675567000000009	1.7722220000000000
S	11.2773350000000008	36.496082999999987	1.9930520000000000
S	9.484994999999996	39.3362290000000030	1.9040440000000001
S	16.162873999999986	33.720981999999993	2.3018550000000002
S	14.5166380000000004	36.495666999999974	1.8723770000000000
S	12.8489140000000006	39.262383999999973	2.383011999999999
S	41.352775999999986	-1.970788999999999	2.8991590000000000
S	40.343229999999984	0.984932999999999	4.821698999999997
S	38.896385000000022	3.8816310000000001	4.768921999999999
S	37.423423999999971	6.7301760000000002	4.698776999999998
S	35.5928710000000024	9.5987950000000009	4.8114900000000000
S	34.216169999999982	12.575139999999993	4.4722900000000001
S	32.582574000000010	15.378610999999994	4.485281999999998
S	30.971264000000015	18.164338000000008	4.441874999999996
S	29.3484890000000007	20.8991030000000002	4.4602110000000001
S	27.722280999999988	23.634931999999992	4.5041500000000001
S	26.1296520000000001	26.399184999999992	4.462679999999998
S	24.5875260000000004	29.200824999999983	4.3203440000000004
S	38.418447999999979	0.0409530000000000	2.055403999999998
S	37.083508999999994	2.969472999999998	2.0042930000000001

S	35.583703999999973	5.814162999999997	2.225439999999999
S	34.009340999999992	8.607530999999998	2.331592999999998
S	32.400427000000005	11.577830000000005	1.901775000000000
S	30.818477999999989	14.404662999999993	1.813709000000000
S	29.227911999999999	17.157537999999988	1.809914000000000
S	27.627279000000015	19.889250000000005	1.812511000000000
S	26.041817000000018	22.626387000000011	1.799608000000001
S	24.424468000000010	25.332822000000002	1.779528999999999
S	22.769396000000004	28.076623999999989	1.798097000000001
S	21.127788999999999	30.939008999999987	2.003236999999999
S	22.985604999999996	31.971522000000002	4.505806999999999
S	21.137892999999983	34.804093999999992	4.677575000000000
S	19.661356999999989	37.702162000000013	4.674986999999998
S	19.518581000000011	33.838064000000028	2.264154000000000
S	17.772245999999991	36.569271999999980	2.133354999999999
S	16.130523000000002	39.326234999999969	2.036468000000002
S	11.157978000000000	42.027216000000028	2.099511999999998
S	16.439493999999998	43.112093999999990	4.698039999999998
S	14.725212000000009	45.822279999999992	5.001080000000000
S	12.807567999999998	48.287537999999979	3.141118000000001
S	14.430728999999995	40.042783000000000	5.254000999999997
S	12.891916999999994	42.901671999999978	5.613357999999998
S	11.015031000000005	45.786064000000032	5.046191999999996
S	11.251303999999993	40.092252999999995	5.254293999999998
S	9.353267000000007	43.063698999999997	4.772020000000004
S	7.608068000000003	40.463290000000006	4.371710000000002

$W_{105}S_{210}$; $E_{tot} = -49\,817\,927.231\,413\,83\text{ eV}$; $E_{rel} = 28.831\,634\,295\,2\text{ meV/f.u.}$

W	21.044955999999991	-0.395372000000000	3.378832000000001
W	19.292636000000017	2.228915999999999	3.372131000000000
W	17.684006000000001	4.944096000000000	3.391582999999998
W	16.105488999999986	7.690062000000002	3.388207000000000

W	14.510367999999997	10.436076999999992	3.346287999999999
W	12.909986000000000	13.189467999999997	3.299249999999998
W	11.321688999999992	15.943568000000009	3.280536999999998
W	9.748856999999992	18.693111999999993	3.282300999999999
W	8.196179000000000	21.438880000000010	3.285388999999999
W	6.671904999999998	24.172326999999992	3.279920000000002
W	5.143473000000000	26.911228000000013	3.172690999999999
W	3.583946000000000	29.742585999999993	2.969093000000000
W	2.057955000000000	32.406775000000032	3.094796000000000
W	24.235172999999996	-0.555406000000000	3.391636000000000
W	22.280041000000000	1.937028000000000	3.364418999999998
W	20.623017999999983	4.528139999999996	3.348590000000002
W	18.951879999999992	7.345095999999998	3.335240000000000
W	17.288170999999984	10.230029999999993	3.335248000000000
W	15.671034999999998	13.040535000000002	3.327147000000000
W	14.095359000000000	15.758442999999998	3.315466999999999
W	12.534425999999998	18.460629999999983	3.314784000000000
W	10.963749999999992	21.197092999999989	3.317035999999999
W	9.403297999999995	23.941086999999996	3.295227000000000
W	7.870880999999998	26.692774000000000	3.235444999999999
W	6.280605000000000	29.880193999999995	3.194408000000000
W	5.078521000000000	32.256295000000015	3.123904000000000
W	27.294700999999999	-0.550827000000000	3.390547999999999
W	28.818380999999987	1.705864000000000	3.526142000000000
W	25.646229999999992	1.716259999999999	3.458911000000000
W	24.221391000000000	5.134216000000000	3.447385999999998
W	22.661735000000000	7.788534000000000	3.465093000000000
W	21.081882000000000	10.510061999999996	3.449352000000000
W	19.481624000000000	13.288890000000000	3.461119000000000
W	17.886579999999986	16.061128000000000	3.480074000000000
W	16.312114999999986	18.802975000000000	3.486305999999999
W	14.740045999999995	21.539287999999991	3.476386999999999
W	13.144102999999994	24.321857999999989	3.460388000000000

W	11.5325570000000006	27.1534730000000017	3.4166189999999999
W	10.0062680000000004	29.8501660000000015	3.3402759999999998
W	8.1615570000000002	32.2914129999999986	3.2571639999999999
W	30.3471609999999998	-0.5506470000000000	3.5743209999999999
W	27.4452710000000017	5.1741750000000000	3.4512510000000001
W	25.4143660000000011	7.5837709999999996	3.3838080000000001
W	23.8253430000000002	10.2775660000000002	3.3435820000000001
W	22.2250499999999995	13.0357489999999991	3.3302100000000001
W	20.6347249999999995	15.8092249999999996	3.3556270000000001
W	19.0654919999999990	18.5643209999999996	3.3852280000000001
W	17.4998460000000016	21.2941970000000005	3.3825680000000000
W	15.9146029999999996	24.0223009999999988	3.3449369999999998
W	14.3064990000000005	26.8050420000000003	3.2943750000000001
W	12.7600870000000004	29.6429800000000014	3.2918790000000002
W	11.2852580000000007	32.2961030000000022	3.2550450000000000
W	33.6557910000000007	-0.5969630000000000	3.9631460000000001
W	35.0748699999999971	2.1036380000000001	3.6369699999999998
W	32.4146810000000016	2.0181239999999998	3.6085950000000002
W	30.5415470000000013	5.1069849999999999	3.4968680000000001
W	29.1355800000000009	7.7644950000000001	3.5074700000000001
W	27.5757550000000009	10.6600579999999994	3.5161560000000001
W	25.9963750000000005	13.4190109999999994	3.5293380000000001
W	24.4251870000000011	16.1453740000000003	3.5532740000000000
W	22.8525759999999991	18.8841320000000010	3.5771850000000001
W	21.2708019999999998	21.6515750000000011	3.5818289999999999
W	19.6779089999999997	24.4221910000000015	3.5565590000000000
W	18.0830820000000010	27.1428019999999997	3.4927250000000001
W	16.5037260000000003	29.8194079999999992	3.4055529999999998
W	14.3179669999999994	32.3389200000000017	3.1774480000000001
W	37.2031180000000035	-0.4756110000000000	3.8739150000000002
W	33.4690980000000025	4.7145390000000003	3.4558920000000000
W	31.9213549999999984	7.4821080000000002	3.4404469999999998
W	30.3554700000000004	10.3023489999999995	3.4068870000000002

W	28.7827570000000001	13.1058420000000009	3.4156640000000000
W	27.2043830000000000	15.8793989999999994	3.4544160000000002
W	25.6130390000000006	18.6450570000000013	3.4787080000000001
W	24.0137399999999985	21.4159739999999985	3.4788160000000001
W	22.4095039999999983	24.1969180000000001	3.4545340000000002
W	20.7930109999999999	26.9826210000000017	3.4144030000000001
W	19.1896360000000001	29.7530239999999999	3.3674810000000002
W	17.8953360000000004	32.4699370000000016	3.0540859999999999
W	40.0373379999999983	-0.4813300000000000	3.8927930000000002
W	41.4493530000000021	2.1117330000000001	3.8158240000000001
W	38.8153250000000014	2.0517120000000002	3.7406799999999998
W	37.1625670000000028	5.1806460000000003	3.7062020000000002
W	35.6058000000000021	7.9268340000000004	3.6437059999999999
W	34.0858550000000022	10.6325109999999992	3.6084849999999999
W	32.5751109999999997	13.3415750000000006	3.5836769999999998
W	31.0115939999999988	16.1099810000000012	3.5731160000000002
W	29.3964059999999989	18.9455549999999988	3.5828080000000000
W	27.7576439999999991	21.7896150000000013	3.6024780000000001
W	26.1109819999999999	24.6174040000000005	3.6170279999999999
W	24.5109519999999996	27.3891519999999993	3.6236950000000001
W	22.9539089999999995	30.0662410000000015	3.6298059999999999
W	21.3157619999999994	32.7134849999999986	3.6529630000000002
W	42.9971129999999988	-0.5505130000000000	3.7652239999999999
W	39.9295710000000028	4.8971720000000003	3.6827529999999999
W	38.3933180000000007	7.6419889999999997	3.6315759999999999
W	36.8778750000000031	10.3806360000000009	3.6704260000000000
W	35.3413660000000007	13.1456540000000004	3.6522630000000000
W	33.7729690000000033	15.9159790000000001	3.5982580000000000
W	32.1908919999999981	18.6811940000000014	3.5563060000000002
W	30.6113959999999992	21.4387560000000015	3.5604399999999998
W	29.0407909999999987	24.1949280000000009	3.6086770000000001
W	27.4635500000000015	26.9520720000000011	3.6636340000000001
W	25.8765199999999993	29.7093109999999996	3.7002500000000000

W	22.6523520000000005	34.9218860000000006	3.7417520000000000
W	24.2487500000000011	32.3967049999999972	3.7216779999999998
S	22.2684819999999988	-2.0202670000000000	4.3002029999999998
S	20.6561239999999984	1.1614560000000000	5.0847400000000000
S	18.9965159999999997	3.8475890000000001	5.0876099999999997
S	17.3736849999999983	6.5856420000000000	5.0924930000000002
S	15.7588480000000004	9.3429590000000005	5.0783980000000000
S	14.1427320000000005	12.0903279999999995	5.0459480000000001
S	12.5352379999999997	14.8228779999999993	5.0241040000000003
S	10.9429820000000007	17.5533310000000000	5.0201140000000004
S	9.3715869999999999	20.2923019999999994	5.0265279999999999
S	7.8296460000000003	23.0460220000000007	5.0225260000000000
S	6.3198939999999997	25.8525150000000004	4.9645450000000002
S	4.7991180000000000	28.6951169999999998	4.7733800000000004
S	25.6227429999999998	-2.1735099999999998	4.2067220000000001
S	23.9566289999999995	1.0592189999999999	5.0314110000000003
S	22.4315260000000016	3.9115799999999998	4.8165190000000004
S	20.7823859999999989	6.6317690000000002	4.7075449999999996
S	19.1564380000000014	9.4034010000000006	4.6622960000000004
S	17.5495759999999983	12.1957679999999993	4.7029850000000000
S	15.9635929999999995	14.9589649999999992	4.7447499999999998
S	14.3943549999999991	17.6972489999999993	4.7484830000000002
S	12.8217920000000003	20.4434299999999993	4.7327640000000004
S	11.2347359999999998	23.2133639999999986	4.7235790000000000
S	9.6573180000000001	25.9920839999999984	4.6838139999999999
S	8.0763359999999995	28.7884250000000002	4.5314949999999996
S	19.0052470000000007	-0.2285030000000000	2.5098699999999998
S	17.1961019999999998	2.6284839999999998	2.5626039999999999
S	15.5756280000000000	5.4559049999999996	2.5476380000000001
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S	12.3750060000000008	11.0353379999999994	2.4398689999999998
S	10.7705789999999997	13.8017550000000000	2.4036879999999998
S	9.1873559999999994	16.5607700000000015	2.3829240000000000

S	7.612000000000001	19.312141000000004	2.3889190000000000
S	6.072604000000001	22.097469000000002	2.3313429999999999
S	4.4493729999999996	24.8644959999999990	2.4398749999999998
S	2.9870500000000000	27.7243640000000013	2.1319729999999999
S	1.4940840000000000	30.6104279999999989	1.8956299999999999
S	22.6007579999999990	0.1091290000000000	1.6991410000000000
S	20.7884080000000004	2.8420690000000000	1.6672760000000000
S	19.1483199999999982	5.6210550000000001	1.6818919999999999
S	17.5323929999999990	8.4542400000000004	1.6865669999999999
S	15.9167970000000008	11.2587390000000003	1.6488609999999999
S	14.3307350000000007	14.0235889999999994	1.6025400000000001
S	12.7644160000000007	16.7683309999999999	1.5859710000000000
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S	9.6502630000000007	22.2654950000000014	1.5899420000000000
S	8.0819480000000006	25.0125840000000004	1.5460680000000000
S	6.5178330000000004	27.9010110000000005	1.6173200000000001
S	4.9476540000000000	30.7219310000000014	1.3494060000000001
S	3.3623949999999998	31.5475299999999983	4.7779509999999998
S	6.5679689999999997	31.6389640000000014	4.9069219999999998
S	0.3628660000000000	33.4694110000000009	3.8580390000000002
S	3.4417000000000000	33.7794430000000006	2.0043180000000000
S	28.8685529999999986	-2.1611579999999999	4.2950929999999996
S	27.2133509999999994	1.0101739999999999	5.1887090000000002
S	25.7051979999999993	3.8613770000000001	4.7935590000000001
S	24.0078989999999983	6.7195590000000003	5.1807280000000002
S	22.3931910000000016	9.4426740000000002	5.1518879999999996
S	20.8042990000000003	12.1945040000000002	5.1319809999999997
S	19.2123090000000012	14.9656850000000006	5.1532590000000003
S	17.6317340000000016	17.7274679999999982	5.1805320000000004
S	16.0567649999999986	20.4784509999999997	5.1813019999999996
S	14.4728560000000002	23.2462969999999984	5.1492149999999999
S	12.8786210000000008	26.0549239999999998	5.1037350000000004
S	11.3036829999999995	28.8397730000000010	5.0855329999999999

S	32.078009999999990	-2.0776740000000000	4.5816960000000000
S	30.514576999999992	1.1029929999999999	5.1452730000000004
S	28.8628420000000006	3.8572199999999999	4.8541379999999998
S	27.285655999999995	6.8546769999999997	5.0006860000000000
S	25.6936420000000005	9.5646339999999999	4.8095960000000000
S	24.1086010000000002	12.3025570000000002	4.7517019999999999
S	22.5273660000000007	15.0449710000000003	4.7604810000000004
S	20.9493389999999984	17.7973719999999993	4.8007559999999998
S	19.3627709999999986	20.5631799999999991	4.8185269999999996
S	17.7621029999999998	23.3271659999999983	4.7878809999999996
S	16.1638780000000004	26.0853719999999996	4.7151319999999997
S	14.6055299999999999	28.8611159999999991	4.6897440000000001
S	25.7561420000000005	0.0453120000000000	1.6617850000000001
S	24.1105869999999989	3.0134110000000001	2.0687540000000002
S	22.4078739999999996	5.7148320000000004	2.0334560000000002
S	20.7932689999999987	8.4703830000000000	2.0331589999999999
S	19.1729659999999988	11.2711430000000004	2.0509729999999999
S	17.5672150000000009	14.0508509999999998	2.0601159999999998
S	15.9849490000000003	16.7981020000000001	2.0602320000000001
S	14.4177900000000001	19.5341670000000001	2.0613389999999998
S	12.8471480000000007	22.2897570000000016	2.0742829999999999
S	11.2695139999999991	25.0663629999999991	2.0575329999999998
S	9.7192139999999991	27.8464320000000001	1.9227600000000000
S	8.1941360000000003	30.5992910000000009	1.7476849999999999
S	28.9334629999999997	0.0229350000000000	1.7478340000000001
S	27.3254130000000011	2.9829240000000001	2.1233040000000001
S	25.7693919999999999	5.8115530000000000	1.7667320000000000
S	24.0983400000000003	8.5827299999999997	1.6592890000000000
S	22.5013749999999995	11.3486530000000005	1.6493730000000000
S	20.8928809999999991	14.1249990000000007	1.6596390000000001
S	19.3009419999999992	16.8839100000000002	1.6794220000000000
S	17.7300900000000006	19.6156520000000008	1.6855389999999999
S	16.1554690000000001	22.3407359999999997	1.6686589999999999

S	14.563148999999999	25.0998370000000008	1.6471290000000001
S	12.957088999999999	27.894400999999984	1.6296590000000000
S	11.426709999999999	30.7054580000000001	1.5545480000000000
S	9.6938080000000006	31.6892840000000007	4.9744299999999999
S	12.8893050000000002	31.6135869999999990	4.9119640000000002
S	6.5998270000000003	33.8589569999999966	2.3478560000000002
S	9.723684999999997	33.9168880000000001	2.5312800000000002
S	35.416637999999990	-1.9918340000000001	4.5666570000000002
S	33.7345070000000007	1.1315900000000001	5.4739920000000000
S	32.02692600000000031	3.9085320000000001	5.1216470000000003
S	30.4668409999999987	6.7264530000000002	5.2447229999999996
S	28.937965999999994	9.5347969999999993	5.1651999999999996
S	27.3482340000000015	12.3247490000000006	5.2149830000000001
S	25.7676000000000016	15.0770189999999999	5.2467350000000001
S	24.1868419999999986	17.8241890000000005	5.2686950000000001
S	22.599188999999991	20.5891270000000013	5.2708159999999999
S	20.9986730000000001	23.3678169999999987	5.2535800000000004
S	19.3922670000000004	26.1424790000000016	5.2184650000000001
S	17.786298999999996	28.9014290000000003	5.1483730000000003
S	38.5583389999999966	-2.0366059999999999	4.8774220000000001
S	36.95910400000000035	1.2731730000000001	5.2618000000000000
S	35.2966300000000004	4.0420689999999997	5.0232450000000002
S	33.7521759999999986	6.7534789999999996	4.8791159999999998
S	32.21183700000000027	9.5442920000000004	4.8365790000000004
S	30.6769849999999984	12.3229019999999991	4.8157740000000002
S	29.1106629999999988	15.0954270000000008	4.8400140000000000
S	27.51875400000000013	17.8807890000000000	4.8677380000000001
S	25.9083949999999987	20.6687480000000008	4.8814299999999999
S	24.29109800000000016	23.4519330000000004	4.8738340000000004
S	22.67497200000000003	26.2275600000000004	4.8414359999999999
S	21.0419629999999991	28.9882419999999996	4.8285090000000004
S	32.19755200000000017	0.0313200000000000	2.1030750000000000
S	30.54039500000000002	2.9337190000000000	2.2485710000000001

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S	22.548045999999994	16.9059020000000011	2.1283820000000002
S	20.9664520000000003	19.6591969999999989	2.1564199999999998
S	19.3873010000000008	22.4103679999999983	2.1512970000000000
S	17.799123999999991	25.1574910000000003	2.0942680000000000
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S	14.589022999999992	30.6065649999999998	1.7875509999999999
S	35.4001019999999968	0.0346840000000000	2.2964129999999998
S	33.7723670000000027	2.9536609999999999	1.8453960000000000
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S	30.6113539999999986	8.6211629999999992	1.7518119999999999
S	29.0453760000000010	11.4140139999999999	1.7238260000000001
S	27.4614529999999988	14.2044230000000002	1.7423480000000000
S	25.8777760000000008	16.9708089999999991	1.7732260000000000
S	24.2898740000000011	19.7308899999999987	1.7911940000000000
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S	16.0828370000000014	33.8442590000000010	2.4976340000000001
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S	40.1786349999999999	1.1428400000000001	5.5481249999999998
S	38.5642879999999977	3.9874540000000001	5.3013690000000002
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S	35.4127909999999986	9.5869590000000002	5.3589149999999997
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S	30.778493999999985	17.868303000000009	5.254550000000001
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S	27.561478000000010	23.472041000000008	5.285318000000002
S	25.939855999999989	26.263902999999991	5.323716000000001
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S	44.705897999999977	-1.541687999999999	2.938810000000001
S	43.555835000000019	1.263714999999999	4.933726000000001
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S	40.616881999999968	7.001178000000003	4.386180000000004
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S	37.462139000000005	12.530905000000006	4.544750999999998
S	35.896217999999975	15.296991000000002	4.513939999999998
S	34.327060000000030	18.077453999999995	4.439236000000002
S	32.745547000000020	20.862055999999990	4.402878000000003
S	31.149615000000007	23.648755999999988	4.436086000000004
S	29.548100999999991	26.439973999999994	4.499661999999998
S	27.963709000000015	29.242929000000002	4.511299000000002
S	38.574098999999968	0.265679000000000	2.104664999999998
S	36.989280999999983	3.070122000000000	2.385006000000002
S	35.389868999999974	5.857134000000003	2.249947999999998
S	33.822164999999983	8.620355000000000	2.176877999999999
S	32.279006000000025	11.402898999999997	2.145776000000001
S	30.718537000000013	14.172335999999996	2.161874000000001
S	29.133737000000000	16.955272999999983	2.216880999999999
S	27.532699999999984	19.746256999999999	2.253180000000000
S	25.930001000000007	22.535665000000016	2.253458000000002
S	24.328658999999983	25.320851000000011	2.212933000000000
S	22.730304000000003	28.092372999999985	2.163377999999998
S	21.146097999999985	30.867944000000014	2.141500000000002
S	41.676233000000034	0.339124000000000	2.113134000000001
S	40.239502000000017	3.202313999999999	2.047820999999999
S	38.678133000000025	5.969663999999999	1.940220000000001
S	37.196537999999968	8.768993000000000	1.921152000000000

S	35.701284999999986	11.524260999999992	1.9180320000000000
S	34.155611999999979	14.2747430000000008	1.8890780000000000
S	32.5547880000000021	17.0323409999999988	1.8524769999999999
S	30.9453430000000012	19.8034649999999992	1.8413980000000001
S	29.3503520000000009	22.5827579999999983	1.8707620000000000
S	27.7651250000000012	25.3558270000000014	1.9228930000000000
S	26.1901060000000001	28.1126280000000008	1.9602640000000000
S	24.637606999999991	30.8324460000000009	1.9613449999999999
S	22.6346309999999988	31.7468359999999983	5.3646360000000000
S	26.3447920000000018	32.0343039999999988	4.5082719999999998
S	24.380639999999996	34.5879589999999979	5.0517729999999998
S	19.4468330000000016	33.8288439999999966	2.1802120000000000
S	23.0513960000000004	33.5549200000000027	1.9405289999999999
S	20.7999749999999999	34.8516679999999965	4.9317039999999999

$W_{105}S_{210}$; $E_{tot} = -49\,817\,928.633\,448\,50$ eV; $E_{rel} = 15.478\,923\,152\,3$ meV/f.u.

W	59.066153999999974	-66.1604520000000065	3.4974710000000000
W	57.3187050000000013	-63.4284620000000032	3.4828000000000001
W	60.5080570000000009	-63.9528899999999965	3.4700650000000000
W	55.7606859999999998	-60.7410679999999985	3.5183010000000001
W	54.2191869999999980	-58.0628749999999982	3.5121540000000002
W	52.6660839999999979	-55.3569579999999988	3.4687209999999999
W	51.2150200000000027	-52.4665139999999965	3.4524590000000002
W	62.2266479999999973	-66.3594350000000048	3.5434450000000002
W	58.5322060000000022	-61.0161330000000035	3.4267059999999998
W	56.9266810000000021	-58.2751710000000003	3.4331719999999999
W	55.3532020000000031	-55.4632390000000015	3.4377300000000002
W	53.8464150000000004	-52.3629260000000016	3.4917470000000002
W	52.6215309999999974	-49.6464950000000016	3.4419040000000001
W	65.5591749999999962	-66.4181190000000043	3.5128840000000001
W	63.4157980000000023	-63.9242289999999969	3.4533630000000000
W	62.3251009999999965	-60.7034519999999986	3.4586530000000000

W	60.731485999999967	-57.976722999999998	3.5259369999999999
W	59.1933580000000035	-55.2502970000000033	3.5277379999999998
W	57.572437999999982	-52.4932960000000008	3.4271080000000000
W	55.271267999999992	-49.6281350000000003	3.4892859999999999
W	54.165843999999999	-46.932839999999988	3.3783439999999998
W	68.717709999999967	-66.380116999999985	3.4672310000000000
W	67.0581880000000012	-64.1215579999999932	3.5319180000000001
W	65.3478470000000016	-60.6867650000000012	3.3743120000000002
W	63.486173999999983	-58.257229999999998	3.3632510000000000
W	62.0077050000000014	-55.548229999999967	3.3954119999999999
W	60.271256999999985	-52.304851999999968	3.4892599999999998
W	59.107647999999975	-49.790863999999991	3.3788200000000002
W	56.871999999999999	-46.853302999999968	3.4794710000000002
W	55.7681240000000003	-44.245486999999971	3.3546090000000000
W	71.8390160000000009	-66.398347999999986	3.4535740000000001
W	70.246073999999930	-64.1077120000000065	3.4967030000000001
W	68.3667630000000059	-60.7273860000000028	3.4887310000000000
W	67.236447999999958	-58.242640999999990	3.4017890000000000
W	65.195753999999938	-55.019204999999995	3.4129600000000000
W	64.008139999999974	-52.5623610000000028	3.3504960000000001
W	61.819926999999999	-49.580551999999973	3.5293779999999999
W	60.674276999999965	-47.076825999999970	3.3984139999999998
W	58.7763520000000028	-43.7363050000000015	3.4406919999999999
W	57.349671999999982	-41.4983110000000011	3.4311630000000002
W	74.9648760000000038	-66.3998090000000047	3.4411950000000000
W	73.426479999999980	-64.154174999999951	3.4939209999999998
W	72.037970999999989	-60.703358999999990	3.4972080000000001
W	70.007705999999989	-58.083953999999985	3.5441199999999999
W	68.8394020000000069	-55.5869950000000017	3.4050220000000002
W	66.7174420000000055	-52.3882890000000003	3.4416080000000000
W	65.554884999999987	-49.9286310000000029	3.3482569999999998
W	63.4209230000000019	-46.8621800000000022	3.5153059999999998
W	62.265152999999980	-44.396495999999991	3.4250479999999999

W	60.402786999999965	-41.1622780000000006	3.4656780000000000
W	59.0992320000000007	-38.8681249999999991	3.4731390000000002
W	78.110928999999987	-66.419032999999989	3.5400049999999998
W	76.622270999999978	-64.1248250000000013	3.5363970000000000
W	75.1658900000000045	-60.682454999999974	3.4547780000000001
W	73.617823999999988	-58.444293999999993	3.6064729999999998
W	71.564038999999940	-55.347028999999991	3.6039770000000000
W	70.411816999999992	-52.856017999999988	3.4858140000000000
W	68.2905740000000065	-49.788153999999987	3.4084219999999998
W	67.141779999999971	-46.726813999999974	3.4124850000000002
W	65.557700999999945	-44.343989999999980	3.4866959999999998
W	63.678359999999979	-40.959938999999985	3.4402349999999999
W	62.284588999999969	-38.686872999999985	3.4800119999999999
W	81.470112999999978	-66.321517999999975	3.6387710000000002
W	80.2404370000000000	-63.8587840000000000	3.4948950000000001
W	78.2734190000000041	-60.6581260000000029	3.4918369999999999
W	76.7593310000000031	-58.399659999999972	3.6060520000000000
W	75.2765160000000009	-55.044449999999977	3.6184349999999998
W	73.664345999999948	-52.2918340000000015	3.5527790000000001
W	72.113721999999957	-49.542217999999983	3.5213019999999999
W	70.485675999999980	-46.8110670000000013	3.5032899999999998
W	68.538675999999953	-44.3320950000000025	3.4654910000000001
W	66.888791999999951	-40.931351999999968	3.4279320000000002
W	65.3753090000000014	-38.676670999999989	3.5480740000000002
W	84.602110999999936	-66.271512999999988	3.8865560000000001
W	83.1765610000000066	-63.9789320000000004	3.6575869999999999
W	81.3374570000000006	-60.733680999999971	3.5605929999999999
W	79.855806999999987	-58.405543999999990	3.5985250000000000
W	78.0224180000000018	-55.2916480000000021	3.5433770000000000
W	76.4384340000000009	-52.5549510000000026	3.4369170000000002
W	74.8535250000000048	-49.807276999999991	3.3996400000000002
W	73.262575999999957	-47.064754999999981	3.3766539999999998
W	71.656672999999978	-44.343260999999983	3.4208080000000001

W	70.5371020000000044	-41.1037850000000020	3.4772509999999999
W	68.4593090000000046	-38.6512999999999991	3.5056409999999998
W	88.3145350000000064	-66.5557900000000018	3.9156520000000001
W	86.1808850000000035	-63.5635380000000012	3.6402540000000001
W	89.8400270000000063	-63.8882100000000008	3.8580160000000001
W	84.9971720000000062	-60.7768429999999995	3.6589999999999998
W	83.4198769999999996	-58.3129009999999965	3.5646909999999998
W	81.7908910000000020	-55.0496020000000001	3.5632299999999999
W	80.2527249999999981	-52.2405019999999993	3.5177429999999998
W	78.6628230000000030	-49.4749669999999995	3.5130620000000001
W	77.0633490000000023	-46.7284649999999999	3.5022240000000000
W	75.4330929999999995	-43.9853999999999985	3.5030809999999999
W	73.4567200000000042	-41.0998960000000011	3.4543990000000000
W	71.6839140000000015	-38.6633580000000023	3.4371550000000002
W	87.7251169999999973	-60.8581610000000026	3.8565839999999998
W	86.1908899999999960	-58.1349099999999979	3.6618550000000001
W	84.5361950000000064	-55.2116419999999977	3.5683280000000002
W	82.9627650000000045	-52.4734690000000015	3.4748359999999998
W	81.4240259999999978	-49.7280709999999999	3.4828399999999999
W	79.8493880000000047	-46.9957119999999975	3.4905819999999999
W	78.2457780000000014	-44.2888260000000002	3.4536859999999998
W	76.6414970000000011	-41.5734410000000025	3.4577979999999999
W	74.8528539999999936	-38.8572080000000000	3.4321060000000001
S	60.2408829999999966	-67.8467849999999970	4.3561199999999998
S	58.7413230000000013	-64.5271489999999943	5.1450810000000002
S	57.0526899999999983	-61.8336439999999996	5.2215680000000004
S	55.4602170000000001	-59.1279159999999990	5.2329780000000001
S	53.9120720000000020	-56.3842659999999967	5.2114349999999998
S	52.4164060000000021	-53.5758089999999996	5.1355120000000003
S	50.3433490000000035	-50.6038780000000017	4.3010440000000001
S	63.6774100000000018	-67.9070839999999976	4.3502840000000003
S	62.0111589999999993	-64.7262699999999995	5.2060540000000000
S	60.4717819999999975	-61.8297910000000002	4.7307199999999998

S	58.8348200000000006	-59.0437039999999982	4.8167099999999996
S	57.2401070000000018	-56.2703840000000000	4.8009490000000001
S	55.6709829999999997	-53.4390730000000005	4.7953270000000003
S	53.8902659999999969	-50.6205599999999976	5.1730380000000000
S	51.9466389999999976	-47.6107889999999969	4.2740549999999997
S	66.9876000000000005	-67.9935129999999930	4.2885749999999998
S	65.2981379999999945	-64.7566120000000041	5.0709340000000003
S	63.7613180000000028	-61.9233720000000005	4.9006129999999999
S	62.0843029999999985	-59.0868210000000005	5.1817810000000000
S	60.5274829999999966	-56.2558319999999981	5.1985760000000001
S	58.9165459999999968	-53.4633070000000004	5.1519190000000004
S	57.1754529999999974	-50.5920580000000015	4.8054930000000002
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S	63.7391840000000016	-56.2905689999999979	4.9151520000000000
S	62.1258709999999965	-53.4464320000000015	4.7034820000000002
S	60.4914739999999966	-50.6605410000000020	5.2034580000000004
S	58.7741200000000035	-47.8248669999999976	4.8239250000000000
S	57.2193049999999985	-44.9540810000000022	5.0027619999999997
S	55.2185300000000012	-41.9606089999999980	4.1433109999999997
S	73.4370530000000059	-67.9565039999999954	4.3652889999999998
S	71.8251709999999974	-64.7582510000000013	5.1910639999999999
S	70.2165559999999971	-61.9015399999999971	4.7469359999999998
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S	60.4512360000000015	-44.9870469999999969	4.8327609999999996

S	58.831930999999973	-42.082895000000006	5.1418130000000000
S	57.046798000000026	-39.076433000000015	4.3206329999999999
S	76.669051999999935	-68.003226999999954	4.2911089999999996
S	75.027583000000070	-64.807738000000005	5.2076320000000003
S	73.488647000000003	-62.010137999999978	4.8093019999999997
S	71.848910000000036	-59.057929999999989	5.1311080000000002
S	70.216566000000003	-56.377473999999994	5.2623970000000000
S	68.548119999999973	-53.485522000000031	4.7678820000000002
S	66.963705000000045	-50.701343000000014	5.1536320000000000
S	65.370296999999937	-47.874071999999982	4.7203010000000001
S	63.813389000000008	-45.072301000000031	5.0991720000000003
S	62.159106999999988	-42.270634999999986	4.8201859999999996
S	60.645401999999971	-39.352266999999977	5.1650210000000003
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S	78.338605999999986	-64.764330000000011	5.1044489999999998
S	76.688152000000023	-61.969307000000006	4.8828440000000004
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S	73.493784000000051	-56.289819000000014	4.8856960000000003
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S	70.247131999999935	-50.707121000000008	4.7482239999999996
S	68.653126000000003	-47.894222999999967	4.8947229999999999
S	67.033686000000030	-45.085191999999993	5.1758329999999999
S	65.384521000000066	-42.194352000000021	4.8117590000000003
S	63.784269999999994	-39.278857999999996	5.2315829999999997
S	83.192205000000013	-67.923015000000066	4.5013620000000003
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S	76.666895999999942	-56.285504000000031	5.1525840000000001
S	75.057281000000032	-53.351998999999993	5.2680330000000000
S	73.428454000000021	-50.600974999999983	5.2218619999999998
S	71.839568999999973	-47.840164999999989	5.1865430000000003
S	70.178212999999995	-45.049453999999972	5.1457590000000000

S	68.6216320000000053	-42.1593629999999990	4.7040199999999999
S	66.9482330000000019	-39.2706500000000034	5.2311240000000003
S	86.4242849999999976	-67.4742260000000016	4.9124080000000001
S	84.7875570000000067	-64.5188870000000065	5.3973760000000004
S	83.1376659999999958	-61.8307969999999969	4.8778620000000004
S	81.6254289999999969	-58.9979579999999970	5.1531200000000004
S	79.9382640000000038	-56.1958580000000012	4.8487869999999997
S	78.3868439999999964	-53.3176899999999989	4.8115649999999999
S	76.7682690000000036	-50.5484579999999966	4.8081560000000003
S	75.1646109999999936	-47.7831130000000002	4.7865679999999999
S	73.5362130000000036	-45.0211230000000029	4.8002469999999997
S	71.8883000000000010	-42.2607519999999965	4.9694399999999996
S	70.1372109999999935	-39.3259910000000019	5.1231600000000004
S	57.0526219999999995	-65.8775470000000070	2.5789670000000000
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S	51.9570750000000032	-57.3657189999999986	2.6959909999999998
S	50.4333570000000009	-54.3532030000000006	2.5436879999999999
S	60.6182149999999993	-65.7885890000000018	1.7887200000000001
S	58.8564110000000014	-62.8458589999999973	1.8673700000000000
S	57.1595200000000006	-59.9951420000000013	1.7328140000000001
S	55.5599249999999998	-57.1968859999999992	1.7511330000000001
S	53.9503910000000033	-54.3117200000000011	1.8571420000000001
S	52.3764340000000033	-51.3729020000000034	1.7409129999999999
S	63.8324950000000015	-65.7663990000000069	1.8941830000000000
S	62.0710750000000004	-62.7968710000000030	1.9377880000000001
S	60.4184259999999966	-59.9964310000000012	2.0953529999999998
S	58.8199410000000000	-57.1967939999999970	2.1277149999999998
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S	55.6381119999999996	-51.5392519999999976	2.0434559999999999
S	53.8792439999999999	-48.6176859999999991	1.7064450000000000
S	67.0795970000000068	-65.8552940000000007	1.7764670000000000
S	65.3313579999999945	-62.9122429999999966	2.2391719999999999

S	63.7765580000000014	-59.9760920000000013	1.6859029999999999
S	62.1317769999999996	-57.2200630000000032	1.6746509999999999
S	60.5349519999999970	-54.3177289999999999	1.8774649999999999
S	58.8351309999999970	-51.5026780000000031	1.6889230000000000
S	57.1781319999999980	-48.7517429999999976	2.0901160000000001
S	55.4734979999999993	-45.8919569999999979	1.6785350000000001
S	70.2605460000000051	-65.8817880000000002	1.7353609999999999
S	68.5662959999999941	-62.8657249999999976	2.1365639999999999
S	66.9371150000000057	-59.9648329999999987	1.7132400000000001
S	65.3567560000000043	-57.1626059999999967	2.1340889999999999
S	63.6756180000000001	-54.3899339999999967	1.7738339999999999
S	62.1080869999999976	-51.5415300000000016	2.0465710000000001
S	60.4010850000000019	-48.7180320000000009	1.6994020000000001
S	58.7857369999999975	-45.9126389999999986	2.2179540000000002
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S	73.4110060000000004	-65.8964639999999946	1.7191030000000000
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S	70.2159630000000021	-60.0395159999999990	2.0107219999999999
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S	67.0372849999999971	-54.4316109999999966	2.0485980000000001
S	65.3171159999999986	-51.5674410000000023	1.6051670000000000
S	63.7019999999999982	-48.7975569999999976	2.0753590000000002
S	62.0248009999999965	-46.0013909999999981	1.7081489999999999
S	60.5340339999999983	-43.1482889999999983	1.9794920000000000
S	58.7485950000000017	-40.4210679999999982	1.7541009999999999
S	76.6163370000000015	-65.8554029999999955	1.7717719999999999
S	75.0851590000000044	-62.8792860000000005	2.1554620000000000
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S	71.9002490000000023	-57.2775760000000034	2.1764299999999999
S	70.2449330000000032	-54.4845619999999968	1.7547509999999999
S	68.6409950000000038	-51.6772739999999970	2.0206710000000001
S	66.9694939999999974	-48.7447000000000017	1.7848370000000000
S	65.3344199999999944	-46.0369590000000031	1.9158700000000000

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S	76.7131909999999948	-60.0324349999999995	1.7833140000000001
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S	63.6842860000000002	-37.0631589999999989	2.7020970000000002
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S	81.6509219999999942	-62.7974000000000032	2.0385179999999998
S	79.8903190000000052	-60.0552459999999968	1.7997970000000001
S	78.3374079999999964	-57.2096310000000017	2.0683690000000001
S	76.7334969999999998	-54.3163529999999994	1.7979330000000000
S	75.1247960000000035	-51.5419240000000016	1.7427600000000001
S	73.5440930000000037	-48.7394710000000018	1.6973980000000000
S	71.9123469999999969	-45.9711590000000001	1.7141759999999999
S	70.2266359999999992	-43.0927269999999965	2.0138550000000000
S	68.6541339999999991	-40.2731939999999966	1.8966799999999999
S	66.9610279999999989	-37.0573400000000035	2.7139430000000000
S	89.5667289999999952	-68.2647350000000017	4.1655129999999998
S	88.6314509999999984	-64.9382820000000009	5.5466930000000003
S	86.3132980000000032	-61.8710760000000022	5.3917400000000004
S	84.8585250000000002	-59.0388129999999975	5.3531510000000004
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S	81.6020199999999960	-53.3366169999999968	5.2309250000000000
S	80.0112450000000024	-50.5506010000000003	5.2143280000000001
S	78.3985169999999982	-47.7822869999999966	5.2126780000000004

S	76.791257999999991	-45.006810999999990	5.2000520000000003
S	75.095933999999997	-42.1639679999999970	5.0702119999999997
S	73.3208900000000057	-39.2708170000000010	5.1496639999999996
S	91.9573800000000006	-64.0791629999999941	4.0350520000000003
S	89.6870710000000031	-61.7967900000000014	4.8745760000000002
S	88.4628809999999959	-58.7926879999999983	4.4153969999999996
S	86.7327709999999996	-56.0415860000000023	4.4302349999999997
S	85.2021249999999952	-53.1624580000000009	4.2962699999999998
S	83.5714650000000034	-50.3822860000000006	4.3907670000000003
S	81.9717270000000013	-47.5706249999999997	4.3993380000000002
S	80.3383089999999953	-44.7671380000000028	4.3842260000000000
S	78.7314120000000059	-41.9250919999999994	4.2222450000000000
S	76.8652680000000004	-39.1012509999999978	4.3540859999999997
S	86.4347790000000060	-65.6912140000000022	2.3936999999999999
S	84.7420500000000061	-62.7502509999999987	2.1118500000000000
S	83.2241080000000011	-60.0357040000000026	2.0417730000000001
S	81.6137700000000024	-57.1825299999999999	2.3045659999999999
S	79.9743760000000066	-54.3139169999999964	2.1675019999999998
S	78.3720809999999943	-51.5064339999999987	2.1424280000000002
S	76.7731869999999930	-48.7294729999999987	2.1221220000000001
S	75.1630420000000044	-45.9574289999999976	2.1166179999999999
S	73.4995629999999949	-43.1928339999999977	2.1582669999999999
S	71.9324199999999934	-40.2610930000000025	1.7455660000000000
S	70.2294890000000009	-37.0780820000000020	2.6843210000000002
S	89.4738229999999959	-65.4900880000000001	2.1753220000000000
S	88.1386049999999983	-62.7227290000000011	2.3571629999999999
S	86.5581169999999958	-59.8702120000000022	1.9799469999999999
S	84.8436310000000020	-57.0646869999999993	1.9999309999999999
S	83.3026749999999936	-54.1801159999999982	1.8053220000000001
S	81.7647630000000021	-51.3552030000000030	1.7534860000000001
S	80.2100230000000067	-48.6023970000000034	1.7612909999999999
S	78.6198779999999999	-45.8932209999999969	1.7483200000000001
S	76.9549650000000014	-43.1841819999999998	1.7353749999999999

S	75.2198300000000017	-40.4841910000000027	1.7837390000000000
S	73.6528349999999961	-37.1791929999999979	2.5889380000000002

$W_{105}S_{210}$; $E_{tot} = -49\,817\,929.051\,481\,15$ eV; $E_{rel} = 11.497\,659\,819\,0$ meV/f.u.

W	21.1998460000000009	-0.4888000000000000	3.3524989999999999
W	19.4574730000000002	2.2731279999999998	3.3640349999999999
W	17.8721110000000003	4.9987389999999996	3.3882629999999998
W	16.2492790000000014	7.6621079999999999	3.3495490000000001
W	14.6327630000000006	10.3478519999999996	3.3607570000000000
W	13.0650720000000007	13.0491100000000007	3.3930650000000000
W	11.4810529999999993	15.7654250000000005	3.2938540000000001
W	9.6709599999999991	18.7410209999999999	3.0128590000000002
W	8.0272349999999992	21.8389239999999987	3.1729189999999998
W	6.5370939999999997	24.4909800000000004	3.2430300000000001
W	5.0041140000000004	27.0804060000000000	3.1261540000000001
W	3.2188750000000002	30.2384069999999987	3.0281479999999998
W	1.7432500000000000	32.9421960000000027	3.0947760000000000
W	0.2357090000000000	35.4425179999999997	3.0341559999999999
W	-1.3432249999999999	38.0140889999999985	3.1304650000000001
W	24.3405309999999986	-0.6576400000000000	3.4688279999999998
W	22.6918100000000003	1.6729099999999999	3.4521430000000000
W	20.7006019999999999	4.7818430000000003	3.3686440000000002
W	19.0400080000000003	7.4544370000000004	3.3456850000000000
W	17.4056099999999994	10.1445790000000002	3.3379430000000001
W	15.7874440000000007	12.8477859999999993	3.3463919999999998
W	14.2128619999999994	15.5809719999999992	3.3534180000000000
W	12.6900980000000008	18.8967339999999986	3.3038400000000001
W	11.3021619999999992	21.1851459999999996	3.3781289999999999
W	9.5437139999999996	24.5158890000000014	3.3255699999999999
W	8.0202860000000005	26.8061480000000003	3.3828130000000001
W	6.4035940000000000	30.1977089999999997	3.2314660000000002
W	2.9656570000000002	35.6843569999999985	3.1912330000000000

W	4.8667860000000003	32.4660560000000018	3.2797960000000002
W	1.7248980000000000	38.0222279999999984	3.0818710000000000
W	27.4717969999999987	-0.7097340000000000	3.5833360000000001
W	28.8844460000000005	1.6028439999999999	3.6041040000000000
W	25.7801310000000008	1.5919250000000000	3.5307689999999998
W	24.3184019999999990	5.0233499999999998	3.3454190000000001
W	22.7442659999999997	7.2760740000000004	3.3946679999999998
W	21.1147460000000002	10.7031939999999999	3.3552000000000000
W	19.5951099999999983	13.3372189999999993	3.4654389999999999
W	18.0065619999999988	15.9198029999999999	3.4139599999999999
W	15.8553040000000003	18.9486519999999992	3.4046660000000002
W	14.3836099999999991	21.2057180000000010	3.4993379999999998
W	12.8003879999999999	24.6047629999999984	3.3438819999999998
W	11.1322170000000007	26.8242609999999999	3.4793280000000002
W	9.5756840000000008	30.2502600000000008	3.3149920000000002
W	7.9533370000000003	32.4822950000000006	3.4097970000000002
W	6.5655010000000003	35.8867309999999975	3.2514460000000001
W	4.9054710000000004	38.1347379999999987	3.2670219999999999
W	30.6224589999999992	-0.6847380000000000	3.6128749999999998
W	27.4463000000000008	5.0367030000000002	3.4108239999999999
W	25.8649309999999986	7.2724330000000004	3.5134460000000001
W	24.2815420000000017	10.7176840000000002	3.3689659999999999
W	22.7143400000000000	12.9515809999999991	3.4891570000000001
W	20.8085750000000012	16.0814309999999985	3.4614850000000001
W	19.4523359999999990	18.7031169999999989	3.4641109999999999
W	17.4855480000000014	21.1963380000000008	3.5678999999999998
W	16.0717789999999994	24.6340399999999988	3.4252319999999998
W	14.3957970000000000	26.8414460000000012	3.5655359999999998
W	12.7956459999999996	30.2682900000000004	3.3927710000000002
W	9.7293760000000002	35.9317500000000010	3.3296280000000000
W	11.1441359999999996	32.5021559999999994	3.5105430000000002
W	8.0278220000000005	38.2016530000000003	3.3612180000000000
W	33.8703239999999965	-0.6814020000000000	3.7171439999999998

W	35.5980449999999990	1.9229900000000000	3.7032490000000000
W	31.9667819999999985	1.6659150000000000	3.6459470000000000
W	30.5977749999999986	5.0672420000000002	3.4993639999999999
W	29.0006370000000011	7.2912679999999996	3.5896010000000000
W	27.4299299999999988	10.7317630000000008	3.4136639999999998
W	25.8500790000000009	12.9621820000000003	3.5310959999999998
W	23.8131500000000003	16.0784309999999984	3.5084200000000001
W	22.2798720000000010	18.6206859999999992	3.4193120000000001
W	20.7608870000000003	21.2124309999999987	3.5037729999999998
W	19.2831709999999994	24.6590460000000000	3.4917799999999999
W	17.6474879999999992	26.8767439999999986	3.6313780000000002
W	16.0442070000000001	30.2853789999999989	3.4639210000000000
W	14.3724969999999992	32.5076150000000013	3.5812330000000001
W	12.8707659999999997	35.9362050000000011	3.3862489999999998
W	11.1365180000000006	38.2360820000000032	3.3751310000000001
W	36.8158469999999980	-0.7100820000000000	3.8938440000000001
W	33.7053020000000032	5.0896070000000000	3.6255069999999998
W	32.1765860000000004	7.3500569999999996	3.6817989999999998
W	30.5238720000000008	10.7370020000000004	3.5143040000000001
W	29.0361319999999985	13.0029669999999999	3.5950839999999999
W	27.6469629999999995	16.3281470000000013	3.5195520000000000
W	26.0923009999999991	19.0422680000000000	3.5075989999999999
W	24.4547600000000003	21.7160229999999999	3.5313140000000001
W	22.4112800000000014	24.7093139999999991	3.5612819999999998
W	20.8313459999999999	26.9445009999999989	3.6770999999999998
W	19.1749490000000016	30.3260770000000015	3.5494699999999999
W	15.9321240000000000	35.8723770000000002	3.4240770000000000
W	17.6730419999999988	32.6025100000000023	3.5775459999999999
W	14.2645730000000004	38.2063059999999979	3.4228170000000002
W	39.7395509999999987	-0.8254860000000001	3.7493870000000000
W	38.2306290000000004	1.8493210000000000	3.7402839999999999
W	36.8430719999999994	4.4907630000000003	3.7253470000000002
W	35.3681059999999974	7.3189770000000003	3.9104459999999999

W	33.615628999999984	10.4539840000000002	3.8075040000000002
W	32.2159040000000019	12.9681549999999994	3.7957420000000002
W	30.4055639999999983	16.1369259999999990	3.6259440000000001
W	28.8024519999999988	18.8401619999999994	3.4355300000000000
W	27.2355680000000007	21.4993739999999995	3.4356969999999998
W	25.6394510000000011	24.1624249999999989	3.5571199999999998
W	24.0059709999999988	26.9595009999999995	3.8502850000000000
W	22.1982430000000015	30.0876589999999986	3.8028520000000001
W	20.6531850000000006	32.6591009999999997	3.6543000000000001
W	19.1271179999999994	35.2614659999999986	3.6091500000000001
W	17.4187420000000017	38.0380480000000034	3.4879730000000002
S	22.3137420000000013	-2.1638679999999999	4.2793799999999997
S	20.8473830000000007	1.1288810000000000	5.0261449999999996
S	19.1943179999999991	3.8823040000000000	5.0839670000000003
S	17.4764480000000013	6.5819640000000001	5.1003040000000004
S	15.8571740000000005	9.2481860000000005	5.0864640000000003
S	14.2727039999999992	11.9503579999999996	5.1078229999999998
S	12.6600959999999993	14.7244410000000006	5.0869249999999999
S	11.0205000000000002	17.6716329999999999	4.7608540000000001
S	9.3686769999999999	20.4989489999999996	4.7500210000000003
S	7.9112000000000000	23.4281569999999988	4.9252010000000004
S	6.2283260000000000	26.1996029999999998	4.9609030000000001
S	4.5994149999999996	28.9785290000000018	4.6299370000000000
S	25.6814740000000015	-2.2544160000000000	4.4243819999999996
S	24.1448299999999989	0.9597540000000000	5.1999839999999997
S	22.5616810000000001	3.8305720000000001	4.6647040000000004
S	20.8941769999999991	6.6598080000000000	4.8608140000000004
S	19.3195850000000000	9.4605669999999993	4.7127900000000000
S	17.6792330000000000	12.1580390000000005	4.7239719999999998
S	16.0561189999999989	14.8850569999999998	4.7424830000000000
S	14.2828040000000005	17.6561120000000003	4.7485200000000001
S	12.7443869999999997	20.4945810000000002	5.1243340000000002
S	11.1775719999999996	23.3032429999999984	4.6997030000000004

S	9.528840999999999	26.172841999999993	5.1268180000000001
S	7.9315150000000001	28.9649310000000000	4.6802919999999997
S	19.1601709999999983	-0.1414510000000000	2.4710580000000002
S	17.3745079999999987	2.6659560000000000	2.5990540000000002
S	15.7796319999999994	5.4513230000000004	2.4400710000000001
S	14.1198800000000002	8.1944300000000005	2.4281670000000002
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S	10.8245660000000008	13.7367589999999993	2.5356540000000001
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S	5.9620850000000001	22.3076800000000013	2.3405830000000001
S	4.3650260000000003	25.0153360000000013	2.3530630000000001
S	3.0029849999999998	27.9506470000000000	2.2240720000000000
S	1.1534409999999999	30.7036639999999998	2.2297229999999999
S	22.7810139999999990	-0.0783990000000000	1.6857500000000001
S	21.0399530000000006	2.8840390000000000	1.8530510000000000
S	19.3203759999999996	5.7340710000000001	1.6462920000000001
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S	16.0505059999999986	11.1836409999999997	1.6324449999999999
S	14.4345979999999994	13.9263890000000004	1.6370920000000000
S	12.8333359999999992	16.7935200000000009	1.7641460000000000
S	11.1624800000000004	19.5931050000000013	1.5078149999999999
S	9.6680430000000008	22.4815199999999997	1.7939380000000000
S	8.0022859999999998	25.1671970000000016	1.5695600000000001
S	6.5007180000000000	28.0405589999999982	1.7527230000000000
S	4.8113830000000002	30.8231350000000006	1.4667559999999999
S	3.0644710000000002	31.8336940000000013	4.8094760000000001
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S	0.0714430000000000	37.3029179999999982	4.7888440000000001
S	6.3315440000000001	31.8130500000000005	5.0428639999999998
S	4.8044490000000000	34.6547120000000035	4.4985819999999999
S	3.2582979999999999	37.5019020000000012	4.8665529999999997
S	-0.3459390000000000	33.3920480000000026	2.1010550000000001

S	-1.890663999999999	36.160201999999982	1.992521000000000
S	-3.061847000000000	39.005336999999973	3.933870999999999
S	3.298125999999999	33.713883000000027	1.665667999999999
S	1.533546000000000	36.422080999999986	1.364462000000000
S	-0.052133000000000	39.414799999999996	1.970100000000000
S	28.936668000000009	-2.238264000000000	4.530082000000002
S	27.328379000000018	0.934176000000000	5.289477999999999
S	25.784127000000016	3.764845999999999	4.798721999999997
S	24.206285999999986	6.632795999999999	5.159198000000000
S	22.608167000000017	9.443830000000002	4.752580000000000
S	21.019946999999984	12.288994999999999	5.133112999999998
S	19.334703000000011	15.041843000000001	5.157441999999996
S	17.559194000000015	17.774521000000000	4.837334000000002
S	15.930018000000005	20.534953000000016	5.238042000000001
S	14.382659000000003	23.370620999999999	4.745289999999998
S	12.733873000000009	26.196107999999988	5.179365999999999
S	11.149241000000000	29.008378000000004	4.739911000000002
S	32.187828000000032	-2.307475000000002	4.288908000000002
S	30.504681000000015	0.903464000000000	5.351581999999996
S	28.954057999999999	3.766175000000001	4.863293999999998
S	27.398263000000000	6.662911000000003	5.244214000000004
S	25.810410000000010	9.457471999999992	4.799095000000003
S	24.260359999999986	12.331526000000002	5.203106000000000
S	22.481823999999996	15.013284999999998	5.020423000000001
S	20.898066000000000	17.786294999999991	5.181300000000002
S	19.234446999999994	20.495557999999991	5.146080999999997
S	17.613669999999990	23.374031999999997	4.844367000000001
S	16.002102000000007	26.235731999999987	5.259864999999996
S	14.388799999999998	29.029987999999995	4.814612000000003
S	25.940032999999997	-0.201899000000000	1.792181000000000
S	24.272498999999998	2.843897000000001	2.035453000000000
S	22.565540999999996	5.612306000000002	1.769063000000001
S	20.964743999999996	8.494467999999995	2.101792999999998

S	19.2517710000000015	11.3145159999999994	2.0240459999999998
S	17.6662439999999989	13.9910119999999996	2.0488569999999999
S	16.0264820000000014	16.7847389999999983	2.1270970000000000
S	14.3392900000000001	19.5885870000000004	1.6704300000000001
S	12.8255029999999994	22.4221490000000010	1.9940300000000000
S	11.1943870000000008	25.2352960000000017	1.6784509999999999
S	9.5998629999999991	28.0638320000000014	2.0009410000000001
S	8.0086340000000007	30.8625189999999989	1.5905350000000000
S	29.0668040000000012	-0.1699840000000000	1.8767149999999999
S	27.4320729999999990	2.8298049999999999	2.1352039999999999
S	25.8825679999999991	5.6492680000000002	1.6731650000000000
S	24.2486360000000012	8.5503610000000005	2.0830709999999999
S	22.6319189999999999	11.3285739999999997	1.6748069999999999
S	21.1054710000000014	14.1319700000000008	1.9189529999999999
S	19.3141220000000011	16.8844209999999997	1.7347159999999999
S	17.6278049999999986	19.5523659999999992	1.8917400000000000
S	16.0478799999999993	22.4583469999999998	2.1308099999999999
S	14.4546290000000006	25.2429510000000015	1.7345610000000000
S	12.8083189999999991	28.0795810000000010	2.1474479999999998
S	11.2137539999999998	30.8835550000000012	1.6867310000000000
S	9.5173729999999992	31.8644579999999991	5.1385920000000000
S	8.0088340000000002	34.6795649999999966	4.6898369999999998
S	6.4294430000000000	37.5977779999999981	5.0254589999999997
S	12.7411700000000003	31.8866119999999995	5.2141359999999999
S	11.1853330000000000	34.7087209999999970	4.7849459999999997
S	9.5740649999999992	37.6860619999999997	5.0863199999999997
S	6.4689880000000004	33.7310280000000020	1.8989900000000001
S	4.8067469999999997	36.4892460000000014	1.6675890000000000
S	3.1879249999999999	39.5931709999999981	2.2387049999999999
S	9.6424319999999994	33.7609690000000029	2.0598359999999998
S	8.1065790000000000	36.6178939999999997	1.5969650000000000
S	6.3856270000000004	39.7934199999999976	2.5673219999999999
S	35.2876260000000003	-2.3117489999999998	4.6427310000000004

S	33.788770999999970	1.023552999999999	5.2240830000000003
S	32.1139650000000003	3.8044760000000002	4.9968880000000002
S	30.5796770000000002	6.685788999999998	5.3167890000000000
S	28.979883999999984	9.4793350000000007	4.889548999999997
S	27.4431900000000013	12.3562320000000003	5.240110999999997
S	25.777868999999990	15.161094999999995	4.7451910000000002
S	24.2144030000000008	17.9684260000000009	4.8360750000000001
S	22.605288999999991	20.6185720000000003	4.886123999999997
S	20.854652999999990	23.377372999999986	4.908916999999998
S	19.244036999999987	26.2557280000000013	5.330390999999997
S	17.612628999999983	29.0654730000000008	4.943325999999999
S	38.412495999999973	-2.1619780000000000	4.9945830000000004
S	36.926718999999985	0.9298720000000000	5.5138730000000002
S	35.2773480000000035	3.8083770000000001	5.222357999999998
S	33.777712999999985	6.7023120000000000	5.454521999999999
S	32.095990999999979	9.4943320000000000	5.1509840000000002
S	30.645317999999996	12.3538420000000002	5.346805999999999
S	29.0063350000000000	15.127133999999999	5.1290610000000001
S	27.4463030000000003	17.996090999999998	5.2205700000000004
S	25.8585190000000011	20.7369430000000001	5.225534999999998
S	24.0957410000000003	23.5009550000000011	5.1226770000000004
S	22.4428920000000005	26.301947999999994	5.4144300000000003
S	20.7154300000000013	29.1028190000000002	5.172805999999996
S	32.261775999999976	-0.0822160000000000	1.9694090000000000
S	30.578762999999986	2.8649320000000000	2.200083999999999
S	29.058099999999996	5.660893999999999	1.764062999999999
S	27.458681999999996	8.551945999999992	2.137690999999998
S	25.862107999999992	11.3380880000000008	1.6946470000000000
S	24.2902640000000005	14.163821999999997	2.0301190000000000
S	22.471160999999986	16.908436999999993	1.754621999999999
S	20.8792350000000013	19.674575999999983	1.7311500000000000
S	19.247589999999989	22.4874860000000005	2.192791999999999
S	17.6932890000000000	25.284116999999984	1.791663999999999

S	16.0400320000000001	28.0996430000000004	2.2248700000000001
S	14.4441699999999997	30.8912970000000016	1.7652520000000000
S	35.3783049999999974	0.0812450000000000	2.0758809999999999
S	33.7792790000000025	2.8981650000000001	2.3960059999999999
S	32.2382350000000031	5.7141900000000003	1.8684160000000001
S	30.6588400000000014	8.5773349999999997	2.2312150000000002
S	29.0562709999999988	11.3893749999999994	1.7716980000000000
S	27.5151509999999995	14.2306260000000009	2.1650250000000000
S	25.7984739999999988	17.0269429999999993	2.1050320000000000
S	24.1617539999999984	19.7575369999999992	2.1284339999999999
S	22.5209499999999991	22.5516539999999992	2.2647539999999999
S	20.8902080000000012	25.3475169999999999	1.8453260000000000
S	19.2679590000000012	28.1688760000000009	2.2567580000000000
S	17.6449180000000005	30.9041969999999999	1.8077900000000000
S	16.0070020000000000	31.8994250000000008	5.2329790000000003
S	14.3581959999999995	34.7034000000000020	4.8801300000000003
S	12.6984080000000006	37.7068659999999980	5.1260779999999997
S	19.2109099999999984	31.9847119999999983	5.3486890000000002
S	17.5062530000000010	34.6526130000000023	5.0396039999999998
S	15.8635359999999999	37.6397320000000022	5.1808800000000002
S	12.8237909999999999	33.7541530000000023	2.1601650000000001
S	11.2860209999999999	36.6070100000000025	1.6551240000000000
S	9.6335630000000005	39.7799079999999989	2.4458250000000001
S	15.9982120000000005	33.7342820000000003	2.1803770000000000
S	14.4589009999999991	36.5963270000000023	1.6900029999999999
S	12.8947880000000001	39.7921160000000000	2.4937749999999999
S	41.4174130000000034	-1.8830730000000000	2.9437039999999999
S	40.3337390000000013	1.0198810000000000	4.8615349999999999
S	38.8557440000000014	3.9002479999999999	4.7669269999999999
S	37.4660190000000028	6.7399550000000001	4.5524699999999996
S	35.6525079999999974	9.5692350000000008	4.6770079999999998
S	34.3524069999999995	12.5156080000000003	4.5862259999999999
S	32.4393889999999985	15.1891549999999995	4.6018090000000003

S	31.044375999999997	18.197233000000007	4.3087749999999998
S	29.353826000000015	20.947908999999992	4.3987679999999996
S	27.753980999999996	23.746925000000009	4.3058050000000003
S	26.083103999999987	26.462295000000010	4.5191650000000001
S	24.188769000000006	29.220686000000006	4.7130720000000004
S	38.431035000000014	0.049586000000000	2.0827589999999998
S	37.062832999999977	2.939549000000000	1.976820000000000
S	35.528112999999976	5.721256999999996	2.0962510000000001
S	33.995387999999984	8.557731000000004	2.300200999999999
S	32.344200000000007	11.321528000000007	1.993079000000000
S	30.823508000000004	14.195985000000003	2.1773889999999998
S	29.206467000000000	17.125551000000015	1.7885420000000001
S	27.571139999999998	19.897897000000004	1.705271000000000
S	25.922550999999986	22.625149000000004	1.763317000000000
S	24.206008000000006	25.393177999999989	2.014654999999999
S	22.605230999999999	28.207212999999994	2.2734760000000001
S	20.958846000000012	30.925179000000000	1.963387000000000
S	22.827068000000006	32.162888999999998	4.5584189999999998
S	21.209555999999992	34.895164999999987	4.452105000000004
S	19.492169000000005	37.672780000000030	4.340385000000004
S	19.268398000000012	33.621904999999982	1.924269000000000
S	17.782343999999984	36.385666999999980	1.867802000000000
S	16.289063999999998	39.690224999999981	2.5444239999999998

$\mathbf{W}_{105}\mathbf{S}_{210}$; $E_{tot} = -49\,817\,929.081\,115\,17\text{ eV}$; $E_{rel} = 11.215\,431\,057\,1\text{ meV/f.u.}$

W	19.594957000000008	1.674411000000001	3.2413530000000002
W	18.037655000000009	4.426016999999999	3.3429470000000001
W	16.448980999999999	7.201455000000002	3.400919000000000
W	14.783011000000001	10.030806000000001	3.365451999999999
W	13.183372999999996	12.776289999999995	3.3544890000000001
W	11.653112999999994	15.513749999999999	3.3640460000000001
W	10.110073999999991	18.253009999999997	3.1996989999999998

W	8.2786340000000003	21.3444590000000005	2.9153530000000001
W	6.7201769999999996	24.2665830000000007	3.1510110000000000
W	5.2897429999999996	26.7338279999999990	3.1934909999999999
W	3.7468880000000002	29.2852679999999985	3.3918919999999999
W	6.8314209999999997	29.2769580000000005	3.2591839999999999
W	22.3946089999999991	1.4908650000000001	3.3012549999999998
W	20.8797810000000013	4.1341749999999999	3.3311380000000002
W	19.3347680000000004	6.8533439999999999	3.3591419999999999
W	17.5436550000000011	10.0288160000000008	3.4125429999999999
W	15.9566350000000003	12.6145650000000007	3.3861919999999999
W	14.3882110000000001	15.2647049999999993	3.3556300000000001
W	12.8367550000000001	18.0271280000000012	3.2752050000000001
W	11.4288109999999996	21.3975089999999994	3.1932070000000001
W	9.9567680000000003	23.6627280000000013	3.2961200000000002
W	8.0659369999999999	26.9295510000000000	3.2939029999999998
W	28.9331800000000001	1.4855290000000001	3.3786700000000001
W	26.1970300000000016	1.7608159999999999	3.4994299999999998
W	24.6105690000000017	4.5210809999999997	3.5326100000000000
W	22.9860660000000010	7.3081829999999997	3.5319219999999998
W	21.3729419999999983	10.0605010000000004	3.5076470000000000
W	19.7852500000000013	12.8942259999999997	3.5646230000000001
W	18.1573570000000011	15.6651150000000001	3.5108100000000002
W	16.5950769999999999	18.3475709999999985	3.3587400000000001
W	14.5869250000000008	21.4386049999999990	3.2799489999999998
W	13.0626479999999994	23.6727080000000001	3.3977330000000001
W	11.6063189999999992	27.0839180000000006	3.2917700000000001
W	10.0502000000000002	29.3541029999999985	3.3543859999999999
W	27.3719479999999997	4.2334509999999996	3.3862440000000000
W	25.7461160000000007	7.0060079999999996	3.4042289999999999
W	24.1557050000000011	9.8581199999999995	3.4314019999999998
W	22.6793869999999984	12.4621560000000002	3.4606020000000002
W	20.8574379999999984	15.6089199999999995	3.4590220000000000
W	19.3945490000000014	18.1323819999999998	3.3887550000000002

W	17.712122999999983	21.3955330000000004	3.3444479999999999
W	16.2223180000000013	23.6823699999999988	3.4608880000000002
W	14.7681349999999991	27.1147029999999987	3.3502280000000000
W	13.1882680000000008	29.3756960000000014	3.4111140000000000
W	32.6034340000000000	1.2955650000000001	3.4366819999999998
W	30.9560859999999991	4.7103370000000000	3.4140990000000002
W	29.5612549999999992	7.3667420000000003	3.5725140000000000
W	28.0135579999999997	9.9791030000000003	3.5348679999999999
W	25.7147499999999987	12.4696960000000008	3.4010600000000002
W	24.6940649999999984	15.7244949999999992	3.6028889999999998
W	22.3370579999999990	18.2648299999999999	3.3730690000000001
W	21.2609549999999992	21.4056980000000010	3.4086949999999998
W	19.4809739999999998	23.6710719999999988	3.5211030000000001
W	17.9441109999999995	27.1257850000000005	3.3974210000000000
W	16.3108380000000004	29.3984379999999987	3.4119579999999998
W	34.1840559999999982	4.6512770000000003	3.3378950000000001
W	32.5951349999999991	6.9049810000000003	3.4910169999999998
W	30.7350379999999994	10.1021180000000008	3.5686760000000000
W	29.5040440000000004	12.6641370000000002	3.5255700000000001
W	27.6336280000000016	15.7944890000000004	3.5710109999999999
W	26.1800059999999988	18.3114920000000012	3.5328020000000002
W	24.3191470000000010	21.4475520000000017	3.4403860000000002
W	22.6937800000000003	23.7101840000000017	3.5187719999999998
W	21.1550229999999999	27.1312819999999988	3.4219879999999998
W	19.4508159999999997	29.4047850000000004	3.4389829999999999
W	35.6690809999999985	7.5024319999999998	3.4849880000000000
W	34.5143259999999970	10.0183680000000006	3.4673360000000000
W	32.1855189999999993	12.7798390000000008	3.5603579999999999
W	30.5096319999999999	15.5000499999999999	3.4492370000000001
W	28.9196869999999997	18.2553720000000013	3.4517899999999999
W	27.3226839999999989	20.9536990000000003	3.4113419999999999
W	25.7776190000000014	23.7004249999999992	3.4811690000000000
W	24.3925249999999991	27.1102279999999993	3.4189479999999999

W	22.601939999999990	29.4048130000000008	3.4619439999999999
W	37.174154999999989	10.168587999999997	3.5716130000000001
W	35.948158999999969	12.706711999999996	3.4637090000000001
W	34.3067040000000034	15.9015310000000003	3.5159129999999998
W	32.704523999999993	18.643415999999984	3.5128219999999999
W	31.0673390000000005	21.404607999999996	3.5067349999999999
W	29.352910999999989	24.253181999999989	3.4995690000000002
W	27.620862999999999	26.9070220000000013	3.4590280000000000
W	25.7568470000000005	29.405250999999998	3.4351430000000001
W	38.5659580000000020	12.939645999999998	3.5485989999999998
W	37.017307999999999	15.7953700000000001	3.4742920000000002
W	35.426966999999977	18.4629380000000012	3.4239649999999999
W	33.855246999999985	21.1220810000000014	3.4336720000000001
W	32.286923999999991	23.8163650000000011	3.4411030000000000
W	30.7094710000000006	26.556208999999991	3.4769399999999999
W	28.941494999999997	29.212621999999996	3.4518080000000002
S	20.7940100000000001	0.5312920000000000	4.9786390000000003
S	19.252738999999983	3.2636500000000002	5.0265230000000001
S	17.723701999999994	6.083319999999996	5.0789720000000003
S	16.101967999999994	8.908082999999995	5.0744980000000002
S	14.406667999999998	11.6576880000000003	5.0950240000000004
S	12.812167999999998	14.3925630000000009	5.0967729999999998
S	11.2791610000000002	17.2315150000000017	5.0226620000000004
S	9.6630070000000003	20.189783999999995	4.6173869999999999
S	8.072006999999993	22.966796999999997	4.7276179999999997
S	6.677458999999998	25.7993470000000009	4.9416969999999996
S	5.217863999999996	28.551545999999983	4.9910769999999998
S	24.242907999999999	0.6899300000000000	4.7453770000000004
S	22.6675940000000011	3.4189829999999999	4.7916420000000004
S	21.0762880000000017	6.1563270000000001	4.7972840000000003
S	19.4077510000000011	8.9591820000000002	4.6647319999999999
S	17.8213860000000004	11.8290780000000009	4.8727289999999996
S	16.2312590000000014	14.566395999999992	4.8157310000000004

S	14.628475999999991	17.331959999999987	4.7187830000000002
S	12.957368999999999	20.146803999999995	4.6244839999999998
S	11.4191400000000005	22.997541999999993	5.0271590000000002
S	9.8929220000000004	25.832143999999996	4.5650000000000004
S	8.4142740000000007	28.725567999999991	4.9821869999999997
S	17.471382999999994	2.3306589999999998	2.3585479999999999
S	15.8423920000000003	5.0838690000000000	2.5968059999999999
S	14.2685180000000003	7.8468460000000002	2.6143529999999999
S	12.6509630000000008	10.649402999999995	2.4392049999999998
S	11.055654999999998	13.444777999999995	2.4023379999999999
S	9.424585999999997	16.213291999999991	2.4971869999999998
S	8.049989999999997	19.1741320000000002	2.1700539999999999
S	6.1814910000000003	21.990860999999989	2.3285450000000001
S	4.6746040000000004	24.711500000000009	2.1695679999999999
S	3.1444320000000001	27.455781999999992	2.2331799999999999
S	21.0397220000000011	2.5122650000000002	1.5655180000000000
S	19.4421679999999988	5.2229520000000003	1.6263040000000000
S	17.8375449999999987	8.0904220000000002	1.8115500000000000
S	16.1695470000000014	10.858159999999998	1.6581850000000000
S	14.614896999999991	13.576852999999998	1.6390929999999999
S	13.047439999999999	16.327283999999998	1.6085010000000000
S	11.4854210000000005	19.2581360000000004	1.6712620000000000
S	9.8524650000000005	22.0928600000000017	1.4220370000000000
S	8.3135150000000007	24.9736520000000013	1.7353510000000001
S	6.578231999999999	27.7111300000000007	1.5202860000000000
S	5.0124620000000002	30.6939850000000014	2.2174130000000001
S	27.5112640000000006	0.6780130000000000	5.1846719999999999
S	25.9480359999999983	3.4544100000000002	5.1949529999999999
S	24.3199879999999986	6.2205380000000003	5.2069219999999996
S	22.6878059999999984	8.9676189999999991	5.1998259999999998
S	21.0938650000000010	11.7706000000000000	5.1970859999999997
S	19.4910430000000012	14.5879630000000002	5.2104330000000001
S	17.8447490000000002	17.4080200000000005	5.1485300000000001

S	16.1925080000000001	20.2299439999999997	4.8346590000000003
S	14.6142769999999995	23.0447009999999999	5.1146710000000004
S	13.0949010000000001	25.8506539999999987	4.6968180000000004
S	11.5884309999999999	28.7679720000000003	5.0890779999999998
S	30.7583370000000009	0.6557110000000000	4.8541030000000003
S	29.2721620000000016	3.5022780000000000	4.8028079999999997
S	27.6580620000000010	6.2500819999999999	4.7719430000000003
S	26.0572440000000007	9.0030750000000008	4.7988140000000001
S	24.2991260000000011	11.6972410000000000	5.1203870000000000
S	22.7638250000000006	14.6127859999999998	4.7440030000000002
S	21.0022950000000002	17.4070670000000014	5.1245139999999996
S	19.4583259999999996	20.2420180000000016	4.6686139999999998
S	17.8494980000000005	23.0256240000000005	5.1344900000000004
S	16.2819399999999987	25.8630010000000006	4.7544670000000000
S	14.7409800000000004	28.8554320000000004	5.1288530000000003
S	24.2953149999999987	2.5427279999999999	2.0908509999999998
S	22.7021300000000004	5.2752610000000004	2.1220289999999999
S	21.1065760000000004	8.0386699999999998	2.0796039999999998
S	19.4654680000000013	10.9045059999999996	2.1212249999999999
S	17.8639609999999998	13.6306200000000004	2.1468720000000001
S	16.2421979999999984	16.3639459999999985	2.0675560000000002
S	14.6758050000000004	19.2185069999999989	2.0471330000000001
S	13.0362650000000002	22.0610630000000008	1.5593649999999999
S	11.5036769999999997	24.9349640000000008	1.9172940000000001
S	9.8638580000000005	27.7385060000000010	1.7229200000000000
S	8.2757629999999995	30.8435319999999997	2.4088579999999999
S	27.6389040000000001	2.5703130000000001	1.6876500000000001
S	26.0205969999999986	5.3180449999999997	1.7237549999999999
S	24.3909570000000002	8.0890269999999997	1.7582480000000000
S	22.7877960000000002	10.8462309999999995	1.6962470000000001
S	21.1975850000000001	13.7057380000000002	1.9053730000000000
S	19.5025219999999990	16.4509030000000003	1.6574370000000000
S	17.9427030000000016	19.3278560000000006	1.7839039999999999

S	16.209040999999991	22.062888000000009	1.617806000000001
S	14.696042999999995	24.964064000000005	2.035355000000000
S	13.160005000000000	27.800648999999999	1.628718000000001
S	11.501516999999998	31.001101999999995	2.666506000000000
S	32.640056000000013	3.412739000000002	4.758619999999996
S	31.017426000000004	6.287181999999996	5.209514000000004
S	29.375036000000015	9.045921999999991	5.271219000000003
S	27.602965999999986	11.822952000000008	4.962595999999996
S	26.023855000000011	14.540611999999994	5.029444999999999
S	24.284911999999985	17.517302000000008	4.966803999999998
S	22.675381000000016	20.231107999999990	4.914505000000001
S	21.089517000000007	23.056039999999994	5.187439000000004
S	19.495884000000002	25.878029999999990	4.779501999999999
S	17.877673000000015	28.886202999999983	5.150401999999997
S	34.362710999999973	6.285413000000001	5.104158000000000
S	32.644832000000010	9.056331000000001	4.770628000000003
S	30.912413000000008	11.812037000000001	5.307863000000002
S	29.153980000000007	14.579596999999997	5.107032000000002
S	27.586324000000012	17.462731000000016	5.312678000000000
S	25.843455999999998	20.230146999999988	5.053193000000003
S	24.294142999999983	23.091135999999988	5.229942999999996
S	22.713090999999986	25.886821999999987	4.798477000000001
S	21.037639999999997	28.875826000000000	5.171824000000000
S	30.880542999999994	2.534743999999999	2.145651000000000
S	29.253123999999997	5.406898000000000	2.007115000000002
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S	26.049371000000007	10.725450999999996	1.990027000000000
S	24.336148000000014	13.721196000000008	2.045065000000001
S	22.772352000000015	16.425088999999998	2.048331000000001
S	21.012779999999993	19.347947000000013	1.876679999999999
S	19.496562999999983	22.084969000000010	1.794014000000000
S	17.914291999999997	24.947213999999989	2.125287999999998
S	16.346720000000012	27.772048000000016	1.677646000000000

S	14.727750000000003	30.9509429999999988	2.5047419999999998
S	34.182594999999992	2.5054270000000001	1.9399329999999999
S	32.6022219999999976	5.2582399999999998	1.7100599999999999
S	31.0511200000000009	8.2007169999999991	1.9734929999999999
S	29.3117939999999990	10.9687239999999999	1.7949150000000000
S	27.5773140000000012	13.6604379999999992	2.2861080000000000
S	26.0379509999999996	16.5239760000000011	1.8487180000000001
S	24.2902880000000003	19.2727070000000005	2.2199420000000001
S	22.7696320000000014	22.1028570000000002	1.6984969999999999
S	21.1172980000000017	24.9606880000000011	2.1291989999999998
S	19.5361089999999997	27.7702920000000013	1.7184170000000001
S	17.9412799999999990	30.9696479999999994	2.5402209999999998
S	35.9388569999999987	9.0738819999999993	5.2585459999999999
S	34.1506570000000025	11.9200450000000000	4.9429480000000003
S	32.4776620000000023	14.7944370000000003	4.8638539999999999
S	30.8443369999999994	17.5111759999999990	4.8195280000000000
S	29.1948019999999993	20.3145479999999985	4.8279139999999998
S	27.6020450000000004	23.0564689999999999	4.8542949999999996
S	25.9118770000000005	25.8318370000000002	4.8461540000000003
S	24.2249650000000010	28.8482699999999994	5.1689369999999997
S	37.4146879999999982	11.8600630000000002	5.2741850000000001
S	35.7489780000000010	14.7263070000000003	5.0644039999999997
S	34.1042109999999994	17.6049539999999993	5.2095149999999997
S	32.4474930000000015	20.3488299999999995	5.1961440000000003
S	30.8199070000000006	23.1509250000000009	5.1538620000000002
S	29.1820929999999983	25.9788780000000017	5.1444359999999998
S	27.3818319999999993	28.7502330000000015	5.1353299999999997
S	36.1214340000000007	5.3729500000000003	2.3353750000000000
S	34.1644209999999973	8.1672419999999999	1.8994110000000000
S	32.6026840000000036	10.9682510000000004	2.1065520000000002
S	30.8499349999999986	13.7555320000000005	1.8213010000000001
S	29.1652769999999997	16.5101170000000010	1.7896749999999999
S	27.5484900000000010	19.3013800000000018	1.7505919999999999

S	25.945060000000016	22.069507999999990	1.7499130000000001
S	24.315979999999997	24.983181999999993	2.0869680000000002
S	22.7490330000000007	27.785889999999984	1.7417810000000000
S	21.1550790000000006	30.9870130000000010	2.5969560000000000
S	37.817163999999982	8.066943999999994	2.6618810000000002
S	35.883204999999967	11.019653999999992	1.7568630000000001
S	34.094597999999977	13.806096999999994	2.2291680000000000
S	32.4281560000000013	16.587970999999996	2.1559750000000002
S	30.7967030000000008	19.346364999999987	2.1519520000000001
S	29.181145999999983	22.1411580000000008	2.1727799999999999
S	27.5234290000000001	24.885346999999994	2.0583640000000001
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S	24.395842999999993	31.0325670000000002	2.6803759999999999
S	39.2895120000000020	14.8696120000000001	4.4104239999999999
S	37.696886999999967	17.807296999999984	4.2476380000000002
S	35.9991160000000008	20.5701520000000002	4.3535469999999998
S	34.388838999999973	23.360486999999991	4.2980660000000004
S	32.8073610000000002	26.1836020000000005	4.2095390000000004
S	30.963951999999990	29.023682999999983	4.3541930000000004
S	39.437274999999996	11.0556520000000003	2.7116039999999999
S	37.3325000000000031	13.9795820000000006	1.8419449999999999
S	35.7648310000000009	16.7888920000000006	1.7259249999999999
S	34.172001999999991	19.5105660000000007	1.7087909999999999
S	32.5725120000000032	22.206206999999991	1.7230470000000000
S	30.9571390000000015	24.9372420000000012	1.7543210000000000
S	29.322209999999983	27.6248830000000005	1.7752310000000000
S	27.7677380000000014	30.854064999999985	2.5278040000000002
W	26.0337360000000011	-9.180021999999992	3.0623950000000000
W	22.7880320000000012	-3.7675320000000001	3.2745700000000002
W	24.4049680000000002	-6.467469999999996	3.2284739999999998
W	27.423328999999990	-6.950022999999998	3.1607210000000001
W	25.5376210000000015	-3.915652999999998	3.2290239999999999
W	29.2846580000000003	-3.6848500000000000	3.3254779999999999

W	21.1810830000000010	-1.0654060000000001	3.2246049999999999
W	23.9336869999999990	-1.1924310000000000	3.2784650000000002
W	27.7443239999999989	-0.9670500000000000	3.4552390000000002
W	30.6155900000000010	-1.3255230000000000	3.3334540000000001
S	25.7110680000000009	-11.4147099999999995	1.9199269999999999
S	23.9664999999999999	-8.6620749999999997	2.1748159999999999
S	27.5180469999999993	-8.5598559999999999	1.3351219999999999
S	22.2382090000000012	-5.9921550000000003	2.5002589999999998
S	25.8829950000000011	-5.7289209999999997	1.6229789999999999
S	29.0633499999999998	-5.7227560000000004	1.6665200000000000
S	20.6597469999999994	-3.1976110000000002	2.3200440000000002
S	24.1740460000000006	-2.9336820000000001	1.5427080000000000
S	27.4963569999999997	-2.9248259999999999	1.9195009999999999
S	30.7974029999999992	-2.9874630000000000	1.5317590000000001
S	25.7153039999999997	-7.6025419999999997	4.8512219999999999
S	24.0805140000000009	-4.8557490000000003	4.9726939999999997
S	27.4441169999999985	-4.8638399999999997	4.5216079999999996
S	22.6115870000000001	-0.1949620000000000	1.5506300000000000
S	25.8719639999999984	-0.2015940000000000	2.0407459999999999
S	29.2042539999999988	-0.2036240000000000	1.6999880000000001
S	32.4060619999999986	-0.3441180000000000	1.7349209999999999
S	22.3935350000000000	-2.1618930000000001	4.9829689999999998
S	25.8165949999999995	-2.0581839999999998	4.6917350000000004
S	29.1077610000000000	-2.1230220000000002	5.0738620000000001
S	19.0320239999999998	-0.4507940000000000	2.3441640000000001
W	29.0089749999999995	-9.2602530000000005	2.9732680000000000
W	27.5709400000000002	-11.8559079999999994	3.0686770000000001
W	30.4503950000000003	-6.8266929999999997	3.0425710000000001
S	27.5773499999999991	-13.8401999999999994	3.8693439999999999
S	27.4740499999999983	-10.2855580000000000	4.7394119999999997
S	29.4495509999999996	-11.4259959999999996	1.9081010000000000
S	29.0938249999999989	-7.6479689999999998	4.7862510000000000
S	31.1024640000000012	-8.7666550000000001	1.9967210000000000

S	30.8718040000000009	-5.0278359999999997	4.6483290000000004
W	32.3180839999999989	-3.7831120000000000	3.0642900000000002
S	32.6717299999999966	-6.0420749999999996	2.4435500000000001
S	32.3253130000000013	-2.2775240000000001	4.9013629999999999
W	33.7870909999999967	-1.2090930000000000	3.3621219999999998
S	34.4473989999999972	-3.3168440000000001	2.3473850000000001
S	33.9632580000000033	0.3314470000000000	5.2305970000000004
W	35.2801850000000030	1.3768510000000000	3.6388520000000000
S	36.0866650000000035	-0.5454900000000000	2.7333479999999999
S	36.1801829999999995	3.1384129999999999	4.6394719999999996
S	2.0586169999999999	30.2589509999999997	4.2747010000000003

$W_{105}S_{210}$; $E_{tot} = -49\,817\,929.241\,150\,29$ eV; $E_{rel} = 9.691\,287\,057\,1$ meV/f.u.

W	21.0117130000000003	-0.6420100000000000	3.2997619999999999
W	19.3752059999999986	2.0302039999999999	3.2440600000000002
W	17.7312240000000010	4.7787810000000004	3.2448210000000000
W	16.0809040000000003	7.6225849999999999	3.3162289999999999
W	14.4840210000000003	10.4016140000000004	3.3551839999999999
W	12.8859060000000003	13.1420290000000008	3.3517310000000000
W	11.3174569999999992	15.8842169999999996	3.3785479999999999
W	9.8053380000000008	18.6304529999999993	3.3927990000000001
W	8.2976749999999999	21.3858449999999998	3.2455669999999999
W	6.4973609999999997	24.4173240000000007	2.9046620000000001
W	4.8926829999999999	27.4256959999999985	3.0566990000000001
W	3.4922589999999998	29.8982689999999991	3.0116719999999999
W	1.9648399999999999	32.4549919999999972	3.0983070000000001
W	23.7620560000000012	-0.7832310000000000	3.2672080000000001
W	22.1544470000000011	1.9077310000000001	3.2997230000000002
W	20.6064079999999983	4.5312510000000001	3.3126169999999999
W	19.0588009999999990	7.1989140000000003	3.3341390000000000
W	17.2833010000000016	10.1637079999999997	3.3329749999999998
W	15.6539880000000000	12.9369409999999991	3.3511479999999998

W	14.069333999999996	15.6627170000000007	3.3657370000000002
W	12.5135780000000008	18.3884709999999991	3.3715649999999999
W	11.0210430000000006	21.1522889999999997	3.3277040000000002
W	9.6023940000000003	24.5251149999999996	3.2210179999999999
W	8.1697819999999997	26.8071790000000014	3.2855200000000000
W	6.2793850000000004	30.0772410000000008	3.1832790000000002
W	5.0520569999999996	32.4218959999999967	3.0722619999999998
W	27.5694510000000008	-0.5191780000000000	3.4262779999999999
W	28.7246859999999984	2.1240329999999998	3.3918379999999999
W	25.9990810000000003	2.1486850000000000	3.4745339999999998
W	24.3619540000000008	4.8983829999999999	3.5316709999999998
W	22.6882130000000011	7.6976789999999999	3.5379000000000000
W	21.0505910000000007	10.4580120000000001	3.4982989999999998
W	19.4636509999999987	13.2270400000000006	3.5015090000000000
W	17.8826430000000016	15.9765210000000000	3.5056259999999999
W	16.3271610000000003	18.7040970000000009	3.5107610000000000
W	14.7879939999999994	21.4254479999999994	3.4347639999999999
W	12.8021870000000000	24.5335129999999992	3.3230610000000000
W	11.3006069999999994	26.7832849999999993	3.4243199999999998
W	9.8087070000000001	30.2022469999999998	3.2488649999999999
W	8.2616329999999998	32.4748030000000014	3.2457750000000001
W	30.5462689999999988	-1.0151710000000000	3.3741870000000000
W	27.1598889999999997	4.6817669999999998	3.4003060000000001
W	25.4079489999999986	7.5246350000000000	3.4162390000000000
W	23.7915260000000011	10.2765579999999996	3.4193760000000002
W	22.2084609999999998	13.0051009999999998	3.4179110000000001
W	20.6418229999999987	15.7275559999999999	3.4188269999999998
W	19.0879200000000004	18.4353419999999986	3.4092950000000002
W	17.5500919999999994	21.1466549999999991	3.3916810000000002
W	15.9437940000000005	24.4366489999999992	3.4032860000000000
W	14.4501980000000003	26.7553710000000002	3.5018419999999999
W	12.9501340000000003	30.2143140000000017	3.3321619999999998
W	11.3892260000000007	32.4815169999999966	3.3458049999999999

W	33.7438860000000034	-0.5121430000000000	3.4751180000000002
W	35.2740859999999969	2.1272940000000000	3.5494520000000001
W	32.5532129999999995	1.9165200000000000	3.4077530000000000
W	30.2355909999999994	4.8595100000000002	3.4379219999999999
W	29.1747750000000003	7.8252210000000000	3.5139330000000002
W	27.6280390000000011	10.5525070000000003	3.5819850000000000
W	26.0337250000000004	13.3123280000000008	3.6178629999999998
W	24.4336589999999987	16.0802760000000013	3.6247889999999998
W	22.8314629999999994	18.8484130000000007	3.6183269999999998
W	21.2199090000000012	21.6117449999999991	3.5942159999999999
W	19.6268239999999992	24.3230170000000001	3.5159140000000000
W	17.6017779999999995	26.7352980000000002	3.5170889999999999
W	16.0803189999999994	30.2106859999999990	3.3868239999999998
W	14.4914210000000008	32.4889190000000028	3.3729480000000001
W	34.1236379999999997	4.6636499999999996	3.4423940000000002
W	31.8986710000000002	7.6637069999999996	3.4426709999999998
W	30.3690280000000001	10.3233999999999995	3.4466869999999998
W	28.7915880000000008	13.0451589999999999	3.4775299999999998
W	27.1845280000000002	15.8154939999999993	3.4907149999999998
W	25.5736789999999985	18.5965880000000006	3.4868410000000001
W	23.9609020000000008	21.3703849999999989	3.4690259999999999
W	22.3771370000000012	24.1009050000000009	3.4500240000000000
W	20.8430210000000002	26.7736580000000011	3.4590820000000000
W	19.2568230000000007	30.1907439999999987	3.4142100000000002
W	17.5955300000000001	32.4693469999999991	3.4372630000000002
W	36.7997500000000031	4.7781079999999996	3.5000270000000002
W	35.6342420000000004	7.7154509999999998	3.5080819999999999
W	34.2109859999999983	10.3766630000000006	3.5172479999999999
W	32.5768380000000022	13.3786369999999994	3.5704449999999999
W	30.9599769999999985	16.1977200000000003	3.5855790000000001
W	29.3693379999999991	18.9520529999999994	3.5944410000000002
W	27.7913430000000012	21.6773470000000010	3.5920939999999999
W	26.1805160000000008	24.4050550000000008	3.5753800000000000

W	24.1755980000000008	27.4450530000000015	3.4660449999999998
W	22.7138199999999983	29.9838139999999989	3.4755370000000001
W	20.7144520000000014	32.4650990000000021	3.4525060000000001
W	38.2713480000000033	7.6112289999999998	3.4974560000000001
W	36.8837460000000021	10.4520420000000005	3.5204620000000002
W	35.3013300000000001	13.2576800000000006	3.5201180000000001
W	33.7078559999999996	15.9905179999999998	3.5377909999999999
W	32.1380849999999967	18.7209879999999984	3.5805889999999998
W	30.5629670000000004	21.4418340000000001	3.5906380000000002
W	28.9808239999999984	24.1455920000000006	3.5546700000000002
W	27.3994460000000011	26.8717059999999996	3.5482600000000000
W	25.6888189999999987	29.7028059999999989	3.5486339999999998
W	23.9315190000000015	32.3283890000000014	3.5004379999999999
S	22.2958280000000002	-1.7452049999999999	5.0017829999999996
S	20.5954179999999987	0.9446440000000000	5.0103309999999999
S	18.9649940000000008	3.6421410000000001	4.9813520000000002
S	17.3706910000000008	6.4255160000000000	4.9790809999999999
S	15.7566380000000006	9.2444819999999996	5.0497139999999998
S	14.1220580000000009	12.0117440000000002	5.0789020000000002
S	12.5230210000000000	14.7415230000000008	5.0982599999999998
S	10.9754039999999993	17.5002129999999987	5.1213460000000000
S	9.4510489999999994	20.3471690000000009	5.0639110000000001
S	7.8533499999999998	23.3294330000000016	4.6559520000000001
S	6.2361990000000000	26.1216889999999999	4.6537249999999997
S	4.8352649999999997	28.9895169999999993	4.8140080000000003
S	25.6907139999999998	-1.7420990000000001	4.5378470000000002
S	24.0559429999999992	1.0838019999999999	4.7351880000000000
S	22.4079860000000011	3.8146320000000000	4.7860709999999997
S	20.7849420000000009	6.5322740000000001	4.7977920000000003
S	19.1242720000000013	9.2953119999999991	4.6693590000000000
S	17.5332000000000008	12.1095150000000000	4.7304250000000003
S	15.9483099999999993	14.8812169999999995	4.7636900000000004
S	14.3723919999999996	17.6477639999999987	4.7796789999999998

S	12.8000670000000003	20.4341900000000010	4.7683580000000001
S	11.1432819999999992	23.2735050000000001	4.6610279999999999
S	9.6059249999999992	26.1463530000000013	5.0335310000000000
S	8.0715769999999996	28.9848129999999991	4.5246180000000003
S	18.9071180000000005	-0.1404590000000000	2.3265579999999999
S	17.2522969999999987	2.5971549999999999	2.3552499999999998
S	15.6204459999999994	5.3972519999999999	2.4380359999999999
S	13.9679289999999998	8.1702429999999993	2.5107080000000002
S	12.3787149999999997	10.9781820000000003	2.4267110000000001
S	10.7516680000000004	13.7608320000000006	2.4507720000000002
S	9.1716029999999993	16.5682049999999990	2.4596369999999999
S	7.5861260000000001	19.3651620000000015	2.5293269999999999
S	6.1791630000000000	22.2713539999999988	2.2243610000000000
S	4.4012560000000001	25.1288960000000010	2.3187389999999999
S	2.8817810000000001	27.8504970000000007	2.0176729999999998
S	1.3866620000000001	30.6048149999999985	1.9594879999999999
S	22.4095089999999999	0.1886180000000000	1.5630630000000001
S	20.8003800000000005	2.8895320000000000	1.5595129999999999
S	19.1797849999999990	5.5820090000000002	1.5825130000000001
S	17.5527090000000001	8.3720529999999993	1.6977979999999999
S	15.9000350000000008	11.1957699999999996	1.6460920000000001
S	14.3143069999999994	13.9684980000000003	1.6434299999999999
S	12.7336860000000005	16.7159440000000004	1.6526850000000000
S	11.1845879999999998	19.4764780000000002	1.6358470000000001
S	9.6762650000000008	22.3913569999999993	1.7170420000000000
S	8.0560030000000005	25.2090169999999993	1.4233330000000000
S	6.5309869999999997	28.0846300000000006	1.6713270000000000
S	4.8405870000000002	30.8242459999999987	1.3575560000000000
S	3.3797050000000000	31.7509259999999998	4.7640130000000003
S	6.5856310000000002	31.8998890000000017	4.8503020000000001
S	0.2548620000000000	33.4617440000000030	3.8982019999999999
S	3.2773800000000000	33.8267260000000007	1.9331330000000000
S	28.9330959999999990	-1.8929469999999999	4.8899200000000000

S	27.3831230000000012	1.0657479999999999	5.1497960000000003
S	25.6967339999999993	3.8462170000000002	5.1799700000000000
S	24.0347779999999993	6.6069449999999996	5.2038820000000001
S	22.3720140000000001	9.3810690000000001	5.2027590000000004
S	20.7631779999999999	12.1246670000000005	5.1931099999999999
S	19.1808860000000010	14.8887450000000001	5.2032819999999997
S	17.6152389999999990	17.6456739999999996	5.2116550000000004
S	16.0556500000000000	20.4360229999999987	5.1844089999999996
S	14.3873259999999998	23.3082929999999990	4.8940109999999999
S	12.8189229999999998	26.1464490000000005	5.1551020000000003
S	11.2889049999999997	28.9786280000000005	4.7013579999999999
S	32.2465199999999967	-1.6241950000000001	5.0703360000000002
S	30.5980249999999998	1.0773940000000000	4.6692929999999997
S	28.8481950000000005	3.8942969999999999	5.0808039999999997
S	27.3231320000000011	6.7047530000000002	4.7710319999999999
S	25.7077120000000008	9.4660799999999998	4.8176459999999999
S	24.1051049999999982	12.2174610000000001	4.8501360000000000
S	22.5188559999999995	14.9740190000000002	4.8616299999999999
S	20.9277729999999984	17.7330159999999992	4.8638009999999996
S	19.3362610000000004	20.4829159999999995	4.8565670000000001
S	17.6943979999999996	23.2728539999999988	4.7055290000000003
S	16.0479459999999996	26.0833520000000014	5.1849020000000001
S	14.4724540000000008	28.9653969999999994	4.7736349999999996
S	25.7258129999999987	0.2085810000000000	1.9982690000000001
S	24.0718299999999985	2.9448010000000000	2.0801620000000001
S	22.4390959999999993	5.6677359999999997	2.1281650000000001
S	20.8115519999999989	8.4053260000000005	2.0874579999999998
S	19.1683780000000006	11.2018330000000006	2.0750560000000000
S	17.5546660000000010	13.9670389999999998	2.0908419999999999
S	15.9681560000000005	16.7241940000000007	2.0991100000000000
S	14.3959770000000002	19.4800560000000011	2.1118630000000000
S	12.8696050000000000	22.3224240000000016	2.0997319999999999
S	11.2493090000000002	25.1603479999999990	1.6035930000000000

S	9.7268190000000008	28.0329249999999988	1.9179809999999999
S	8.1045119999999997	30.8368609999999990	1.6321660000000000
S	29.0654879999999984	0.2497570000000000	1.8043169999999999
S	27.3674940000000007	3.0270920000000001	1.6499960000000000
S	25.7114800000000017	5.7673839999999998	1.7736460000000001
S	24.0684930000000001	8.5457330000000002	1.7340070000000001
S	22.4723919999999993	11.3042149999999992	1.7161160000000000
S	20.8913769999999985	14.0487549999999999	1.7108650000000001
S	19.3165629999999986	16.7781500000000001	1.7055860000000000
S	17.7401920000000004	19.5076929999999997	1.6893640000000001
S	16.1410580000000010	22.3867590000000014	1.8192200000000001
S	14.4413579999999993	25.1362610000000011	1.6694040000000001
S	12.9098670000000002	28.0472029999999997	2.0550739999999998
S	11.3786000000000005	30.8790650000000007	1.5811050000000000
S	9.7677700000000005	31.9115900000000003	5.0179919999999996
S	12.9139590000000002	31.9851099999999988	5.0899450000000002
S	6.5240549999999997	33.9688299999999970	2.2353540000000001
S	9.7295409999999993	34.1057059999999979	2.5508139999999999
S	33.9528219999999976	1.0665240000000000	5.2298030000000004
S	32.1919990000000027	3.8737740000000001	4.7858460000000003
S	30.5451809999999995	6.6257359999999998	5.1141139999999998
S	28.9700820000000014	9.4565269999999995	5.2509930000000002
S	27.3686439999999997	12.2246480000000002	5.2864509999999996
S	25.7667199999999994	15.0007789999999996	5.3027970000000000
S	24.1645299999999992	17.7763409999999986	5.3015930000000004
S	22.5565080000000009	20.5515059999999998	5.2842200000000004
S	20.9283360000000016	23.3253130000000013	5.2534470000000004
S	19.2826069999999987	26.1032100000000007	5.1497909999999996
S	17.6611720000000005	28.9553559999999983	4.7888599999999997
S	35.5306629999999970	3.7798159999999998	5.2473520000000002
S	33.7903659999999988	6.6736740000000001	4.7992970000000001
S	32.2918340000000015	9.4948549999999994	4.8800860000000004
S	30.7139840000000000	12.2818159999999992	4.8758450000000000

S	29.1043619999999983	15.0699079999999999	4.8671410000000002
S	27.4948790000000010	17.8479519999999994	4.8645870000000002
S	25.8870970000000007	20.6233760000000004	4.8583160000000003
S	24.2663839999999986	23.3932499999999983	4.8735759999999999
S	22.6121459999999992	26.1703329999999994	4.9148550000000002
S	20.8843850000000018	28.9260939999999991	4.7642559999999996
S	32.2667140000000003	0.1138460000000000	1.8207199999999999
S	30.6747629999999987	2.9580240000000000	2.0641799999999999
S	28.8577529999999989	5.8440320000000003	1.8965500000000000
S	27.3002180000000010	8.5875380000000003	2.1110329999999999
S	25.7135520000000000	11.3292149999999996	2.1903670000000002
S	24.1293930000000003	14.0777750000000008	2.2135600000000002
S	22.5452119999999994	16.8266939999999998	2.2110680000000000
S	20.9567000000000014	19.5751840000000001	2.1900949999999999
S	19.3700800000000015	22.3256090000000000	2.1027269999999998
S	17.7566190000000006	25.0883949999999984	1.8906650000000000
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S	14.5364950000000004	30.8458700000000015	1.6427200000000000
S	35.8794260000000023	-0.0968790000000000	2.7343050000000000
S	33.9557080000000013	2.9373649999999998	1.7325170000000001
S	32.2407210000000006	5.7055239999999996	2.1161110000000001
S	30.6154879999999991	8.6295979999999997	1.7175940000000001
S	29.0560639999999992	11.3782440000000005	1.7683979999999999
S	27.4579759999999986	14.1286660000000008	1.8079050000000001
S	25.8559610000000006	16.9000580000000014	1.8150120000000001
S	24.2519179999999999	19.6732289999999992	1.8036520000000000
S	22.6513740000000006	22.4370420000000017	1.7726139999999999
S	21.0518099999999997	25.1746699999999990	1.7298970000000000
S	19.2794920000000012	28.0215670000000010	2.1225600000000000
S	17.7047500000000007	30.8453260000000000	1.6970550000000000
S	16.0257269999999998	31.9795820000000006	5.1387270000000003
S	19.1738029999999995	31.9136440000000015	5.1758730000000002
S	12.9405339999999995	34.0325589999999991	2.4099629999999999

S	16.1475960000000001	34.0371329999999972	2.4764290000000000
S	37.0542810000000031	6.5284529999999998	5.1824560000000002
S	35.6015900000000016	9.4567289999999993	5.2145729999999997
S	33.9919429999999991	12.2619100000000003	5.1704829999999999
S	32.3411019999999994	15.0999490000000005	5.2567769999999996
S	30.7200600000000001	17.8756489999999992	5.2948979999999999
S	29.1176250000000003	20.6363410000000016	5.3080480000000003
S	27.5271019999999993	23.4083630000000014	5.2912020000000002
S	25.8244240000000005	26.2613759999999985	5.1006090000000004
S	24.1618290000000009	29.0794789999999992	5.2039840000000002
S	39.1565769999999986	9.4599309999999992	4.3597710000000003
S	37.5736390000000000	12.4667580000000005	4.3043370000000003
S	35.9468770000000006	15.2958689999999997	4.3468760000000000
S	34.3082589999999996	18.0735869999999998	4.4492599999999998
S	32.6945350000000019	20.8560499999999998	4.4989410000000003
S	31.0711559999999984	23.6367380000000011	4.5019169999999997
S	29.4769439999999996	26.4511560000000010	4.3610329999999999
S	27.7583750000000009	29.2484760000000001	4.3526889999999998
S	37.5078329999999980	2.7472099999999999	2.7193700000000001
S	35.5263929999999988	5.8062870000000002	1.8586879999999999
S	33.8488490000000013	8.5618599999999994	2.0319400000000001
S	32.3094480000000033	11.3811599999999995	2.2263160000000002
S	30.6940029999999986	14.1664069999999995	2.2370600000000000
S	29.0850079999999984	16.9377609999999983	2.2152040000000000
S	27.4864509999999989	19.7022869999999983	2.2019310000000001
S	25.8853049999999989	22.4655139999999989	2.2016030000000000
S	24.2743310000000001	25.2707310000000014	2.2646549999999999
S	22.5234270000000016	28.0437219999999989	1.9528900000000000
S	20.9790199999999984	30.8365679999999998	1.8361270000000001
S	39.0512069999999980	5.7302910000000002	2.5805920000000002
S	37.1248500000000021	8.7372069999999997	1.7975449999999999
S	35.5983480000000014	11.5312950000000001	1.8373960000000000
S	34.0428619999999995	14.3388059999999999	1.8202590000000001

S	32.478760000000012	17.109024999999990	1.836989999999999
S	30.926075999999983	19.840205999999985	1.855142000000001
S	29.348252999999997	22.543806000000000	1.843652000000001
S	27.721125000000007	25.268238000000002	1.832175000000001
S	25.981401000000017	28.008638999999987	1.906347000000000
S	24.371351000000007	30.787632999999996	1.797051000000000
S	22.346538999999999	31.809536000000014	5.145775000000004
S	25.979881999999999	32.158864999999987	4.357491999999997
S	19.360227999999993	34.101860999999995	2.693258000000002
S	22.711317999999986	33.931924999999997	2.555613999999998
W	22.641383000000011	-3.322365000000000	3.236329000000000
S	22.203917000000006	-5.539176999999996	2.186167999999999
S	20.487607000000006	-2.900981999999999	2.525914000000002
S	24.154081000000015	-2.587219999999999	1.677222000000000
S	24.004301000000017	-4.491576000000002	4.809643000000003
W	24.294992000000006	-6.054619999999999	2.986838999999998
W	25.779360000000005	-3.823290000000001	3.190633000000001
S	23.917260999999999	-8.236126999999998	1.795474000000000
S	25.766612999999995	-5.370732000000003	1.302630000000000
S	25.646062000000006	-7.216313000000004	4.694372000000004
S	27.329070000000015	-2.515359999999998	1.763952000000000
S	27.414861999999994	-4.645418000000003	4.800271000000004
W	25.716287000000012	-8.758732999999994	3.005710000000001
W	27.240982999999999	-6.129369999999998	2.941117000000002
W	28.796345999999998	-3.638723000000002	3.119068000000000
S	25.612666999999983	-10.757996000000003	3.761807999999998
S	27.636828000000013	-8.354146000000001	1.924501999999999
S	29.106964999999989	-5.543527000000001	1.731579999999999
S	30.605474999999984	-2.711444000000002	1.637453000000000
W	32.066301000000028	-3.220187999999998	3.373586000000000
S	31.020589999999986	-4.906845999999998	4.311271999999998
S	34.154989999999980	-2.933545000000001	2.643635999999999

$W_{105}S_{210}$; $E_{tot}=-49\,817\,929.493\,715\,67\text{ eV}$; $E_{rel}=7.285\,902\,485\,7\text{ meV/f.u.}$

W	21.1119960000000013	-0.5663250000000000	3.4467420000000000
W	19.3599029999999992	2.0617749999999999	3.4231360000000000
W	17.6627599999999987	4.9032910000000003	3.4403890000000001
W	16.0975579999999994	7.6455650000000004	3.4476010000000001
W	14.5471009999999996	10.3601690000000008	3.4148420000000002
W	13.0332629999999998	13.0816239999999997	3.3979080000000002
W	11.5174070000000004	15.8109330000000003	3.2793040000000002
W	9.8345099999999999	18.6942309999999985	2.9393359999999999
W	8.2433999999999994	21.8786120000000004	3.0358230000000002
W	6.8414609999999998	24.3750679999999988	3.0306320000000002
W	5.3028769999999996	26.8781859999999995	3.1226240000000001
W	24.3464139999999993	-0.6987040000000000	3.4348320000000001
W	22.3146799999999992	1.7747970000000000	3.4487269999999999
W	20.8570810000000009	4.3158190000000003	3.4748960000000002
W	18.8880629999999989	7.3750390000000001	3.4038469999999998
W	17.3001490000000011	10.1160350000000001	3.4021029999999999
W	15.7534360000000007	12.8459420000000009	3.3783910000000001
W	14.2306130000000000	15.5988299999999995	3.3193429999999999
W	12.6919930000000001	18.8726550000000017	3.2807640000000000
W	11.5039770000000008	21.2636609999999990	3.2715079999999999
W	9.7303239999999995	24.5481489999999987	3.1739370000000000
W	8.3918850000000003	26.8517340000000004	3.0777860000000001
W	27.4507539999999999	-0.6993290000000000	3.3805170000000002
W	28.9787029999999994	1.5545819999999999	3.4738039999999999
W	25.8309330000000017	1.5603469999999999	3.4705819999999998
W	24.1958510000000011	4.9667219999999999	3.4769040000000002
W	22.6820149999999998	7.6447550000000000	3.5028500000000000
W	21.1225479999999983	10.3962289999999999	3.5109130000000000
W	19.5156540000000014	13.2064319999999995	3.5008930000000000
W	17.9221380000000003	16.0255130000000001	3.4650789999999998
W	16.3693290000000005	18.7474929999999986	3.4002520000000001

W	14.4827680000000001	21.1781369999999995	3.4049079999999998
W	12.8778410000000001	24.6161069999999995	3.2236229999999999
W	11.5685830000000003	26.9705520000000014	3.1816110000000002
W	30.5040200000000006	-0.6640590000000000	3.3564669999999999
W	27.4531939999999999	5.0228400000000004	3.4047950000000000
W	25.4397979999999997	7.3909430000000000	3.4202040000000000
W	23.8768740000000008	10.1064279999999993	3.3594909999999998
W	22.2717729999999996	12.9010759999999998	3.3478340000000002
W	20.6770780000000016	15.6986939999999997	3.3314879999999998
W	19.1333330000000004	18.5291560000000004	3.3393480000000002
W	17.5346499999999992	21.2121490000000001	3.3390970000000002
W	16.2241430000000015	24.6010799999999996	3.2851300000000001
W	14.7515029999999996	26.8913849999999996	3.3163649999999998
W	33.6317030000000017	-0.5519450000000000	3.3286720000000001
W	35.9052190000000024	2.0527530000000000	3.7299080000000000
W	32.1025810000000007	1.6171450000000001	3.4932550000000000
W	30.5904319999999998	5.0207280000000001	3.4207130000000001
W	29.0821690000000004	7.3306950000000004	3.4979749999999998
W	27.5236620000000016	10.5700360000000000	3.4974870000000000
W	26.0060420000000008	13.2999600000000004	3.5067719999999998
W	24.4622579999999985	16.0951829999999987	3.5049929999999998
W	22.8136429999999990	18.8365369999999999	3.4185859999999999
W	21.1922159999999984	21.1625669999999992	3.3925630000000000
W	19.4349710000000009	24.5756550000000011	3.3610139999999999
W	17.8913860000000007	26.8464500000000008	3.3635109999999999
W	33.6575559999999996	5.0050340000000002	3.5192510000000001
W	32.0666960000000003	7.3178419999999997	3.5137250000000000
W	30.3483659999999986	10.1564150000000009	3.4291570000000000
W	28.8073669999999993	12.9503190000000004	3.4036040000000001
W	27.2970910000000018	15.6657039999999999	3.4231549999999999
W	25.7526179999999982	18.8573230000000009	3.4460289999999998
W	24.2742620000000002	21.1820120000000003	3.5141290000000001
W	22.6255309999999987	24.6378300000000010	3.4051740000000001

W	21.019007999999995	26.880966000000008	3.391538000000002
W	41.974203000000028	2.217886000000000	3.755262999999998
W	38.893031999999980	2.205430999999999	3.778907999999999
W	37.349786000000017	4.732329000000000	3.620861999999998
W	35.689306000000020	7.691429000000003	3.576997000000000
W	34.135944000000021	10.554945000000000	3.574037000000001
W	32.575018999999975	13.336213000000008	3.559766000000002
W	30.995985999999985	16.111650999999984	3.537055000000001
W	29.394532000000017	18.809385999999999	3.514136999999998
W	27.352957000000000	21.196542999999984	3.523820999999999
W	25.794596999999996	24.663284999999983	3.416760000000000
W	24.161200000000009	26.923059999999995	3.426263000000001
W	40.069110000000020	4.669724999999997	3.596623000000001
W	38.476823000000031	7.367229000000000	3.475843999999999
W	36.886040000000013	10.216132999999992	3.426836999999999
W	35.309854000000014	13.040514999999992	3.424569000000000
W	33.732593000000014	15.826921999999997	3.422428000000000
W	32.198168000000026	18.580864999999993	3.406648999999998
W	30.512740000000009	21.273731000000015	3.416465000000001
W	28.977861000000008	24.660271000000016	3.421174999999999
W	27.293548000000013	26.931239000000015	3.463446999999999
W	48.121453000000025	2.233645999999998	3.886288000000000
W	45.091842999999972	2.312037000000001	3.849927999999998
W	43.815275999999972	4.650353000000000	3.739551000000001
W	42.182822999999991	7.830033000000002	3.648893999999999
W	40.657462999999999	10.574484999999992	3.576458999999998
W	39.117749000000034	13.318479999999992	3.541901999999999
W	37.543120000000018	16.090254999999991	3.539969000000001
W	35.549509000000005	19.146298000000016	3.396408000000001
W	34.193373999999986	21.841219999999999	3.482463000000001
W	32.566634999999980	24.399996000000016	3.493631999999998
W	30.432936000000015	26.947666000000017	3.435620000000001
W	46.514426999999977	4.843481999999998	3.970149999999998

W	44.913527999999995	7.631484999999996	3.726397000000000
W	43.377626999999996	10.348015999999994	3.590371999999999
W	41.862234999999998	13.054933000000001	3.549773000000001
W	40.337879999999998	15.759605000000005	3.524378000000000
W	38.836387000000002	18.514423000000007	3.586430000000000
W	37.124996000000003	21.474323999999993	3.596045000000002
W	35.447766999999998	24.189985000000001	3.465187999999999
W	33.698341999999996	26.781452000000016	3.407408000000002
S	22.377470999999999	-2.164976999999999	4.357723000000000
S	20.690319999999998	0.970863000000000	5.159374999999998
S	19.075337000000001	3.757304000000000	5.070406000000002
S	17.358404000000002	6.512563000000001	5.157402000000003
S	15.748594000000006	9.250329000000007	5.159844999999998
S	14.203602999999993	11.980157000000002	5.139866999999997
S	12.694214000000006	14.786970000000002	5.075110999999997
S	11.093880000000004	17.683911999999994	4.782640999999999
S	9.538544999999992	20.529675000000010	4.620478000000003
S	8.222746000000008	23.464715999999992	4.784305999999999
S	6.734587000000003	26.202667999999992	4.786031000000004
S	25.746984000000012	-2.320167999999998	4.197738000000002
S	24.101551000000006	0.927675000000000	5.049434999999999
S	22.528342999999996	3.707732000000000	4.977358999999999
S	20.792926000000014	6.486635999999998	4.697180000000004
S	19.202138999999990	9.312331999999996	4.786381999999997
S	17.609982999999997	12.101627000000006	4.796064999999996
S	16.035118000000006	14.895889000000004	4.751371999999999
S	14.430199999999992	17.693570000000011	4.607356000000002
S	12.872422000000003	20.492934000000018	5.052690000000001
S	11.380060999999995	23.371363999999998	4.623948999999996
S	9.936367999999999	26.382576000000002	4.843467999999997
S	19.057264000000000	-0.393028000000000	2.603953999999999
S	17.277816000000014	2.533561000000002	2.638631000000002
S	15.578592000000004	5.349249000000004	2.642291999999999

S	14.006881999999992	8.184552000000000	2.497221000000000
S	12.426850999999992	10.994692999999998	2.457665000000000
S	10.812430000000000	13.776961000000000	2.547562999999998
S	9.327180999999995	16.620985000000010	2.268482999999998
S	7.770717999999996	19.598389000000000	2.333193000000000
S	6.208350000000000	22.295508999999991	2.071489999999998
S	4.730292000000000	25.015219999999993	1.993297000000000
S	3.585850999999999	27.860776999999988	3.942642000000000
S	22.675732000000000	-0.047128000000000	1.777044000000000
S	20.859618999999986	2.682551999999998	1.734815000000000
S	19.223321999999996	5.518025999999999	1.871332999999999
S	17.541564999999985	8.380506000000000	1.700142000000000
S	15.985604999999996	11.150169000000000	1.680210000000000
S	14.423014999999995	13.902544999999999	1.636009000000000
S	12.861553000000000	16.806083999999985	1.715780000000000
S	11.282476000000000	19.636838000000000	1.428604999999999
S	9.888310999999999	22.529424999999998	1.656598000000000
S	8.220463000000000	25.225350999999999	1.380679000000000
S	6.585961000000000	28.235230999999989	1.919929000000000
S	29.033377999999990	-2.233064999999999	4.347222000000000
S	27.393059999999984	0.883241000000000	5.171935000000000
S	25.797187000000000	3.716527000000000	4.783781000000000
S	24.017997999999986	6.556798999999998	5.215177999999999
S	22.447091000000000	9.311496999999992	5.189486999999997
S	20.860645000000000	12.108207999999994	5.170859000000000
S	19.258926999999999	14.920503999999993	5.152547000000000
S	17.689678000000000	17.715592000000000	5.126478999999998
S	16.071217999999982	20.464985999999997	5.087009000000000
S	14.545135999999994	23.390280000000000	4.578860999999998
S	13.070638999999999	26.343503999999994	4.956433999999998
S	32.409432999999999	-2.255892999999999	4.099356000000000
S	30.584990999999987	0.875883000000000	5.176206999999998
S	28.970750999999999	3.724873000000000	4.784783000000000

S	27.289349999999989	6.665476000000000	5.037498000000000
S	25.710125000000014	9.407194000000005	4.830311000000000
S	24.136593999999988	12.169549999999992	4.751483000000003
S	22.564326999999987	14.951496000000006	4.714642000000004
S	20.996831000000002	17.716764000000013	4.728543000000002
S	19.356401000000017	20.501628000000002	4.857885999999997
S	17.760256999999993	23.335847000000011	4.695781000000002
S	16.265905000000001	26.310825000000012	5.053340000000004
S	25.851293999999993	-0.138026000000000	1.684213000000000
S	24.156735000000012	2.819179000000001	2.164333000000001
S	22.438051000000015	5.584862000000002	2.028000000000000
S	20.800270000000011	8.376587000000007	2.096915999999998
S	19.209855999999985	11.154645999999996	2.138167000000002
S	17.633144000000015	13.936419000000008	2.113937000000000
S	16.088999999999986	16.720186000000018	1.997664000000001
S	14.541553999999996	19.496542000000016	1.776277000000001
S	13.015494000000003	22.430130999999994	1.857477000000000
S	11.401538000000004	25.357317999999994	1.507109000000000
S	9.787974000000002	28.456669000000015	2.230875999999999
S	28.972950999999983	-0.130912000000000	1.651214000000000
S	27.400642000000013	2.817076000000001	2.080461999999998
S	25.764518999999999	5.621513000000002	1.773423999999999
S	24.121714999999982	8.402905000000005	1.689012000000000
S	22.516134999999985	11.191922999999992	1.686879999999999
S	20.923833999999994	13.987311999999993	1.671381999999999
S	19.343077999999984	16.799064999999988	1.665481999999999
S	17.808150000000013	19.596211000000003	1.624829000000001
S	16.119081999999988	22.441271000000004	1.933443000000000
S	14.614860999999994	25.282070000000009	1.614309999999999
S	13.049056000000002	28.582159000000008	2.562659000000000
S	35.649175999999971	-0.366719000000000	2.413489999999999
S	33.932913999999967	0.964074000000000	5.043048999999999
S	32.168332999999970	3.727923000000001	4.869368999999998

S	30.5676440000000014	6.6201829999999999	5.2603119999999999
S	28.9379370000000016	9.3274329999999992	5.0796049999999999
S	27.3670340000000003	12.1954700000000003	5.2132610000000001
S	25.7923620000000007	14.9770509999999994	5.2004890000000001
S	24.2557410000000004	17.8104510000000005	5.1279310000000002
S	22.6177320000000002	20.5406340000000007	5.1673119999999999
S	21.0182639999999985	23.3577869999999983	4.7527249999999999
S	19.4371250000000018	26.3612390000000012	5.1061310000000004
S	37.3193079999999995	0.7601830000000001	4.9450459999999996
S	35.4666440000000023	3.8901289999999999	5.0477590000000001
S	33.8025149999999996	6.7018740000000001	5.0992879999999996
S	32.2347249999999974	9.4548179999999995	4.8316980000000003
S	30.6652340000000017	12.2157339999999994	4.7915979999999996
S	29.1070840000000004	14.9945819999999994	4.8340430000000003
S	27.5057270000000003	17.7585690000000014	4.7592990000000004
S	25.8398859999999999	20.5525540000000007	5.2190589999999997
S	24.2282420000000016	23.3903099999999995	4.7975450000000004
S	22.5853800000000007	26.4144259999999989	5.1440710000000003
S	32.1042690000000022	-0.0087880000000000	1.6477560000000000
S	30.6087600000000002	2.8556550000000001	2.0792039999999998
S	29.0025669999999991	5.6570760000000000	1.7248140000000001
S	27.3402789999999989	8.4505370000000006	2.1867450000000002
S	25.7440239999999996	11.2383720000000000	2.0687519999999999
S	24.1672720000000005	14.0142969999999991	2.1000570000000001
S	22.5872099999999989	16.7566629999999996	2.0600589999999999
S	21.0357550000000018	19.4784620000000004	1.8267070000000001
S	19.4187539999999998	22.3682039999999986	2.1093180000000000
S	17.8587740000000004	25.2139139999999990	1.6314280000000001
S	16.2451149999999984	28.4570289999999986	2.4948700000000001
S	33.9763269999999977	2.7638219999999998	2.2976329999999998
S	32.2369770000000031	5.6302969999999997	1.7542629999999999
S	30.5775499999999987	8.3985219999999998	1.8362250000000000
S	29.0519050000000014	11.2570230000000002	1.7195600000000000

S	27.4697560000000003	14.0458850000000002	1.6950140000000000
S	25.8864829999999984	16.8939009999999996	1.8379600000000000
S	24.2799119999999995	19.5934260000000009	1.6708680000000000
S	22.6699710000000003	22.4729109999999999	2.0936930000000000
S	21.0327979999999997	25.2200200000000017	1.6809959999999999
S	19.4241880000000009	28.4040929999999996	2.4413429999999998
S	40.4629679999999965	0.6318790000000000	4.6063250000000000
S	38.6999640000000014	3.8467050000000000	5.4223889999999999
S	37.0599699999999999	6.5748610000000003	5.2171370000000001
S	35.4952079999999981	9.4129109999999994	5.2299429999999996
S	33.8996399999999980	12.2263780000000004	5.2503159999999998
S	32.3136300000000034	15.0214669999999995	5.2349069999999998
S	30.7426169999999992	17.8259299999999996	5.2098030000000000
S	29.0437030000000007	20.5694760000000016	5.1594009999999999
S	27.4197090000000010	23.4160019999999989	4.7950809999999997
S	25.7308330000000005	26.4199330000000003	5.1731020000000001
S	43.6002739999999989	0.6865880000000000	4.6354889999999997
S	41.9098060000000032	3.9534009999999999	5.2066900000000000
S	40.3249289999999974	6.6898809999999997	4.9681829999999998
S	38.7682700000000011	9.4401879999999991	4.8169599999999999
S	37.2116970000000009	12.2476190000000003	4.7943230000000003
S	35.6312489999999968	15.0616380000000003	4.8135060000000003
S	34.0135920000000027	17.8774189999999997	4.8670039999999997
S	32.3784180000000035	20.6907899999999998	4.7716589999999997
S	30.6513010000000001	23.4118290000000009	4.7501509999999998
S	28.9121090000000009	26.3907990000000012	5.1760950000000001
S	37.3260519999999971	2.7822380000000000	2.0146630000000001
S	35.5327839999999995	5.6262869999999996	2.1553939999999998
S	33.8529359999999997	8.4794070000000001	2.2026710000000000
S	32.2782800000000023	11.2721999999999998	2.1817009999999999
S	30.7023060000000001	14.0614260000000009	2.1525479999999999
S	29.1256349999999991	16.8161699999999996	2.0912780000000000
S	27.5245439999999988	19.5455010000000016	1.9043580000000000

S	25.846637999999987	22.476579000000010	2.111067999999999
S	24.218343999999983	25.278403000000008	1.701541000000000
S	22.607780000000018	28.468586999999994	2.520394000000000
S	40.478633999999996	2.813979999999999	2.022571000000001
S	38.778666000000012	5.660765999999997	1.839518999999999
S	37.140946999999970	8.476558000000007	1.793698999999999
S	35.575575000000006	11.328549000000006	1.754319000000000
S	34.008009999999987	14.142238000000008	1.743362000000001
S	32.449567999999993	16.916541999999997	1.720397000000000
S	30.780978999999985	19.638134999999983	1.715390000000000
S	29.007191999999999	22.510616999999999	2.078828999999998
S	27.408581000000016	25.321436999999995	1.717171000000000
S	25.819026000000009	28.495799000000017	2.549631999999999
S	46.767288000000006	0.841398000000000	4.988120999999996
S	45.162241000000016	3.873939000000000	5.604290999999999
S	43.540303999999990	6.651281000000000	5.287300000000001
S	41.968711999999965	9.514063999999994	5.333494000000000
S	40.406765000000000	12.258959000000008	5.273509999999999
S	38.863464000000005	15.035790000000004	5.247887000000004
S	37.226315999999971	17.918994000000014	5.091226999999999
S	35.568539999999987	20.750333999999987	5.184338000000003
S	33.984893999999970	23.530415000000014	5.203106000000000
S	32.132167000000026	26.271670000000003	5.080560000000002
S	49.852589999999993	1.213301000000000	3.148404999999999
S	48.627836000000021	4.055864999999998	5.068640000000003
S	47.088276000000005	6.880194000000004	4.776099000000003
S	45.600692999999997	9.687948999999997	4.441574000000001
S	43.977901000000028	12.438352999999993	4.524293000000001
S	42.412413999999983	15.219290000000009	4.492235000000000
S	40.880927999999973	18.035790999999997	4.412650000000002
S	39.152194000000015	20.851524999999988	4.455638000000004
S	37.601109000000010	23.803459000000001	4.204607000000002
S	35.726588999999970	26.656324999999989	4.301921000000001

S	43.5767540000000011	2.8372489999999999	2.0744220000000002
S	42.0080910000000003	5.7146249999999998	2.3887360000000002
S	40.3791859999999971	8.5197289999999999	2.2068690000000002
S	38.8118910000000028	11.3205039999999997	2.1516449999999998
S	37.2336540000000014	14.1369579999999999	2.1560429999999999
S	35.6536749999999998	16.9854160000000007	2.2231380000000001
S	33.9424640000000011	19.8420999999999985	1.9489520000000000
S	32.3191300000000012	22.4868160000000010	2.0375150000000000
S	30.7245799999999996	25.2902990000000010	1.8770629999999999
S	29.0541079999999994	28.5556459999999994	2.6770559999999999
S	46.7950609999999969	3.0278239999999998	2.1876350000000002
S	45.2818929999999966	5.8330760000000001	2.1460260000000000
S	43.7389319999999984	8.6580040000000000	1.9192560000000001
S	42.2192790000000002	11.4384619999999995	1.8302449999999999
S	40.6868720000000010	14.1766410000000000	1.7959200000000000
S	39.1136720000000011	16.9501230000000014	1.8210800000000000
S	37.4349649999999983	19.7540089999999999	1.9778000000000000
S	35.8483590000000021	22.5493640000000006	1.7937550000000000
S	34.1138779999999997	25.2116429999999987	1.7243910000000000
S	32.4098559999999978	28.3703080000000014	2.4967670000000002

$\mathbf{W}_{105}\mathbf{S}_{210}$; $E_{tot} = -49\,817\,929.859\,050\,31$ eV; $E_{rel} = 3.806\,524\,961\,9$ meV/f.u.

W	20.9401760000000010	-0.5274210000000000	3.2469670000000002
W	19.3011690000000016	2.1442109999999999	3.4162729999999999
W	17.6848780000000012	4.8129000000000000	3.4505210000000002
W	16.1209009999999999	7.5168460000000001	3.4551210000000001
W	14.5810720000000007	10.2515669999999997	3.3486039999999999
W	12.8858350000000002	13.1515210000000007	3.0260870000000000
W	11.2764410000000002	16.3461169999999996	3.1126429999999998
W	9.7963120000000004	19.0387610000000009	3.2093400000000001
W	8.2730619999999995	21.7461589999999987	3.2188010000000000
W	6.7819989999999999	24.4423570000000012	3.0886849999999999

W	5.164530000000001	26.998709999999991	3.048690000000001
W	24.308589999999998	-0.933427000000000	3.225108999999998
W	22.0949890000000018	1.950302000000000	3.329095000000001
W	20.4389830000000003	4.6087930000000004	3.399343000000000
W	18.8453790000000012	7.308548000000000	3.412871000000000
W	17.2911430000000017	10.051486999999998	3.390975000000001
W	15.7341060000000006	13.329841999999993	3.357406000000001
W	14.542897999999992	15.723458000000008	3.351522999999998
W	12.8282950000000007	19.057061000000009	3.271096000000000
W	11.3150410000000008	21.344250999999999	3.320158000000002
W	9.4417100000000005	24.567531999999999	3.184364000000000
W	8.2348610000000004	26.979893000000006	2.960948000000001
W	27.1121230000000004	-0.620705000000000	3.396180000000002
W	28.663738999999996	2.116557999999999	3.470132000000000
W	25.9140300000000003	1.816375000000001	3.305679000000000
W	24.209019999999998	5.074379999999997	3.410304000000000
W	22.6069850000000017	7.767190000000003	3.512551000000002
W	21.0077640000000017	10.464902000000004	3.523244000000000
W	19.4396050000000002	13.169627999999994	3.500532999999999
W	17.503409999999998	15.655354000000009	3.484360999999998
W	16.040013999999993	19.113846999999998	3.288587000000001
W	14.4165170000000007	21.345269999999993	3.415233000000002
W	13.007989999999995	24.760474999999996	3.249518999999998
W	11.4676120000000008	27.025345000000015	3.187949000000001
W	30.8975320000000018	-0.917007000000000	3.304736999999998
W	27.4101280000000003	4.587787999999998	3.367982000000000
W	25.356328999999998	7.591478999999996	3.379058000000001
W	23.7611950000000007	10.251640000000001	3.407795999999998
W	22.1810450000000010	12.921521000000003	3.414429000000002
W	20.613572999999998	15.653975000000009	3.422242999999999
W	19.286943999999998	19.105899000000009	3.342394000000001
W	17.6780870000000014	21.346112000000015	3.486502000000002
W	16.1482190000000010	24.790288000000003	3.333753000000002

W	14.6065120000000004	27.0505360000000010	3.3125260000000001
W	33.6965580000000031	-0.5838110000000000	3.3479559999999999
W	35.2563189999999977	2.1264289999999999	3.3961410000000001
W	32.4772630000000007	1.8522339999999999	3.3780910000000000
W	30.2778929999999988	4.9756520000000002	3.5193189999999999
W	29.1712740000000004	7.7266500000000002	3.4549249999999998
W	27.6215340000000005	10.5293489999999998	3.5633370000000002
W	25.9910059999999987	13.2680570000000007	3.5782219999999998
W	24.4082420000000013	15.9757949999999997	3.4836269999999998
W	22.4508639999999993	19.0776220000000016	3.4021390000000000
W	20.9235840000000017	21.3392860000000013	3.5262690000000001
W	19.2941180000000010	24.7863679999999995	3.3890720000000001
W	17.7340879999999999	27.0720999999999989	3.3472179999999998
W	34.0590040000000016	4.6119190000000003	3.4194900000000001
W	31.9215979999999995	7.7900070000000001	3.5419550000000002
W	30.6208260000000010	10.2508219999999994	3.4861670000000000
W	28.6984689999999993	13.0983579999999993	3.4730919999999998
W	27.1309089999999991	15.7827219999999997	3.4366490000000001
W	25.5722139999999989	18.9595270000000014	3.4676130000000001
W	24.0960709999999985	21.3017029999999998	3.5578759999999998
W	22.4544479999999993	24.7688559999999995	3.4161500000000000
W	20.8759820000000005	27.0624399999999987	3.3878430000000002
W	36.8143859999999989	4.8316699999999999	3.4503240000000002
W	35.6578239999999980	7.3734659999999996	3.4201910000000000
W	33.4977829999999983	10.4582909999999991	3.5460500000000001
W	32.4342210000000009	13.4501910000000002	3.5973370000000000
W	30.8771120000000003	16.1703060000000001	3.6104810000000001
W	29.2726289999999985	18.8677059999999983	3.5793620000000002
W	27.2059469999999983	21.2979529999999997	3.5444840000000002
W	25.6372999999999998	24.7388559999999984	3.4203380000000001
W	24.0069319999999991	27.0276579999999989	3.4387449999999999
W	38.4169550000000015	7.5446650000000002	3.4505789999999998
W	37.3598640000000017	10.5681039999999999	3.4843829999999998

W	35.149918999999970	13.205023999999999	3.480367999999999
W	33.600785999999994	15.937462000000000	3.431153000000000
W	32.020440999999982	18.650141999999989	3.426237000000000
W	30.415964999999999	21.348653999999998	3.466575000000002
W	29.243804000000008	24.579140999999999	3.483031000000000
W	27.152660999999984	27.032251999999997	3.430419999999998
W	40.047027999999974	10.373160999999996	3.416736000000002
W	38.861280999999982	13.103077000000008	3.450508999999998
W	37.368675000000032	16.261966999999985	3.489242000000000
W	35.804872000000031	19.024737999999993	3.490362999999999
W	34.182388000000031	21.748318999999986	3.488245000000000
W	32.187500999999975	24.619680999999999	3.443766000000001
W	30.425419000000015	27.010878999999992	3.395481999999999
W	41.493371000000033	13.186500999999998	3.419474000000001
W	40.056427999999968	16.089728999999984	3.419222000000000
W	38.520282999999992	18.809297999999983	3.383808999999998
W	36.966782999999995	21.483816000000009	3.384280000000000
W	35.373463000000010	24.163554999999988	3.415652000000001
W	33.583959999999976	26.856656999999984	3.403516999999999
S	22.408297000000010	-1.850924000000000	4.677399999999996
S	20.624251000000010	0.982543000000001	5.071731999999999
S	18.927257000000009	3.703742000000001	5.165821000000002
S	17.324742000000005	6.422864999999998	5.183303999999997
S	15.756757999999996	9.213146000000001	5.139662999999996
S	14.143565999999999	12.128907999999991	4.855147999999998
S	12.583093999999991	15.013211999999993	4.699817000000004
S	11.177220999999994	17.944803000000003	4.859001000000001
S	9.549362999999996	20.710826000000008	4.940766000000000
S	8.036384999999992	23.444970999999989	4.879235999999997
S	6.538624999999997	26.282987999999996	4.745976999999999
S	25.724859999999996	-1.713962000000000	5.042772000000003
S	24.003101999999984	1.023327000000001	4.660865000000003
S	22.369637000000009	3.846393000000000	4.773227000000003

S	20.730568999999991	6.593932999999998	4.807605999999998
S	19.1123930000000009	9.3494180000000000	4.8003159999999996
S	17.4692660000000011	12.1414639999999991	4.6823480000000002
S	15.9152860000000000	14.9454209999999996	5.1326229999999997
S	14.4266679999999994	17.8281959999999984	4.6768219999999996
S	12.8177830000000004	20.7125449999999987	5.0733430000000004
S	11.2721289999999996	23.5419769999999993	4.5263650000000002
S	9.7355760000000000	26.4334659999999992	4.7725869999999997
S	18.8273949999999992	-0.1340610000000000	2.5399859999999999
S	17.1888620000000003	2.6451060000000002	2.4906779999999999
S	15.5361899999999995	5.4277959999999998	2.5205039999999999
S	13.8877100000000002	8.2209500000000002	2.6085440000000002
S	12.3897239999999993	11.0929319999999993	2.3149150000000001
S	10.8179420000000004	14.0979679999999998	2.4102480000000002
S	9.2013909999999992	16.8508689999999994	2.3275660000000000
S	7.6377220000000001	19.5937939999999990	2.4514469999999999
S	6.1470339999999997	22.3336269999999999	2.2947000000000002
S	4.6630019999999996	25.1213149999999992	1.9487900000000000
S	3.3967670000000001	27.9513789999999993	3.7912819999999998
S	22.4914069999999988	0.1734830000000000	1.7147610000000000
S	20.7120759999999997	2.9311039999999999	1.6514279999999999
S	19.0848389999999988	5.6376299999999997	1.6992910000000001
S	17.4882840000000002	8.3676460000000006	1.6930820000000000
S	15.9187390000000004	11.2639800000000001	1.7908450000000000
S	14.3202900000000000	14.1052099999999996	1.5080340000000001
S	12.9283769999999993	17.0014070000000004	1.7490500000000000
S	11.2653909999999993	19.6965170000000001	1.5241929999999999
S	9.7722899999999999	22.5587349999999986	1.7261970000000000
S	8.0696230000000000	25.3202229999999986	1.3298479999999999
S	6.4636160000000000	28.3772170000000017	1.8691380000000000
S	29.0201110000000000	-1.7071639999999999	4.6272979999999997
S	27.3346109999999989	1.0306059999999999	5.1307820000000000
S	25.6651789999999984	3.8017859999999999	4.8618660000000000

S	23.9949960000000004	6.6570669999999996	5.1713540000000000
S	22.3438690000000015	9.4008550000000000	5.2218320000000000
S	20.7226539999999986	12.1399530000000002	5.2208930000000002
S	19.1219329999999985	14.9194630000000004	5.1508830000000003
S	17.6068970000000000	17.8472580000000001	4.6831940000000003
S	16.0178060000000002	20.7127009999999991	5.1094650000000001
S	14.4822839999999999	23.5452639999999995	4.7033899999999997
S	12.9596099999999996	26.5172249999999998	4.9840249999999999
S	32.4535959999999974	-1.7416330000000000	5.0460130000000003
S	30.5986340000000006	1.0782689999999999	4.7361930000000001
S	28.9037170000000003	3.8741750000000001	5.1328889999999996
S	27.2764780000000009	6.6822179999999998	4.6900729999999999
S	25.6720390000000016	9.4802429999999998	4.8329329999999997
S	24.0555109999999992	12.2160240000000009	4.8578169999999998
S	22.4593820000000015	14.9821679999999997	4.8086810000000000
S	20.8016620000000003	17.8033549999999998	4.7643279999999999
S	19.2597999999999985	20.7079440000000012	5.1670290000000003
S	17.6770589999999999	23.5494130000000013	4.7729819999999998
S	16.1394950000000001	26.5938039999999987	5.0667780000000002
S	25.6784010000000009	0.1547130000000000	1.5866700000000000
S	24.0278770000000002	2.9639720000000001	2.0823170000000002
S	22.3135499999999993	5.7001739999999996	2.1188870000000000
S	20.7089539999999985	8.4269839999999991	2.1202730000000001
S	19.1321469999999998	11.1824490000000001	2.0788590000000000
S	17.5901069999999997	13.9644370000000002	1.8740390000000000
S	16.0704570000000011	16.8984099999999984	1.9404450000000000
S	14.4554679999999998	19.7469549999999998	1.6116930000000000
S	12.9149490000000000	22.5895979999999987	1.9226010000000000
S	11.2936099999999993	25.3470000000000013	1.6261620000000001
S	9.7020040000000005	28.5055259999999997	2.1502710000000000
S	29.0077129999999990	0.1707300000000000	2.0187339999999998
S	27.2579349999999998	2.9309249999999998	1.6464209999999999
S	25.7209469999999989	5.7645869999999997	1.7913829999999999

S	24.0215110000000003	8.5680160000000001	1.6791680000000000
S	22.4323119999999996	11.2780109999999993	1.7026140000000001
S	20.8513809999999999	14.0298549999999995	1.7125570000000001
S	19.1908420000000000	16.9114679999999993	2.0386639999999998
S	17.6773379999999989	19.7402850000000001	1.6593180000000001
S	16.0957089999999994	22.6134209999999989	2.0838649999999999
S	14.5788569999999993	25.4152799999999992	1.5709990000000000
S	12.9098140000000008	28.6437619999999988	2.4735179999999999
S	35.8117200000000011	-0.0121070000000000	2.4454120000000001
S	34.0422530000000023	0.9846080000000000	5.1103719999999999
S	32.2006080000000026	3.8662980000000000	4.7868930000000001
S	30.5332320000000017	6.6644540000000001	5.1865509999999997
S	28.9894789999999993	9.4495339999999999	5.1784070000000000
S	27.3216059999999992	12.2218540000000004	5.2697640000000003
S	25.7099149999999987	15.0229599999999994	5.2414920000000000
S	24.0303830000000005	17.8549149999999983	4.9737020000000003
S	22.4693439999999995	20.7005090000000003	5.2278739999999999
S	20.8857309999999998	23.5374310000000015	4.8046899999999999
S	19.2824360000000006	26.6105790000000013	5.1085349999999998
S	35.6024409999999989	3.7135780000000000	5.1568540000000000
S	33.8162469999999971	6.6664719999999997	4.8061199999999999
S	32.1736629999999977	9.4796720000000008	5.2352179999999997
S	30.5989019999999989	12.3125560000000007	4.8455789999999999
S	28.9867060000000016	15.0723420000000008	4.8807039999999997
S	27.3527769999999997	17.8325649999999989	4.7986250000000004
S	25.6899160000000002	20.6346540000000012	5.2345290000000002
S	24.0944509999999994	23.5155419999999999	4.8090469999999996
S	22.4255910000000007	26.5652979999999985	5.1488170000000002
S	32.2445179999999993	0.2110880000000000	1.6373350000000000
S	30.5876990000000006	2.9738600000000002	2.1371760000000002
S	28.8872190000000018	5.8235270000000003	1.8394509999999999
S	27.2760849999999984	8.5713279999999994	2.0873080000000002
S	25.6803330000000010	11.2992600000000003	2.1738680000000001

S	24.0583320000000001	14.0311310000000002	2.1670769999999999
S	22.4772040000000004	16.8701749999999997	2.1820230000000000
S	20.8981379999999994	19.7093769999999999	1.6913680000000000
S	19.2967000000000013	22.6110310000000005	2.1372119999999999
S	17.7434879999999993	25.4017429999999997	1.6437759999999999
S	16.1263019999999990	28.6011719999999983	2.3845760000000000
S	33.8213360000000023	2.9668519999999998	1.6929000000000001
S	32.1982709999999983	5.7500780000000002	2.1562670000000002
S	30.5702619999999996	8.5961320000000008	1.7094940000000001
S	29.0256879999999988	11.3339219999999994	1.8581710000000000
S	27.3902760000000001	14.1081550000000000	1.7403450000000000
S	25.7463769999999990	16.9452169999999995	1.8363680000000000
S	24.0735540000000015	19.6860070000000000	1.7375980000000000
S	22.5043129999999998	22.5970750000000002	2.1398169999999999
S	20.9065960000000004	25.3910799999999988	1.6893290000000001
S	19.3265749999999983	28.6191400000000016	2.4532400000000001
S	37.1604129999999984	6.4850159999999999	5.1659420000000003
S	35.4918580000000006	9.4593699999999998	4.7278859999999998
S	33.8009819999999976	12.2489880000000007	5.2008770000000002
S	32.2365210000000033	15.1116980000000005	5.2871969999999999
S	30.6130899999999997	17.8849829999999983	5.2763510000000000
S	28.9114530000000016	20.6559950000000008	5.1859140000000004
S	27.3403929999999988	23.5320800000000006	4.7308820000000003
S	25.6111049999999985	26.4928969999999993	5.1558570000000001
S	38.7259549999999990	9.3153469999999992	5.0946959999999999
S	37.0751599999999968	12.3332549999999994	4.9822050000000004
S	35.5348979999999983	15.1753750000000007	4.8243679999999998
S	33.9435640000000021	17.9536319999999989	4.8238320000000003
S	32.3151439999999965	20.7055240000000005	4.8216359999999998
S	30.6306410000000007	23.4536610000000003	4.9756819999999999
S	28.8480699999999999	26.4029389999999999	5.0707480000000000
S	37.4017109999999988	2.7563830000000000	2.4880019999999998
S	35.4371060000000000	5.7061260000000003	1.7209920000000001

S	33.8193970000000022	8.5332380000000008	2.1125959999999999
S	32.1394390000000030	11.4417130000000000	1.9672879999999999
S	30.5789890000000000	14.1645120000000002	2.1691300000000000
S	28.9881309999999992	16.9051189999999991	2.1515629999999999
S	27.3714249999999986	19.6310670000000016	1.9528310000000000
S	25.7059409999999993	22.5552150000000005	2.1260420000000000
S	24.0863620000000012	25.3913300000000000	1.7131300000000000
S	22.5253329999999998	28.5896499999999989	2.4851079999999999
S	39.0623769999999979	5.5065480000000004	2.6510080000000000
S	37.0968790000000013	8.5730730000000008	1.8754750000000000
S	35.4435450000000003	11.3279580000000006	2.0809679999999999
S	33.8585190000000011	14.2108860000000004	1.7700229999999999
S	32.2669550000000029	16.9738289999999985	1.7492479999999999
S	30.6494190000000017	19.7247100000000017	1.7606139999999999
S	28.9296819999999997	22.5456280000000007	2.0787070000000001
S	27.3863079999999997	25.3668240000000011	1.8621509999999999
S	25.7338239999999985	28.6170709999999993	2.6235670000000000
S	40.3736820000000023	12.0674630000000001	5.1433330000000002
S	38.7811980000000034	15.0712729999999997	5.0536669999999999
S	37.1912349999999989	17.9708080000000017	5.1787419999999997
S	35.5760689999999968	20.7505130000000015	5.1796439999999997
S	33.8527360000000002	23.5700550000000000	5.0492569999999999
S	32.0553870000000032	26.4554709999999993	5.1271440000000004
S	42.2999119999999991	15.0689670000000007	4.3115209999999999
S	40.7900309999999990	18.1030720000000009	4.1658920000000004
S	39.0966420000000028	20.9314560000000007	4.3139830000000003
S	37.4835259999999977	23.8023440000000015	4.1665609999999997
S	35.6131379999999993	26.6197650000000010	4.3017529999999997
S	40.6775379999999984	8.3331180000000007	2.6383420000000002
S	38.7613279999999989	11.3803420000000006	1.7384310000000001
S	37.0548550000000034	14.1901430000000008	2.1667900000000002
S	35.4918850000000035	17.0031539999999985	2.1186460000000000
S	33.8914820000000034	19.7559730000000009	2.1170969999999998

S	32.2271270000000030	22.5090900000000005	2.1651620000000000
S	30.6433320000000009	25.3819200000000009	1.7302620000000000
S	28.9866069999999993	28.5757970000000014	2.6071080000000002
S	42.3299329999999969	11.3166229999999999	2.5512169999999998
S	40.2657949999999971	14.3012020000000000	1.7620590000000000
S	38.8043890000000005	17.1297889999999988	1.6858260000000000
S	37.2690600000000032	19.8704719999999995	1.6721470000000000
S	35.6508079999999978	22.5594560000000008	1.6843649999999999
S	33.9275749999999974	25.2297399999999996	1.7531090000000000
S	32.3867580000000004	28.5179310000000008	2.5339360000000002
W	30.6294089999999990	-6.0749290000000000	3.1501310000000000
W	32.1502559999999988	-3.3041269999999998	3.2827590000000000
W	29.2896460000000012	-3.7248950000000001	3.2161330000000001
W	27.3808250000000015	-11.4769020000000008	3.1291210000000000
W	28.9080189999999995	-8.7814829999999997	3.0711080000000002
W	27.5765649999999987	-6.4677670000000003	3.1787269999999999
W	25.5758970000000012	-3.2962820000000002	3.2927890000000000
W	25.9942670000000007	-8.8837340000000005	3.0524049999999998
W	24.5321059999999989	-6.4174290000000003	3.0842040000000002
W	22.6861770000000007	-3.5703499999999999	2.9404100000000000
S	34.2357060000000004	-2.7867660000000001	2.4030749999999999
S	32.7453550000000035	-5.6177089999999996	2.4836450000000001
S	30.6741999999999990	-2.5774210000000002	1.5759209999999999
S	30.9859399999999994	-8.3741350000000008	2.2047729999999999
S	29.1096110000000010	-5.4007980000000000	1.5194820000000000
S	27.4103400000000015	-2.5962420000000002	1.8944390000000000
S	30.8645999999999994	-4.4959040000000003	4.9417059999999999
S	29.1924579999999985	-11.0452370000000002	1.9182319999999999
S	27.4008530000000015	-8.1123600000000007	1.3842070000000000
S	25.9009870000000006	-5.3254460000000003	1.6828710000000000
S	24.1260440000000003	-2.6220680000000001	1.4333920000000000
S	27.3698820000000005	-13.4575270000000007	3.9425349999999999
S	25.4814469999999993	-11.0317889999999998	2.0078010000000002

S	23.8786020000000008	-8.3886439999999993	2.1083219999999998
S	22.2767769999999992	-5.7484000000000002	2.3702200000000002
S	20.6605510000000017	-2.8022399999999998	2.2350340000000002
S	29.3004409999999993	-7.2022719999999998	4.8166650000000004
S	27.4135269999999984	-4.4281860000000002	4.5822950000000002
S	27.5378320000000016	-9.8987180000000006	4.7897939999999997
S	25.9113469999999992	-7.2388139999999996	4.8115949999999996
S	24.0469159999999995	-4.6295219999999997	4.6975439999999997

$\mathbf{W}_{105}\mathbf{S}_{210}$; $E_{tot} = -49\,817\,930.258\,735\,43\text{ eV}$; $E_{rel} = 0\text{ meV/f.u.}$

W	21.1280609999999989	-0.5562030000000000	3.4121530000000000
W	19.3951600000000006	2.0881859999999999	3.3731140000000002
W	17.7334199999999989	4.9536709999999999	3.4027180000000001
W	16.1999020000000016	7.7211270000000001	3.4299320000000000
W	14.6010810000000006	10.4119209999999995	3.4166949999999998
W	13.0110480000000006	13.1350750000000005	3.4157880000000000
W	11.4985250000000008	15.8797499999999996	3.3844840000000000
W	9.9752550000000006	18.6189120000000017	3.1803089999999998
W	8.1545380000000005	21.6889899999999993	2.8528989999999999
W	6.5635310000000002	24.6115929999999992	3.0384009999999999
W	5.1213430000000004	27.0730520000000006	3.0262009999999999
W	3.5611150000000000	29.6094520000000010	3.1625390000000002
W	24.3614970000000000	-0.7368710000000001	3.4467080000000001
W	22.3538679999999985	1.7770410000000001	3.4355090000000001
W	20.8966160000000016	4.3229249999999997	3.4394979999999999
W	18.9812009999999987	7.4136970000000000	3.3675009999999999
W	17.3919339999999991	10.1838169999999995	3.4055460000000002
W	15.7628909999999998	12.9013089999999995	3.3958360000000001
W	14.2012630000000009	15.6437430000000006	3.3635020000000000
W	12.6931130000000003	18.4185340000000011	3.2958820000000002
W	11.2954319999999999	21.7651550000000000	3.1780290000000000
W	9.8120259999999995	24.0265379999999986	3.2536820000000000

W	7.9018670000000002	27.2841079999999998	3.1914340000000001
W	6.6477029999999999	29.6168550000000010	3.1174949999999999
W	27.4948329999999999	-0.7636860000000000	3.4334680000000000
W	29.0335530000000013	1.4810749999999999	3.5133100000000002
W	25.8406330000000004	1.5181920000000000	3.5047139999999999
W	24.2556669999999990	4.9754490000000002	3.4370799999999999
W	22.7748169999999988	7.5988259999999999	3.5094919999999998
W	21.2431060000000009	10.1242009999999993	3.4110090000000000
W	19.4757730000000002	13.4690569999999994	3.3549259999999999
W	17.9619070000000001	16.0656770000000009	3.4501680000000001
W	16.4639109999999995	18.5747010000000010	3.3834469999999999
W	14.5026720000000005	21.7959700000000005	3.2881800000000001
W	12.9393259999999994	24.0268780000000000	3.3900950000000001
W	11.4280799999999996	27.4430620000000012	3.2512520000000000
W	9.8573360000000001	29.7099669999999989	3.2761600000000000
W	27.4380360000000003	4.9241289999999998	3.4228999999999998
W	25.8886329999999987	7.1809770000000004	3.5720470000000000
W	23.9720270000000006	10.3833420000000007	3.5026150000000000
W	22.7656239999999990	12.8183609999999994	3.4649120000000000
W	20.9588630000000009	16.1081199999999995	3.4094679999999999
W	19.4050820000000002	18.4056210000000000	3.4996499999999999
W	17.7211040000000004	21.8038649999999983	3.3585690000000001
W	16.1199960000000004	24.0467849999999999	3.4600059999999999
W	14.5958410000000001	27.4832479999999997	3.3291249999999999
W	12.9852900000000009	29.7397939999999998	3.3731849999999999
W	35.3070919999999973	1.5924620000000000	3.5222750000000000
W	32.1811039999999977	1.5012239999999999	3.5186259999999998
W	30.6077879999999993	4.9339219999999999	3.4240930000000001
W	29.0355659999999993	7.1642299999999999	3.5993160000000000
W	27.5411080000000013	10.5785470000000004	3.4724149999999998
W	25.9068450000000006	12.8081090000000000	3.5802890000000001
W	24.2718169999999986	16.2376140000000007	3.3937149999999998
W	22.5302979999999984	18.4502360000000003	3.5396200000000002

W	20.9834040000000002	21.8730790000000006	3.3837690000000000
W	19.3308409999999995	24.0889510000000016	3.5039449999999999
W	17.8025370000000009	27.5106210000000004	3.3685860000000001
W	16.0944029999999998	29.7845809999999993	3.3822199999999998
W	33.7787379999999970	4.9624779999999999	3.4443429999999999
W	32.2305149999999969	7.1846040000000002	3.5911529999999998
W	30.6195039999999992	10.6247460000000000	3.4470950000000000
W	28.9987759999999994	12.8730689999999992	3.5889199999999999
W	27.5067500000000003	16.2822649999999989	3.4238689999999998
W	25.8137019999999993	18.4936329999999991	3.5709230000000001
W	24.2041800000000009	21.9059220000000003	3.4108499999999999
W	22.5488989999999987	24.1314430000000009	3.5446970000000002
W	21.0719320000000003	27.5323239999999991	3.3857159999999999
W	19.2298040000000015	29.8297500000000007	3.3807190000000000
W	41.9242289999999969	2.3204330000000000	3.6535190000000002
W	38.9838179999999994	2.0473810000000001	3.6316920000000001
W	36.9773530000000008	5.0402040000000001	3.5432939999999999
W	35.3860030000000023	7.2413699999999999	3.5994579999999998
W	33.7156760000000020	10.6599450000000004	3.4616920000000002
W	32.1087249999999997	12.9058779999999995	3.5819369999999999
W	30.6985750000000017	16.3125970000000002	3.4507240000000001
W	29.0582369999999983	18.5347930000000005	3.5878649999999999
W	27.4405320000000010	21.9275489999999991	3.4359470000000001
W	25.7834229999999991	24.1455540000000006	3.5706280000000001
W	24.2534409999999987	27.5501879999999986	3.3879190000000001
W	22.4063639999999999	29.8772860000000016	3.3621850000000002
W	40.3706770000000006	4.5010360000000000	3.6123650000000000
W	38.4288090000000011	7.6882020000000004	3.6005660000000002
W	37.2613249999999994	10.4183039999999991	3.5600980000000000
W	35.7210820000000027	13.0262150000000005	3.4998010000000002
W	33.7922080000000022	16.3151459999999986	3.4947110000000001
W	32.2478920000000002	18.5858840000000001	3.5968330000000002
W	30.5822970000000005	21.9688000000000017	3.4744389999999998

W	29.055023999999995	24.244582999999987	3.518967000000000
W	27.288464999999986	27.511631999999988	3.374403000000000
W	25.603470000000015	29.858890999999998	3.369530000000001
W	44.981143000000030	2.395430999999999	3.597364999999999
W	43.329720999999993	4.795436999999997	3.770481999999999
W	41.790734000000005	7.289556000000001	3.809759999999998
W	40.025216000000003	10.437243000000005	3.733334000000002
W	38.458140000000002	13.091395000000003	3.510683999999999
W	36.930591999999972	15.811702999999996	3.535508999999998
W	35.453068999999993	18.510971000000014	3.694300999999998
W	33.653978000000022	21.698606999999991	3.692904000000000
W	32.046973999999987	24.306069000000008	3.544261999999998
W	30.484967000000010	26.913333999999990	3.516842000000000
W	28.778057000000004	29.679581999999999	3.396961000000001
S	22.353072000000009	-2.174125000000001	4.338320999999996
S	20.694486000000013	0.983020000000000	5.119811999999996
S	19.116755000000013	3.774071000000002	5.034868000000003
S	17.482117999999998	6.572154000000003	5.122734000000003
S	15.833650000000004	9.311980000000001	5.151525999999996
S	14.222094999999995	12.021015000000002	5.148232000000001
S	12.680754000000003	14.782647000000008	5.128374000000000
S	11.123042999999991	17.609580999999986	5.026556000000002
S	9.513797999999995	20.558540000000007	4.586706000000004
S	7.898894000000003	23.327031999999991	4.645214000000002
S	6.476970999999998	26.158584000000012	4.813420999999999
S	4.993155999999999	28.899536000000012	4.809215000000000
S	25.727785000000008	-2.372761000000001	4.206413000000004
S	24.094884000000004	0.891426000000001	5.062648000000003
S	22.562505000000016	3.723282999999999	4.950027999999997
S	20.863098999999983	6.488495000000003	4.660469000000000
S	19.294377999999983	9.335950000000004	4.785916000000003
S	17.675709000000012	12.184084999999996	4.758573000000002
S	16.076820999999989	14.929937999999999	4.758003000000004

S	14.4700070000000007	17.6857840000000017	4.7512470000000002
S	12.8201699999999992	20.5299179999999986	4.6276650000000004
S	11.26047900000000001	23.3707439999999984	4.9992939999999999
S	9.70627600000000008	26.1974330000000002	4.5114500000000000
S	8.19720300000000000	29.0889139999999990	4.8792080000000002
S	19.0894000000000013	-0.3643180000000000	2.5374669999999999
S	17.3179760000000016	2.5830199999999999	2.5919279999999998
S	15.6539540000000006	5.4191539999999998	2.6204559999999999
S	14.1013699999999993	8.2274999999999991	2.4927720000000000
S	12.4537870000000002	10.9782820000000001	2.5346860000000002
S	10.8736470000000001	13.7889780000000002	2.4858699999999998
S	9.2873590000000004	16.5827460000000002	2.4809739999999998
S	7.9206909999999997	19.5271900000000009	2.1145299999999998
S	6.0538809999999996	22.3267840000000000	2.2491680000000001
S	4.5406690000000003	25.0361499999999992	2.0080010000000001
S	3.0017000000000000	27.7698719999999994	1.9985740000000001
S	1.8402510000000001	30.5758369999999999	3.9909629999999998
S	22.7185570000000006	-0.0495180000000000	1.7671880000000000
S	20.9156489999999984	2.6949770000000002	1.6999569999999999
S	19.2851940000000006	5.5565980000000001	1.8251970000000000
S	17.6453650000000017	8.4707620000000006	1.6856810000000000
S	16.0554820000000014	11.2111330000000002	1.6968559999999999
S	14.4224110000000003	13.9388240000000003	1.6746350000000001
S	12.8852069999999994	16.7150549999999996	1.6245380000000000
S	11.3684329999999996	19.6259720000000009	1.6636679999999999
S	9.7423509999999993	22.4502990000000011	1.3816010000000001
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S	6.4500270000000004	28.0407679999999999	1.3798250000000001
S	4.8502289999999997	31.0173360000000002	2.0134780000000001
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S	22.6498510000000017	14.9347460000000005	4.7699280000000002
S	20.9868650000000017	17.7857699999999994	5.2107840000000003
S	19.3674479999999996	20.5908270000000009	4.7444080000000000
S	17.7217659999999988	23.4386110000000016	5.1542610000000000
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S	25.9022289999999984	-0.1892730000000000	1.7212689999999999
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S	11.3741579999999995	25.2870929999999987	1.8974310000000001
S	9.7159390000000005	28.0882310000000004	1.6465470000000000
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S	16.1383849999999995	22.4042500000000011	1.6480100000000000
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S	30.6206099999999992	12.2319759999999995	5.2908299999999997
S	29.0497909999999990	15.0481330000000000	4.8456780000000004
S	27.4473230000000008	17.8965969999999999	5.2470670000000004
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S	29.0187109999999997	5.5566529999999998	1.7468079999999999

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S	24.206497999999998	19.710467000000013	2.181798999999998
S	22.591205999999997	22.504001999999998	1.725459000000001
S	20.979708999999997	25.371172999999989	2.126560000000000
S	19.372288000000011	28.189538999999999	1.701406999999999
S	17.738452999999998	31.382673000000005	2.516236000000001
S	40.546103000000022	0.837037999999999	4.885670000000002
S	38.651476999999999	3.794439999999998	5.139240000000000
S	37.010150000000030	6.710452000000001	5.289364000000000
S	35.418805999999965	9.422415000000009	4.837982000000002
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S	29.047411000000003	20.715299000000017	4.894871000000002
S	27.422318000000006	23.544543000000009	5.208423999999999
S	25.741067000000010	26.349288000000014	4.871590000000003
S	24.048773000000006	29.345411999999996	5.080417999999999
S	43.738908000000021	0.938187000000000	4.742439000000001
S	41.933343999999982	3.930547999999999	5.391841000000003

S	40.187184999999995	6.5345760000000004	5.1793110000000002
S	38.649467999999998	9.437084999999997	5.297045999999999
S	37.1440169999999981	12.2149710000000002	5.2462090000000003
S	35.4309450000000012	15.032256999999995	5.0143440000000004
S	33.9017150000000029	17.949754999999997	5.308095999999999
S	32.1665240000000026	20.7438690000000001	5.077379999999998
S	30.6274100000000011	23.638201999999997	5.2611210000000002
S	28.8842070000000000	26.3026650000000011	4.969858999999996
S	27.2380110000000002	29.3025449999999985	5.107696999999999
S	37.1178389999999965	2.799056999999999	2.258799999999999
S	35.4580509999999975	5.5774260000000000	1.8126530000000001
S	33.7961630000000000	8.4718699999999991	2.170532999999998
S	32.20127200000000030	11.2994090000000007	1.7490190000000001
S	30.63047800000000001	14.1391570000000009	2.1481560000000002
S	29.0916570000000014	16.9261419999999987	1.7586180000000000
S	27.4393920000000016	19.7443810000000006	2.1957270000000002
S	25.8258699999999983	22.5241560000000014	1.7540890000000000
S	24.1803899999999992	25.3888570000000016	2.1648710000000002
S	22.5880359999999989	28.230541999999998	1.6867460000000001
S	20.9533929999999984	31.422223999999999	2.5115720000000001
S	40.3994969999999967	2.7605019999999998	1.884779999999999
S	38.7588629999999981	5.7085679999999996	2.142917999999999
S	36.9653610000000015	8.5017270000000007	2.0158390000000002
S	35.5174969999999988	11.2632569999999994	1.938226999999999
S	33.8622280000000018	14.130603999999999	2.2885070000000001
S	32.2841159999999974	16.975792999999995	1.7763340000000001
S	30.6763690000000011	19.8087969999999984	2.189004999999999
S	29.0300779999999996	22.540915999999993	1.7571500000000000
S	27.3567299999999989	25.3810040000000008	2.1364220000000000
S	25.7801450000000010	28.2402900000000017	1.6541920000000001
S	24.2288570000000014	31.4400680000000001	2.5011530000000000
S	45.4278189999999995	4.2283730000000004	4.841333999999998
S	43.8978150000000014	6.9271459999999996	4.6461920000000001

S	42.1161010000000005	9.4958969999999994	4.5588590000000000
S	40.6901989999999998	12.4628549999999994	4.4533589999999998
S	39.0957560000000015	15.2342669999999991	4.2891100000000000
S	37.5629399999999976	18.0125549999999990	4.3913209999999996
S	35.6562089999999969	20.8110630000000008	4.5445760000000002
S	34.2508550000000014	23.8004640000000016	4.4043190000000001
S	32.5805530000000019	26.5436550000000011	4.3439560000000004
S	30.8613479999999996	29.3226070000000014	4.2293209999999997
S	43.5474910000000008	3.0776420000000000	1.9474250000000000
S	41.9125209999999981	5.7068479999999999	2.0298010000000000
S	40.3896510000000006	8.5408510000000000	2.2199049999999998
S	38.8356449999999995	11.3559920000000005	1.8692070000000001
S	37.1285540000000012	14.1461550000000003	1.8257749999999999
S	35.5532189999999986	16.9092009999999995	1.8939310000000000
S	34.0274440000000027	19.8023640000000007	2.1622319999999999
S	32.3709199999999981	22.5478510000000014	1.8775850000000001
S	30.6343110000000003	25.2553449999999984	1.8435870000000001
S	29.1171259999999990	28.0192039999999984	1.7797909999999999
S	27.6479329999999983	31.3301160000000003	2.4596209999999998
W	30.6070330000000013	-0.7813030000000000	3.4444560000000002
S	29.0009090000000000	-2.3293370000000002	4.3710630000000004
S	32.1429049999999989	-0.2109580000000000	1.7034330000000000
W	33.6999240000000029	-0.7150339999999999	3.3889459999999998
S	32.2827559999999991	-2.3150870000000001	4.3481470000000000
S	35.2698070000000001	-0.0238180000000000	1.6598710000000001
W	36.8341020000000015	-0.5782220000000000	3.2998530000000001
S	35.6516560000000027	-2.3043130000000001	4.0704269999999996
S	38.8231079999999977	-0.3534210000000000	2.3251890000000000
S	46.7537730000000025	1.5260720000000001	2.7710910000000002

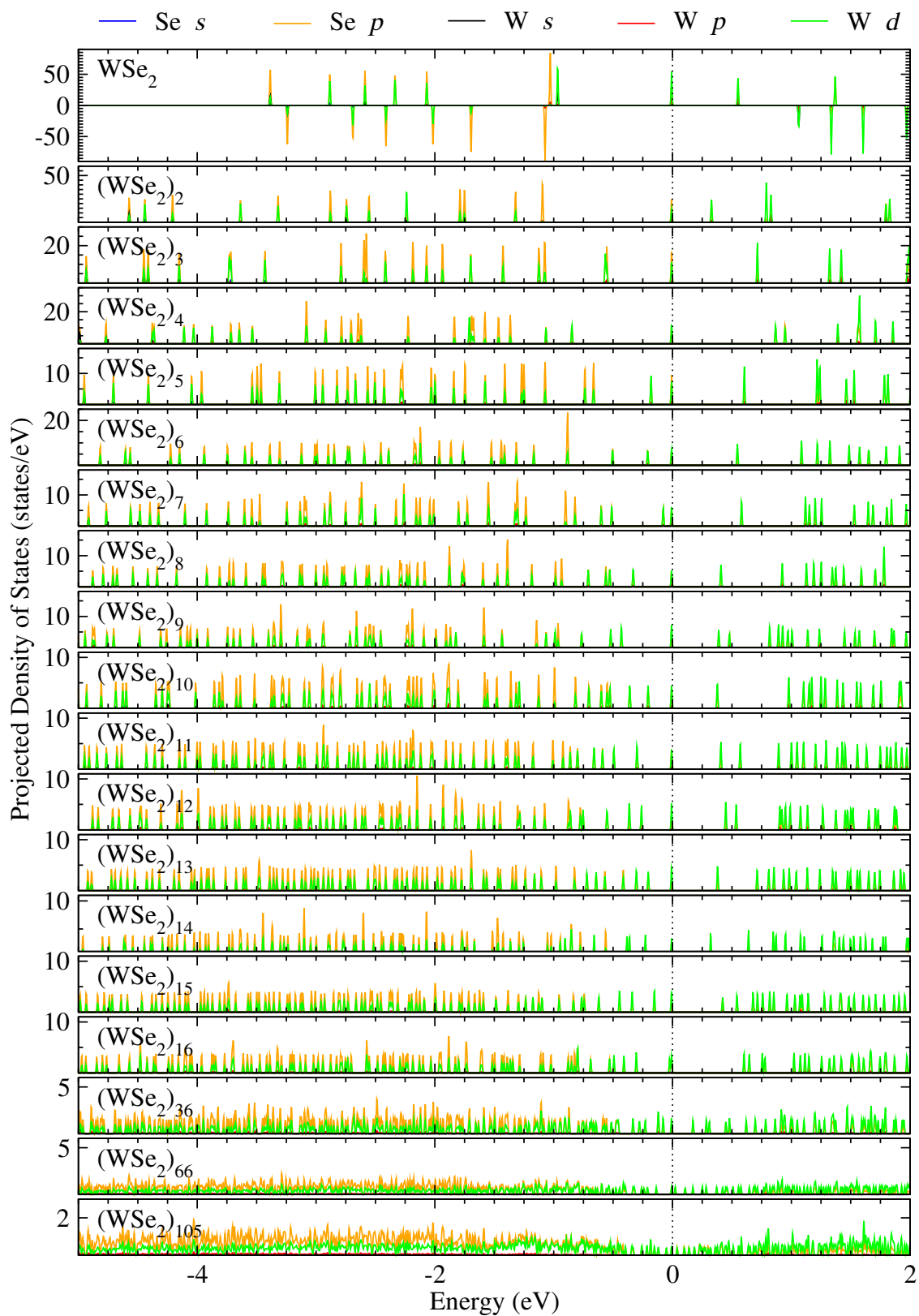


Figure S3: Projected density of states (PDOS) per f.u. of all our WSe_2 pGMCs.

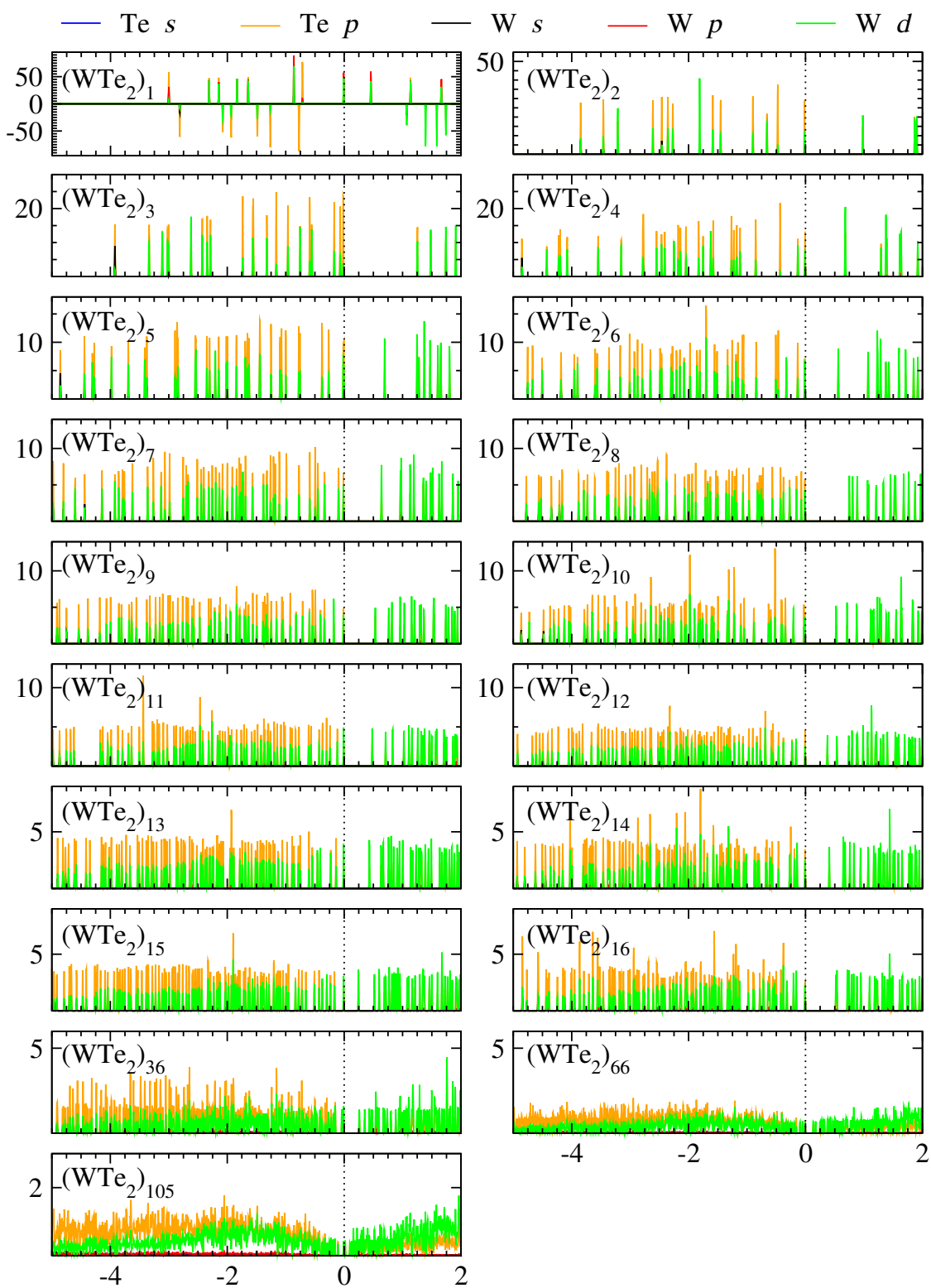


Figure S4: Projected density of states (PDOS) per f.u. of all our WTe_2 pGMCs.

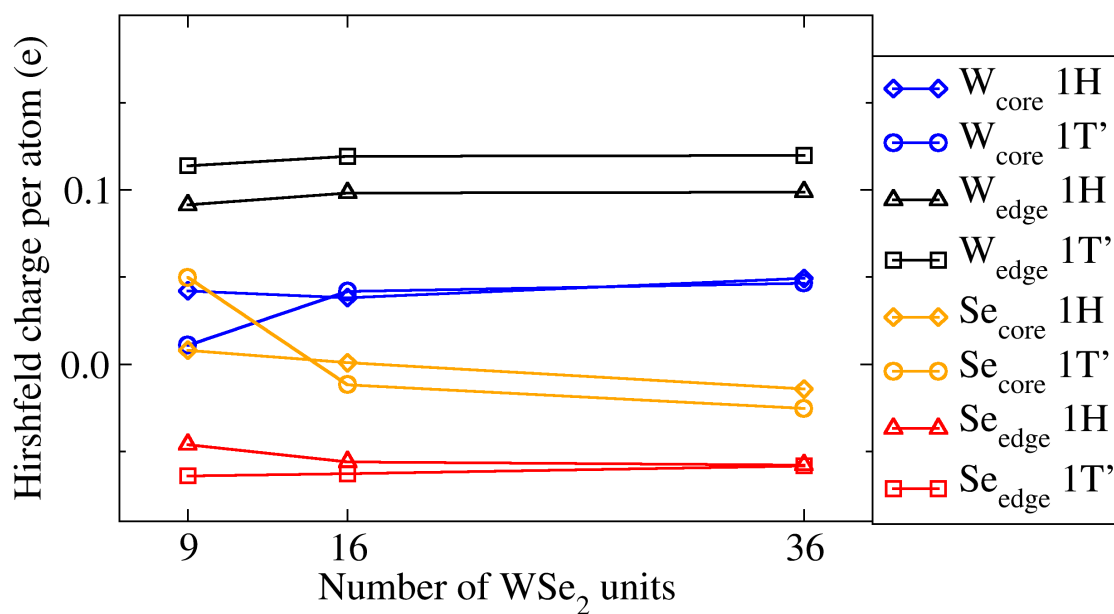


Figure S5: Hirshfeld charges for the WSe₂ as a function of size. For 2D 1T' and 1H nanoflakes, the atoms are divided in core and edge, according to their coordination. Projected density of states (PDOS) per f.u. of all our WTe₂ pGMCs.

W₁Se₂; $E_{tot}=-585\,786.557\,184\,49$ eV; $E_{rel}=0$ meV/f.u.

W	-0.7471090000000000	2.9001999999999999	0.0991500000000000
Se	1.4886640000000000	2.7177539999999998	0.3196100000000000
Se	-1.6878730000000000	1.2033140000000000	-1.0477430000000001

W₂Se₄; $E_{tot}=-1\,171\,577.976\,800\,61$ eV; $E_{rel}=56.080\,620\,500\,0$ meV/f.u.

W	0.6508389999999999	-0.2001480000000000	0.9445760000000000
Se	-0.7716499999999999	1.7252890000000001	1.6468719999999999
Se	-0.4337510000000000	-2.3270160000000000	0.2172230000000000
W	-0.2519010000000000	0.9276070000000000	-0.6588400000000000
Se	2.2424279999999999	0.9516340000000000	-0.5922150000000000
Se	-1.4359649999999999	-1.0773690000000000	-1.5576170000000000

W₂Se₄; $E_{tot}=-1\,171\,578.088\,961\,85$ eV; $E_{rel}=0$ meV/f.u.

W	1.1288590000000001	0.2172830000000000	-0.6348310000000000
Se	1.1734819999999999	2.4281320000000002	-0.0971550000000000
Se	-0.6534600000000000	-0.4598890000000000	-2.1521020000000002
W	-0.7826320000000000	-1.0329530000000000	0.2131920000000000
Se	1.4116979999999999	-1.3214980000000001	1.2336890000000000
Se	-2.2779490000000000	0.1689240000000000	1.4372039999999999

W₃Se₆; $E_{tot}=-1\,757\,370.726\,832\,83$ eV; $E_{rel}=138.034\,723\,666\,6$ meV/f.u.

W	-1.0722449999999999	0.8156330000000001	0.8688030000000000
Se	-2.2098369999999998	1.6938420000000001	-1.1620180000000000
Se	-2.1078929999999998	-0.8178430000000000	2.0665170000000002
W	1.2907660000000001	0.0673610000000000	0.2932570000000000
Se	0.9348940000000000	1.9130929999999999	1.8547220000000000
Se	1.6537580000000001	-2.3193350000000001	0.6790030000000000
W	-0.3970540000000000	0.0393300000000000	-1.4427829999999999
Se	1.8065519999999999	0.9788230000000000	-1.9301029999999999
Se	0.1010580000000000	-2.3709060000000002	-1.2273980000000000

W₃Se₆; $E_{tot}=-1\,757\,371.139\,938\,14$ eV; $E_{rel}=0.332\,953\,666\,6$ meV/f.u.

W	1.4299630000000001	-0.1534170000000000	-0.3212400000000000
Se	3.2709850000000000	-1.4574790000000000	-0.7119510000000000
Se	0.0726680000000000	0.4906070000000000	-2.2581080000000000
W	-0.0523820000000000	0.6424609999999999	1.7265889999999999
Se	-1.9477400000000000	1.8805920000000000	0.8902160000000000
Se	-0.0373260000000000	-1.6966129999999999	1.0018819999999999
W	-1.4068760000000000	-0.1431650000000000	-0.4117440000000000
Se	1.8998500000000000	1.8686100000000001	1.0092030000000001
Se	-3.2291439999999998	-1.4315940000000000	-0.9248470000000000

W₄Se₈; $E_{tot}=-2\,343\,163.292\,045\,39$ eV; $E_{rel}=26.548\,352\,750\,0$ meV/f.u.

W	-2.2172660000000000	1.3274900000000001	0.2271660000000000
Se	-1.4719110000000000	1.8087860000000000	-2.0412800000000000
Se	-3.7861370000000001	2.7797390000000002	1.0352380000000001
W	-0.4582380000000000	-0.8866120000000000	0.7030350000000000
Se	-2.9247049999999999	-1.0029800000000000	0.1909640000000000
Se	1.4720759999999999	-1.8088940000000000	2.0411280000000001
W	2.2173189999999998	-1.3273720000000000	-0.2268020000000000
Se	-0.2411930000000000	1.4395780000000000	1.6565900000000000
Se	3.7856160000000001	-2.7796699999999999	-1.0358010000000000
W	0.4585380000000000	0.8865610000000000	-0.7028460000000000
Se	2.9248509999999999	1.0028600000000001	-0.1909540000000000
Se	0.2410460000000000	-1.4394860000000000	-1.6564369999999999

W₄Se₈; $E_{tot}=-2\,343\,163.398\,238\,80$ eV; $E_{rel}=0$ meV/f.u.

W	1.2622439999999999	-1.6482740000000000	-0.0381780000000000
Se	1.4567200000000000	-3.9033460000000000	-0.3574890000000000
Se	2.5707339999999999	-0.4919040000000000	-1.7360810000000000
W	-1.9499759999999999	0.6722310000000000	-0.2346870000000000
Se	-4.1190559999999996	0.1191730000000000	-0.6984030000000000

Se	-1.8225220000000000	1.5635159999999999	2.0279560000000001
W	0.3969030000000000	0.6714020000000001	1.4194880000000001
Se	-1.1276260000000000	2.1786539999999999	-1.9630300000000001
Se	1.8814270000000000	-1.1148769999999999	2.2560090000000002
W	0.8113690000000000	1.0445560000000000	-0.9424650000000000
Se	1.7916859999999999	2.5425339999999998	0.7126220000000000
Se	-1.1519050000000000	-1.6336660000000001	-0.4457410000000000

W₅Se₁₀; $E_{tot} = -2\,928\,954.275\,590\,47$ eV; $E_{rel} = 202.432\,842\,200\,0$ meV/f.u.

W	-0.4953670000000000	1.8638260000000000	-1.9647159999999999
Se	1.0217449999999999	3.2198410000000002	-0.7275940000000000
Se	0.4495300000000000	0.8384850000000000	-3.7693340000000002
W	-2.2219139999999999	0.7606050000000000	0.3468420000000000
Se	-2.9209390000000002	1.7050850000000000	-1.8078620000000001
Se	-3.4201410000000001	2.0893009999999999	1.7544709999999999
W	-0.4604010000000000	-1.4374180000000001	1.2461760000000000
Se	-2.8914260000000001	-1.5291580000000000	0.8000370000000000
Se	1.2675230000000000	-2.4282439999999998	2.6809150000000002
W	2.2149359999999998	-1.8163380000000000	0.5136920000000000
Se	-0.2683830000000000	0.9055320000000000	2.0296400000000001
Se	3.4888740000000000	-3.4852599999999998	-0.3773230000000000
W	0.7329390000000000	0.6329210000000000	-0.1773870000000000
Se	3.1920910000000000	0.3687480000000000	0.5159530000000000
Se	0.3109320000000000	-1.6879270000000000	-1.0635090000000000

W₅Se₁₀; $E_{tot} = -2\,928\,955.287\,754\,68$ eV; $E_{rel} = 0$ meV/f.u.

W	-2.1593249999999999	2.2980019999999999	0.5488600000000000
Se	0.1055820000000000	3.0327220000000001	0.6384240000000000
Se	-3.7740900000000002	3.8264670000000001	0.0379380000000000
W	-1.7932370000000000	-0.3913890000000000	0.9251170000000000
Se	-2.0596869999999998	0.7282040000000000	-1.3320060000000000
Se	-2.8054589999999999	1.1101770000000000	2.5964489999999998

W	0.4544860000000000	-1.9960230000000001	0.1958460000000000
Se	-1.9418160000000000	-2.6904400000000002	-0.0684150000000000
Se	2.6960780000000000	-2.8137770000000000	0.8114360000000000
W	2.7671709999999998	-1.2174320000000001	-1.0504500000000001
Se	0.4125240000000000	-0.3580360000000000	2.0570379999999999
Se	4.2959470000000000	-1.9359890000000000	-2.5837759999999999
W	0.2907250000000000	0.5471570000000000	-0.3081250000000000
Se	2.9119860000000002	1.0305780000000000	-0.2733920000000000
Se	0.5991160000000000	-1.1702210000000000	-2.1949420000000002

W₆Se₁₂; $E_{tot} = -3\,514\,746.992\,343\,94$ eV; $E_{rel} = 36.238\,360\,166\,6$ meV/f.u.

W	-1.4922740000000001	-2.6091120000000001	1.7015199999999999
Se	0.7287030000000000	-3.0015320000000001	2.3978609999999998
Se	-3.3901550000000000	-1.4554980000000000	2.5364369999999998
W	-1.7563489999999999	2.6817940000000000	-0.0206420000000000
Se	0.4720320000000000	3.4469850000000002	0.1477040000000000
Se	-3.0692970000000002	4.3193320000000002	-0.8743620000000000
W	-1.7266290000000000	-0.2804820000000000	0.8726030000000000
Se	-1.7834420000000000	0.8045909999999999	-1.5582250000000000
Se	-2.7173479999999999	1.8061460000000000	1.9874529999999999
W	0.7056730000000000	-1.6365149999999999	0.0985650000000000
Se	-1.6168469999999999	-2.5121349999999998	-0.6906040000000000
Se	3.1907230000000002	-2.0931419999999998	0.2860620000000000
W	2.9669569999999998	-0.5499230000000001	-1.5326820000000001
Se	0.5649030000000000	0.2964260000000000	1.6731000000000000
Se	4.4611499999999999	-0.9193010000000000	-3.2086380000000001
W	0.6358100000000000	0.9752800000000000	-0.7025410000000000
Se	3.0747770000000001	1.6887989999999999	-0.7128100000000001
Se	0.7516090000000000	-0.9617130000000000	-2.4008010000000000

W₆Se₁₂; $E_{tot} = -3\,514\,747.209\,774\,10$ eV; $E_{rel} = 0$ meV/f.u.

W	-3.7392050000000001	1.5155170000000000	0.6522740000000000
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Se	-5.566330999999999	2.2193619999999998	1.8182250000000000
Se	-3.8346380000000000	-0.7250360000000000	-0.1600260000000000
W	-1.1123010000000000	2.1466870000000000	-0.1487110000000000
Se	1.1105200000000000	2.8044039999999999	0.5602250000000000
Se	-3.1743749999999999	3.1263489999999998	-1.1021069999999999
W	-1.3076319999999999	-0.3533010000000000	0.3988610000000000
Se	-0.7144660000000000	0.5230910000000000	-1.9320459999999999
Se	-1.8493930000000001	1.4524010000000001	2.1764329999999998
W	1.1101610000000000	-2.1469870000000002	0.1434250000000000
Se	-1.1119049999999999	-2.8034599999999998	-0.5674709999999999
Se	3.1692290000000001	-3.1286820000000000	1.1010150000000001
W	3.7400229999999999	-1.5153479999999999	-0.6489590000000000
Se	0.7128090000000000	-0.5250870000000000	1.9285220000000001
Se	5.5739419999999997	-2.2170440000000000	-1.8053800000000000
W	1.3063780000000000	0.3532140000000000	-0.4017780000000000
Se	3.8324210000000001	0.7236740000000000	0.1667250000000000
Se	1.8547650000000000	-1.4497519999999999	-2.1792289999999999

W₇Se₁₄; $E_{tot} = -4\ 100\ 538.049\ 657\ 65\ \text{eV}$; $E_{rel} = 96.713\ 464\ 428\ 5\ \text{meV/f.u.}$

W	-1.3851659999999999	-2.9522910000000002	1.8153340000000000
Se	0.9832910000000000	-3.0669759999999999	2.3694670000000002
Se	-1.8652340000000001	-0.9926070000000000	3.4258690000000001
W	-1.8441529999999999	2.6760510000000002	-0.0786590000000000
Se	0.3831960000000000	3.4661290000000000	0.0219840000000000
Se	-3.1545399999999999	4.2822319999999996	-0.9892190000000000
W	-1.7181999999999999	-0.4112630000000000	0.9001660000000000
Se	-1.8115300000000001	0.7101380000000000	-1.5092209999999999
Se	-2.7096510000000000	1.9031070000000001	1.9579990000000000
W	0.7347440000000000	-1.6368060000000000	0.2214160000000000
Se	-1.4780709999999999	-2.5721579999999999	-0.5848420000000000
Se	3.3449499999999999	-1.8636040000000000	0.4221020000000000
W	3.0343510000000000	-0.4593930000000000	-1.4592860000000001

Se	0.577655999999999	0.360243000000000	1.709370000000001
Se	4.557394999999996	-0.790632000000000	-3.116277999999999
W	0.621487000000000	0.969322000000000	-0.662647000000000
Se	2.995353999999998	1.831153000000000	-0.778712000000000
Se	0.851855999999999	-1.053021000000000	-2.298063000000000
W	-3.667319000000000	-2.224877999999999	2.396450000000002
Se	-3.114732000000001	-4.545415000000002	2.814136000000000
Se	-4.366467000000001	-1.000551000000000	0.520717000000000

W₇Se₁₄; $E_{tot} = -4\ 100\ 538.726\ 651\ 90\ \text{eV}$; $E_{rel} = 0\ \text{meV/f.u.}$

W	-3.467391000000001	3.171726000000000	1.046783000000000
Se	-4.898094999999996	4.890190999999997	0.607020000000000
Se	-1.281372000000000	3.736359000000002	1.743235000000001
W	-3.169972000000000	0.407488000000000	0.865469000000000
Se	-4.597559000000004	1.545256000000000	2.501173999999998
Se	-3.252983000000000	-1.584904000000001	-0.499216000000000
W	-0.856551000000000	1.492110000000000	0.286621000000000
Se	1.537590000000000	1.996337000000000	0.913616000000000
Se	-2.980961000000002	2.055294000000000	-1.067627000000001
W	-0.729304000000000	-1.225965999999999	0.173417000000000
Se	-0.354630000000000	0.289380000000000	-1.850428000000000
Se	-1.258786000000000	0.025011000000000	2.330665000000002
W	1.771940000000001	-2.740037000000001	-0.567877000000000
Se	-0.436732000000000	-3.383417999999998	-1.310317000000000
Se	3.874022000000001	-3.842562000000000	0.044309000000000
W	4.304308999999999	-1.778968000000001	-1.218075999999999
Se	1.363931000000000	-1.639842999999999	1.569412000000000
Se	6.085543999999996	-2.114749000000002	-2.599333999999998
W	1.679766000000001	-0.123803000000000	-0.453417000000000
Se	4.312740999999999	0.177580000000000	0.106457000000000
Se	2.354487999999999	-1.352482000000000	-2.621884999999998

W₈Se₁₆; $E_{tot}=-4\ 686\ 330.095\ 613\ 00\ \text{eV}$; $E_{rel}=37.873\ 656\ 375\ 0\ \text{meV/f.u.}$

W	-1.3250770000000001	-2.9307699999999999	1.6861950000000001
Se	0.9546300000000000	-3.4900730000000002	2.1567880000000001
Se	-1.5964760000000000	-1.0632960000000000	3.2718120000000002
W	-1.6441880000000000	2.6497720000000000	-0.1177170000000000
Se	0.5574249999999999	3.4486990000000000	0.0337120000000000
Se	-2.9770050000000001	4.2390080000000001	-1.0185610000000000
W	-1.7676950000000000	-0.2735820000000000	0.8275000000000000
Se	-1.5504119999999999	0.7873030000000000	-1.6458729999999999
Se	-2.3731100000000001	2.0097640000000001	2.1574629999999999
W	0.9796130000000000	-1.6656860000000000	0.1979790000000000
Se	-1.3250690000000001	-2.3912760000000000	-0.6730280000000000
Se	3.4603419999999998	-2.0093030000000001	0.5732470000000000
W	3.2431960000000002	-0.6009400000000000	-1.3541740000000000
Se	0.6854000000000000	0.3238220000000000	1.6159150000000000
Se	4.7816859999999997	-1.0748489999999999	-2.9627750000000002
W	0.8410590000000000	0.9382230000000000	-0.7258940000000000
Se	3.2305259999999998	1.7305960000000000	-0.7694780000000000
Se	1.0817810000000001	-1.0758570000000001	-2.3045900000000001
W	-3.7242510000000002	-1.8200719999999999	2.3079540000000001
Se	-3.3460730000000001	-4.2681950000000004	1.9969319999999999
Se	-4.1732870000000002	-0.8868490000000000	0.0676970000000000
W	-4.5406789999999999	0.8287110000000000	1.7697950000000000
Se	-6.4297540000000000	1.9371000000000000	1.1503030000000001
Se	-4.9801029999999997	-0.3163620000000000	3.8452320000000002

W₈Se₁₆; $E_{tot}=-4\ 686\ 330.398\ 602\ 25\ \text{eV}$; $E_{rel}=0\ \text{meV/f.u.}$

W	-5.2573829999999999	1.9437120000000001	0.7759210000000000
Se	-7.2611819999999998	2.1901809999999999	1.8326039999999999
Se	-5.0618069999999999	0.1147010000000000	-0.7168570000000000
W	-2.6001180000000002	2.9069870000000000	0.6292560000000000
Se	-4.5859490000000003	4.0689029999999997	-0.2384740000000000

Se	-0.5506030000000000	3.4882640000000000	1.7008909999999999
W	-2.6224900000000000	0.3287770000000000	0.3213020000000000
Se	-3.5723289999999999	1.4318880000000000	2.4532460000000000
Se	-2.2980139999999998	-1.7731669999999999	-1.0837019999999999
W	0.0447360000000000	1.3025329999999999	0.1587270000000000
Se	2.2959510000000001	1.7699840000000000	1.0817280000000000
Se	-1.8134180000000000	1.9480670000000000	-1.4790060000000000
W	-0.0473260000000000	-1.3143050000000001	-0.1506670000000000
Se	0.8258320000000000	0.2227460000000000	-1.9766330000000001
Se	-0.8357390000000000	-0.2367500000000000	1.9811140000000000
W	2.6060479999999999	-2.9124180000000002	-0.6181480000000000
Se	0.5526500000000000	-3.5098870000000000	-1.6752220000000000
Se	4.6070570000000002	-4.0537450000000002	0.2447590000000000
W	5.2583609999999998	-1.9317550000000001	-0.7881980000000000
Se	1.8190130000000000	-1.9465120000000000	1.4865349999999999
Se	7.2572840000000003	-2.1640160000000002	-1.8572130000000000
W	2.6193130000000000	-0.3335780000000000	-0.3225660000000000
Se	5.0616640000000004	-0.0966820000000000	0.6972790000000000
Se	3.5584479999999998	-1.4439270000000000	-2.4566750000000002

W₉Se₁₈; $E_{tot} = -5\,272\,121.852\,813\,44$ eV; $E_{rel} = 84.912\,525\,666\,6$ meV/f.u.

W	4.7518089999999997	-4.2200199999999999	-0.8344110000000000
Se	5.9911779999999997	-6.0450200000000001	-0.2596450000000000
Se	2.7229179999999999	-4.6089000000000002	-1.9742270000000000
W	-5.7573040000000004	2.7106189999999999	0.7648550000000000
Se	-7.7516189999999998	3.0077370000000001	1.8284510000000000
Se	-5.5897709999999998	0.8857810000000000	-0.7207930000000000
W	-3.1167859999999998	3.6144690000000002	0.6732340000000000
Se	-5.0370739999999996	4.8486940000000001	-0.2063620000000000
Se	-1.0601900000000000	4.0961720000000001	1.8145990000000001
W	-3.1016560000000002	1.0098440000000000	0.3400190000000000
Se	-4.1088540000000000	2.0896110000000001	2.4544120000000000

Se	-2.8430300000000002	-1.0632269999999999	-1.0164290000000000
W	-0.5134609999999999	1.9904230000000001	0.2390210000000000
Se	1.7818240000000001	2.4378280000000001	1.1398560000000000
Se	-2.3207640000000000	2.6675700000000000	-1.4314670000000000
W	-0.4827640000000000	-0.7185100000000000	-0.0593260000000000
Se	0.2985920000000000	0.8864880000000001	-1.8651930000000001
Se	-1.3677180000000000	0.3863920000000000	2.0278610000000001
W	2.1373449999999998	-2.4461870000000001	-0.4556840000000000
Se	-0.1201960000000000	-2.8626600000000000	-1.4260079999999999
Se	3.9377430000000002	-3.2027809999999999	1.2296570000000000
W	4.5674910000000004	-1.4530430000000001	-0.5084510000000000
Se	1.2845350000000000	-1.3569580000000001	1.6244950000000000
Se	6.2071339999999999	-2.5761870000000000	-1.9353170000000000
W	2.0414610000000000	0.3055070000000000	-0.1543840000000000
Se	4.4815620000000003	0.4486420000000000	0.9556480000000001
Se	2.9675929999999999	-0.8322870000000000	-2.2444139999999999

W₉Se₁₈; $E_{tot} = -5\,272\,122.617\,026\,17$ eV; $E_{rel} = 0$ meV/f.u.

W	32.7824710000000010	12.7555259999999997	2.6674669999999998
W	31.3988289999999992	15.2810000000000006	3.0583170000000002
W	29.9711280000000002	18.0594970000000004	3.5523030000000002
W	34.1661700000000010	15.2811109999999992	3.0589160000000000
W	32.7819939999999974	18.0292759999999994	3.3917280000000001
W	31.3646950000000011	20.7182920000000017	3.8463759999999998
W	35.5949889999999982	18.0597360000000009	3.5527700000000002
W	34.2004560000000026	20.7187069999999984	3.8460320000000001
W	32.7827580000000012	23.2714980000000011	4.2325290000000004
Se	32.7826310000000021	13.9662849999999992	4.7610820000000000
Se	31.1784880000000015	16.7180819999999990	5.1479670000000004
Se	28.9721450000000011	19.8578049999999990	4.7156789999999997
Se	34.3861970000000028	16.7181260000000016	5.1483600000000003
Se	32.7822850000000017	19.6105179999999990	5.4927950000000001

Se	30.7353470000000009	22.6631169999999997	5.3351590000000000
Se	36.5933739999999972	19.8578380000000010	4.7147059999999996
Se	34.8297519999999992	22.6633509999999987	5.3352659999999998
Se	32.7827180000000027	25.4639929999999985	3.6301660000000000
Se	32.7826850000000007	10.5552039999999998	3.2600600000000002
Se	30.7426390000000005	13.3962789999999998	1.5417240000000001
Se	29.0250379999999986	16.3490199999999994	2.2088310000000000
Se	34.8229600000000019	13.3962550000000000	1.5415010000000000
Se	32.7827070000000020	16.4284530000000011	1.3831580000000001
Se	31.1402639999999984	19.2535139999999991	1.7686400000000000
Se	36.5398240000000030	16.3491019999999985	2.2090239999999999
Se	34.4250759999999971	19.2533080000000005	1.7680149999999999
Se	32.7828289999999996	22.0230269999999990	2.1583869999999998

W₁₀Se₂₀; $E_{tot} = -5\,857\,913.420\,393\,40$ eV; $E_{rel} = 6.039\,706\,100\,0$ meV/f.u.

W	3.2986810000000002	1.6166970000000001	1.4219200000000001
Se	5.2603629999999999	1.1198020000000000	0.1959590000000000
Se	3.7794469999999998	2.9209999999999998	3.2114440000000002
W	4.7024689999999998	-3.8304140000000002	-0.8142030000000000
Se	5.9584929999999998	-5.7110750000000001	-0.5705290000000000
Se	3.1303299999999998	-4.0077059999999998	-2.6004730000000000
W	-6.2569920000000003	2.1878329999999999	0.5962330000000000
Se	-8.1362710000000007	2.5521370000000001	1.8375040000000000
Se	-6.1277629999999998	0.2360380000000000	-0.7256490000000000
W	-3.7222900000000001	3.1957800000000001	0.2615540000000000
Se	-5.7275369999999999	4.2267130000000002	-0.6792160000000000
Se	-1.5830510000000000	3.9147150000000002	1.2330939999999999
W	-3.5568170000000001	0.5767060000000001	0.0949380000000000
Se	-4.4531530000000004	1.7531829999999999	2.2023060000000001
Se	-3.3525369999999999	-1.5821460000000001	-1.2489830000000000
W	-1.1533650000000000	1.8262480000000001	-0.1261090000000000
Se	1.4688099999999999	2.5838709999999998	0.1195830000000000

Se	-3.0167160000000002	2.0855169999999998	-1.8275239999999999
W	-0.9768150000000000	-1.1977519999999999	-0.7463460000000000
Se	-0.0983930000000000	0.6784289999999999	-2.1138279999999998
Se	-1.6434180000000000	0.0648620000000000	1.5871350000000000
W	1.9377400000000000	-2.5763940000000001	-0.8042260000000000
Se	-0.1134580000000000	-2.8265940000000001	-2.3859599999999999
Se	3.3256429999999999	-3.5435099999999999	1.1425719999999999
W	3.9882279999999999	-1.1811449999999999	0.2213400000000000
Se	0.3221250000000000	-2.2723860000000000	1.0719790000000000
Se	6.0497189999999996	-1.8711850000000001	-1.0991670000000000
W	1.2566020000000000	0.0304510000000000	0.0422030000000000
Se	2.6340740000000000	-0.5119830000000000	2.3238129999999999
Se	2.8058519999999998	-0.4576920000000000	-1.8213630000000001

W₁₀Se₂₀; $E_{tot} = -5\ 857\ 913.480\ 790\ 46\ \text{eV}$; $E_{rel} = 0\ \text{meV/f.u.}$

W	6.4142080000000004	-3.3104879999999999	-0.4445810000000000
Se	6.2107479999999997	-1.5324130000000000	1.0938859999999999
Se	8.4917490000000004	-3.6730640000000001	-1.3075190000000001
W	3.6995680000000002	-4.0655029999999996	-0.6056390000000000
Se	5.4858120000000001	-5.4183269999999997	0.3936010000000000
Se	1.7378960000000001	-4.4320579999999996	-1.9034519999999999
W	-6.4195240000000000	3.2944070000000001	0.4480560000000000
Se	-8.5023359999999997	3.6191520000000001	1.3131550000000001
Se	-6.2001169999999997	1.5437820000000000	-1.1187170000000000
W	-3.7066940000000002	4.0635159999999999	0.6246890000000000
Se	-5.5023660000000003	5.4216759999999997	-0.3523260000000000
Se	-1.7489980000000001	4.4184700000000001	1.9314730000000000
W	-3.8620239999999999	1.4960270000000000	0.1918040000000000
Se	-4.9603370000000000	2.5739209999999999	2.2614640000000001
Se	-3.6045400000000001	-0.5616719999999999	-1.2329410000000001
W	-1.1370720000000001	2.2590119999999998	0.3606710000000000
Se	1.0589510000000000	2.6216210000000002	1.3528780000000000

Se	-2.7481460000000002	3.1318090000000001	-1.4242690000000000
W	-1.3881859999999999	-0.3698870000000000	-0.0676040000000000
Se	-0.2331470000000000	1.1716290000000000	-1.7173339999999999
Se	-2.3216899999999998	0.7202140000000000	2.0017980000000000
W	1.1414350000000000	-2.2498279999999999	-0.3593240000000000
Se	-1.0538520000000000	-2.6117729999999999	-1.3574440000000001
Se	2.7539699999999998	-3.1044800000000001	1.4346960000000000
W	3.8657360000000001	-1.4921599999999999	-0.2048620000000000
Se	0.2399630000000000	-1.1504690000000000	1.7099150000000001
Se	4.9542339999999996	-2.6021850000000000	-2.2636219999999998
W	1.3956210000000000	0.3822140000000000	0.0533590000000000
Se	3.6179999999999999	0.5803650000000000	1.2026060000000001
Se	2.3211409999999999	-0.7235050000000000	-2.0144169999999999

W₁₁Se₂₂; $E_{tot} = -6\,443\,704.948\,266\,86$ eV; $E_{rel} = 11.935\,118\,272\,7$ meV/f.u.

W	-6.4675979999999997	3.3270659999999999	0.4716520000000000
W	-3.7740520000000002	4.0522929999999997	0.6510880000000000
W	-3.8968210000000001	1.4740949999999999	0.1841800000000000
W	-1.2419890000000000	2.2822230000000001	0.3312890000000000
W	-1.3595240000000000	-0.3966240000000000	-0.1169160000000000
W	1.2912450000000000	0.4620480000000000	0.0148260000000000
W	1.2495130000000001	-2.2960690000000001	-0.3825760000000000
W	3.8088660000000001	-1.3858090000000001	-0.2770480000000000
W	3.8078910000000001	-4.1444679999999998	-0.6141880000000000
W	6.2736789999999996	-3.2570770000000002	-0.5276690000000001
W	6.3543269999999996	-6.0297770000000002	-0.8766510000000000
Se	-8.5276800000000001	3.7210230000000002	1.3647890000000000
Se	-5.5287369999999996	5.4534940000000001	-0.3185850000000000
Se	-5.0126220000000004	2.5159989999999999	2.2589260000000002
Se	-6.2852090000000000	1.5706979999999999	-1.0912590000000000
Se	-1.8015260000000000	4.3642779999999997	1.9685600000000001
Se	-2.8620749999999999	3.1542110000000001	-1.4321600000000001

Se	-2.3422679999999998	0.6530490000000000	1.9590879999999999
Se	-3.6598039999999998	-0.5560250000000000	-1.2393149999999999
Se	0.9911660000000000	2.6161680000000000	1.3461559999999999
Se	-0.3204190000000000	1.2395270000000000	-1.7574710000000000
Se	0.2593430000000000	-1.1933650000000000	1.6555460000000000
Se	-1.0621370000000001	-2.5558139999999998	-1.3899670000000000
Se	3.6233860000000000	0.7416030000000000	0.9871230000000000
Se	2.2110919999999998	-0.6523940000000000	-2.0593370000000002
Se	1.5883959999999999	-4.4558439999999999	-1.7107260000000000
Se	6.2221650000000004	-1.3652650000000000	0.9384550000000000
Se	2.8697200000000000	-3.0409940000000000	1.4175570000000000
Se	4.7901790000000002	-2.5400019999999999	-2.3327900000000001
Se	4.3731520000000002	-6.3154139999999996	-2.1268120000000001
Se	5.4822259999999998	-4.9911870000000000	1.1549780000000001
Se	7.9297100000000000	-4.4402270000000001	-1.8851979999999999
Se	7.4902069999999998	-7.9106670000000001	-0.2696410000000000

W₁₁Se₂₂; $E_{tot} = -6\,443\,705.079\,553\,16$ eV; $E_{rel} = 0$ meV/f.u.

W	-5.8715669999999998	4.3906549999999998	1.3685920000000000
Se	-7.3080309999999997	6.1200089999999996	0.9804480000000000
Se	-3.7629920000000001	4.8444250000000002	2.3505029999999998
W	3.9540329999999999	0.8166960000000000	1.3855740000000001
Se	5.8370329999999999	0.4653170000000000	-0.0017680000000000
Se	4.5464950000000002	1.8734080000000000	3.2999260000000001
W	5.1423990000000002	-4.3003320000000000	-1.6084609999999999
Se	6.3823590000000001	-6.2064170000000001	-1.6468520000000000
Se	3.4987599999999999	-4.2241499999999998	-3.3328639999999998
W	-5.5514180000000000	1.6901200000000001	0.8330959999999999
Se	-7.0762140000000002	2.5867439999999999	2.5215630000000000
Se	-5.5625679999999997	-0.1231950000000000	-0.7364170000000000
W	-3.2178559999999998	2.8344710000000002	0.6527720000000000
Se	-5.1830850000000002	3.5676660000000000	-0.8280320000000000

Se	-0.8569300000000000	3.3196159999999999	1.4782780000000000
W	-3.0103890000000000	0.1131170000000000	0.1241040000000000
Se	-3.7455530000000001	1.0460910000000001	2.3761700000000001
Se	-2.8722759999999998	-1.9516260000000001	-1.3544900000000000
W	-0.6222850000000000	1.3379430000000001	0.0598860000000000
Se	2.0897619999999999	1.9630719999999999	0.3050740000000000
Se	-2.4618709999999999	1.8952410000000000	-1.5602739999999999
W	-0.4614380000000000	-1.6495470000000001	-0.9758310000000000
Se	0.3767470000000000	0.4154300000000000	-2.0685030000000002
Se	-1.0778589999999999	-0.6674550000000000	1.4915270000000000
W	2.3970630000000002	-3.0258039999999999	-1.3114530000000000
Se	0.2910230000000000	-3.0387979999999999	-2.8457750000000002
Se	3.8476870000000001	-4.2557720000000003	0.4244890000000000
W	4.5218429999999996	-1.8043020000000001	-0.2080650000000000
Se	0.8753470000000000	-2.9362279999999998	0.6653770000000000
Se	6.5162540000000000	-2.3397630000000000	-1.6870890000000001
W	1.8130620000000000	-0.5476470000000000	-0.0945620000000000
Se	3.2873380000000001	-1.4042990000000000	2.0262410000000002
Se	3.2651279999999998	-0.8046840000000000	-2.0831810000000002

$\mathbf{W}_{12}\mathbf{Se}_{24}$; $E_{tot} = -7\,029\,496.521\,113\,23$ eV; $E_{rel} = 136.598\,508\,416\,6$ meV/f.u.

W	-6.4612930000000004	3.3317990000000002	0.4511080000000000
W	-3.7512989999999999	4.0757700000000003	0.6282900000000000
W	-3.9030689999999999	1.5034179999999999	0.1911560000000000
W	-1.2006850000000000	2.2740809999999998	0.3556350000000000
W	-1.4020480000000000	-0.3669840000000000	-0.0949240000000000
W	1.3422490000000000	0.3903990000000000	0.0828800000000000
W	1.1504080000000001	-2.2816310000000000	-0.3958810000000000
W	3.8923340000000000	-1.5243420000000001	-0.1986220000000000
W	3.6995300000000002	-4.1636340000000001	-0.6604290000000000
W	6.3990729999999996	-3.3891300000000002	-0.4575450000000000
W	6.2577439999999998	-5.9609110000000003	-0.9056650000000001

W	8.964708999999992	-5.2134650000000002	-0.6857780000000000
Se	-8.537181999999996	3.6989589999999999	1.3173699999999999
Se	-5.5266950000000001	5.4505030000000003	-0.3543260000000000
Se	-5.0067360000000001	2.5788750000000000	2.2587799999999998
Se	-6.2607980000000003	1.5739980000000000	-1.1080820000000000
Se	-1.7962240000000000	4.4144470000000000	1.9488040000000000
Se	-2.8067790000000001	3.1430140000000000	-1.4278810000000000
Se	-2.3610150000000001	0.7004970000000000	1.9858330000000000
Se	-3.6640259999999998	-0.5455960000000000	-1.2260080000000000
Se	1.0043500000000001	2.6395780000000002	1.3439710000000000
Se	-0.2488190000000000	1.2168850000000000	-1.7113080000000001
Se	0.1812170000000000	-1.2194170000000000	1.6723619999999999
Se	-1.0751390000000001	-2.5246369999999998	-1.4494600000000000
Se	3.5629840000000002	0.6344950000000000	1.1494650000000000
Se	2.3197980000000000	-0.6709770000000000	-1.9789540000000001
Se	1.5072010000000000	-4.5143060000000004	-1.6811560000000001
Se	6.1391890000000000	-1.3496729999999999	0.9664950000000000
Se	2.7281179999999998	-3.1183299999999998	1.4021699999999999
Se	4.8794709999999997	-2.5819770000000002	-2.2697180000000001
Se	4.3190059999999999	-6.2992499999999998	-2.2503579999999999
Se	5.2849550000000001	-5.0376310000000002	1.1405390000000000
Se	8.7401780000000002	-3.4587080000000001	0.8734240000000000
Se	7.5347650000000002	-4.4567490000000003	-2.5117630000000002
Se	8.0198959999999992	-7.3337170000000000	0.1041880000000000
Se	11.0532620000000001	-5.5808130000000000	-1.5198140000000000

W₁₂Se₂₄; $E_{tot} = -7\,029\,498.160\,295\,33$ eV; $E_{rel} = 0$ meV/**f.u.**

W	34.39466500000000034	9.85877600000000006	2.76867500000000000
W	33.0310589999999991	12.50820700000000005	2.94290999999999999
W	31.39588600000000008	15.17422099999999993	3.15314199999999999
W	29.90510000000000009	18.14772100000000007	3.45068800000000000
W	35.80351900000000014	12.43195700000000006	3.12425800000000002

W	34.672496999999999	15.043129999999997	3.3227030000000002
W	32.526870999999999	18.1779970000000013	3.5916489999999999
W	31.3959140000000012	20.7886969999999991	3.7891810000000001
W	37.2941190000000020	15.0735399999999995	3.4642279999999999
W	35.8036710000000014	18.0470480000000002	3.7619520000000000
W	34.1679200000000023	20.7130690000000008	3.9703279999999999
W	32.8045520000000010	23.3627280000000006	4.1419160000000002
Se	34.2783140000000017	11.1917240000000007	4.7811890000000004
Se	32.7096639999999965	14.0189649999999997	4.9077140000000004
Se	30.9848360000000014	16.7589870000000012	5.1530610000000001
Se	29.0055119999999995	19.9415319999999987	4.6920570000000001
Se	36.0628230000000016	13.9099780000000006	5.2317000000000000
Se	34.2369449999999986	16.8808779999999992	5.1360669999999997
Se	32.6628309999999971	19.6951819999999991	5.6372530000000003
Se	30.7673850000000009	22.7692949999999996	5.2460149999999999
Se	38.1684699999999992	17.1250490000000006	4.4354760000000004
Se	36.4557390000000012	20.0259350000000005	4.9731920000000001
Se	34.7164190000000019	22.7518640000000012	5.4342280000000001
Se	32.8128329999999977	25.5527920000000002	3.5226709999999999
Se	34.3864159999999970	7.6681299999999997	3.3844420000000000
Se	32.4828130000000002	10.4710889999999992	1.4763700000000000
Se	30.7437250000000013	13.1961080000000006	1.9410250000000000
Se	29.0307800000000000	16.0960320000000010	2.4800789999999999
Se	36.4319220000000001	10.4532889999999998	1.6644450000000000
Se	34.5367669999999976	13.5274260000000002	1.2765890000000000
Se	32.9624540000000010	16.3403700000000001	1.7787160000000000
Se	31.1360290000000006	19.3097929999999991	1.6826260000000000
Se	38.1940099999999987	13.2798940000000005	2.2214049999999999
Se	36.2148979999999980	16.4622740000000007	1.7615590000000001
Se	34.4899369999999976	19.2016010000000001	2.0061789999999999
Se	32.9209960000000024	22.0281319999999994	2.1302569999999998

$W_{13}Se_{26}$; $E_{tot} = -7\,615\,288.018\,755\,50$ eV; $E_{rel} = 119.424\,446\,230\,7$ meV/f.u.

W	-6.506542999999997	3.366690999999999	0.461154000000000
W	-3.811785000000000	4.079193000000001	0.654498000000000
W	-3.945913000000000	1.504213000000000	0.168961000000000
W	-1.284230000000000	2.290020999999999	0.352762000000000
W	-1.421214999999999	-0.374478000000000	-0.129441000000000
W	1.247459000000001	0.445652000000000	0.065426000000000
W	1.179387000000000	-2.283990999999999	-0.424452000000000
W	3.810547000000001	-1.424203000000001	-0.208959000000000
W	3.789121999999999	-4.192317000000001	-0.612652000000000
W	6.338123999999996	-3.285353000000002	-0.450643000000000
W	6.339885999999999	-6.045078000000002	-0.799083000000000
W	8.808151999999998	-5.168615000000000	-0.650072000000000
W	8.879514000000004	-7.940786000000001	-1.002604000000001
Se	-8.563807000000006	3.767155999999999	1.359148000000000
Se	-5.555519000000003	5.493375000000003	-0.315223000000000
Se	-5.061903000000000	2.542228999999998	2.248832000000002
Se	-6.329208999999996	1.620358000000000	-1.113124000000000
Se	-1.850668000000000	4.377195000000004	1.990221000000000
Se	-2.881923000000000	3.186471000000001	-1.423332000000000
Se	-2.414107000000000	0.655586000000000	1.950957000000001
Se	-3.707249000000000	-0.508463000000000	-1.278802999999999
Se	0.920569000000000	2.598974999999998	1.414258999999999
Se	-0.325895000000000	1.267196000000000	-1.728004000000001
Se	0.156051000000000	-1.240523000000000	1.635891999999999
Se	-1.117877999999999	-2.512324000000000	-1.447093000000000
Se	3.536217999999999	0.728514000000000	1.063800000000001
Se	2.248368000000001	-0.601949000000000	-1.999063000000000
Se	1.494842000000000	-4.456561999999999	-1.658439999999999
Se	2.746277000000001	-3.092194000000001	1.394860000000000
Se	4.778820999999998	-2.536592999999999	-2.264273000000002
Se	4.146979000000000	-6.344078999999998	-1.948096000000000

Se	6.148333000000000	-1.163424999999999	0.799339000000000
Se	5.364193000000000	-4.943659000000000	1.217665000000000
Se	7.368514000000000	-4.434403999999998	-2.485932000000000
Se	6.933422000000000	-8.214092000000000	-2.305575999999998
Se	8.730335999999994	-3.285086999999999	0.822571000000000
Se	7.966480999999999	-6.902400000000000	1.009163000000000
Se	10.492122000000000	-6.359575999999997	-1.966051000000000
Se	9.988576999999994	-9.827341999999998	-0.363566000000000

W₁₃Se₂₆; $E_{tot} = -7\,615\,289.569\,732\,55$ eV; $E_{rel} = 0.118\,519\,307\,6$ meV/f.u.

W	2.214300000000000	-6.278048000000000	-1.476034000000000
Se	1.745376000000000	-8.004075000000000	-2.885724000000000
Se	0.420325000000000	-5.492917000000000	-0.189153000000000
W	-1.120506000000000	4.660727999999998	1.193489000000000
Se	-2.800241999999999	6.032559000000000	0.248704000000000
Se	0.784199000000000	5.052653000000000	2.649156000000000
W	1.544667999999999	3.024458000000000	1.228294000000000
Se	0.166344000000000	3.916996999999998	-0.731781000000000
Se	2.785029000000000	2.013402000000000	-0.746215000000000
W	3.921816999999999	1.262672000000000	1.286906000000000
Se	5.850863999999996	0.322989000000000	0.209717000000000
Se	3.632158000000000	3.195901000000000	2.702602999999999
W	4.156816000000000	-4.431033000000000	-0.636530000000000
Se	4.211701999999998	-6.839414999999998	-0.163025000000000
Se	2.758989000000000	-4.287720000000000	-2.771713999999998
W	-6.418530999999998	2.487731000000000	-0.282263000000000
Se	-8.613704000000000	2.549993999999999	0.307868000000000
Se	-5.956121999999997	0.843219000000000	-1.940196000000000
W	-3.771533999999999	3.552160000000000	0.435138000000000
Se	-5.635620000000000	4.666588000000000	-0.876954000000000
Se	-2.381739000000000	3.089284000000000	2.572798000000000
W	-3.893384999999999	0.832427999999999	-0.377128000000000

Se	-5.1664149999999998	1.7506240000000000	1.6543420000000000
Se	-3.4591219999999998	-1.2121630000000001	-1.8788279999999999
W	-1.2890219999999999	2.0949550000000001	0.4409830000000000
Se	0.4012620000000000	1.1422110000000001	2.1623060000000001
Se	-2.7412150000000000	2.6039889999999999	-1.6211070000000001
W	-1.3952490000000000	-0.9930010000000000	-0.6591430000000000
Se	-0.0052730000000000	0.7386870000000000	-1.4779320000000000
Se	-2.4677699999999998	-0.1222940000000000	1.4472280000000000
W	1.8596770000000000	-3.1611199999999999	-0.6174170000000000
Se	-0.4349960000000000	-2.8184220000000000	-1.9914499999999999
Se	3.2880620000000000	-3.7152050000000001	1.5227370000000000
W	4.0671830000000000	-1.6314070000000001	0.3389360000000000
Se	0.2221800000000000	-2.0813880000000000	1.0846309999999999
Se	5.8199880000000004	-2.7944640000000001	-1.2342089999999999
W	1.8185570000000000	-0.1499270000000000	0.3353010000000000
Se	3.1199360000000000	-0.6791540000000000	2.5186920000000002
Se	2.7610079999999999	-1.1424810000000001	-1.7830269999999999

W₁₄Se₂₈; $E_{tot} = -8\,201\,079.566\,448\,13$ eV; $E_{rel} = 177.343\,202\,214\,2$ meV/f.u.

W	-6.4925750000000004	3.3634189999999999	0.4532600000000000
W	-3.7874379999999999	4.0973269999999999	0.6285849999999999
W	-3.9325709999999998	1.5219579999999999	0.1883420000000000
W	-1.2467420000000000	2.2947340000000001	0.3582220000000000
W	-1.4270879999999999	-0.3583250000000000	-0.1029510000000000
W	1.2850130000000000	0.4136440000000000	0.1000190000000000
W	1.1376230000000001	-2.2781579999999999	-0.4209840000000000
W	3.8367510000000000	-1.5182890000000000	-0.1277560000000000
W	3.7040440000000001	-4.2030310000000002	-0.6717350000000000
W	6.4071579999999999	-3.4242149999999998	-0.4056570000000000
W	6.2576890000000001	-6.0672069999999998	-0.9104360000000000
W	8.9354089999999999	-5.2745249999999997	-0.6664410000000000
W	8.8246120000000001	-7.8461499999999997	-1.1403669999999999

W	11.5191700000000008	-7.0861409999999996	-0.9008020000000000
Se	-8.5603429999999996	3.7415500000000002	1.3334740000000000
Se	-5.5535430000000003	5.4815389999999997	-0.3539680000000000
Se	-5.0374900000000000	2.5934750000000002	2.2552910000000002
Se	-6.3020009999999997	1.6022989999999999	-1.1031340000000001
Se	-1.8293539999999999	4.4243040000000002	1.9543280000000001
Se	-2.8467120000000001	3.1690689999999999	-1.4296240000000000
Se	-2.3966129999999999	0.7024560000000000	1.9790070000000000
Se	-3.7043439999999999	-0.5185580000000000	-1.2338350000000000
Se	0.9530820000000000	2.6290439999999999	1.3928179999999999
Se	-0.2818430000000000	1.2444759999999999	-1.7060360000000001
Se	0.1415750000000000	-1.2403210000000000	1.6582490000000001
Se	-1.1203590000000001	-2.4929540000000001	-1.4608449999999999
Se	3.5222380000000002	0.6663559999999999	1.1552810000000000
Se	2.3197190000000001	-0.6170620000000000	-1.9435060000000000
Se	1.4744139999999999	-4.4369940000000003	-1.7461130000000000
Se	2.6521029999999999	-3.1960660000000001	1.3786579999999999
Se	4.8728899999999999	-2.5301969999999998	-2.1941970000000000
Se	4.0872770000000003	-6.3813680000000002	-2.0104570000000002
Se	6.0676079999999999	-1.3162529999999999	0.9794030000000000
Se	5.2376050000000003	-5.0614280000000003	1.1473590000000000
Se	8.6560799999999993	-3.2631039999999998	0.7833560000000001
Se	7.4346269999999999	-4.4428400000000003	-2.4799920000000002
Se	6.8954420000000001	-8.1772320000000001	-2.5078809999999998
Se	7.8271980000000001	-6.9495430000000002	0.9044320000000000
Se	11.2818980000000000	-5.3396059999999999	0.6657780000000000
Se	10.0927030000000002	-6.3128349999999998	-2.7246229999999998
Se	10.5839549999999996	-9.2176410000000004	-0.1283230000000000
Se	13.6069940000000003	-7.4386780000000003	-1.7433940000000001

$\mathbf{W}_{14}\mathbf{Se}_{28}$; $E_{tot}=-8\ 201\ 082.049\ 252\ 96\ \text{eV}$; $E_{rel}=0\ \text{meV/f.u.}$

W	36.256751999999998	1.4524220000000001	3.4479080000000000
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W	34.8748750000000030	3.8476520000000001	3.4441649999999999
W	39.5455949999999987	1.2290950000000000	3.6208309999999999
W	37.5203190000000006	3.7792710000000000	3.4799829999999998
W	36.3243790000000004	6.8085589999999998	3.6168740000000001
W	42.4849880000000013	1.1508309999999999	3.8416720000000000
W	41.3386560000000003	3.7551130000000001	3.6526679999999998
W	39.4089719999999986	7.0972949999999999	3.6525810000000001
W	37.7262490000000028	9.3921679999999999	3.8416280000000000
W	45.5010290000000026	1.0346820000000001	3.9715720000000001
W	43.9677000000000007	3.7475630000000000	3.8495720000000002
W	42.4741890000000026	6.6383029999999996	3.7601879999999999
W	40.7187600000000032	9.3776080000000004	3.8517210000000000
W	39.1334159999999969	12.0613600000000005	3.9740530000000001
Se	37.5334100000000035	-0.3251670000000000	4.4931250000000000
Se	36.0381259999999983	2.9250609999999999	5.4321229999999998
Se	33.9710759999999965	5.8434939999999997	4.4880950000000004
Se	40.8466740000000001	-0.5954100000000000	4.5752160000000002
Se	39.3497920000000008	2.9641899999999999	5.2290760000000001
Se	37.7277569999999969	5.7724399999999996	5.2274859999999999
Se	35.3940809999999999	8.8466850000000008	4.5709920000000004
Se	44.0512519999999981	-0.4827020000000000	5.0873460000000001
Se	42.5564699999999974	2.7729279999999998	5.6806140000000003
Se	40.9026509999999988	5.7317689999999999	5.3198770000000000
Se	39.1649499999999975	8.6432769999999994	5.6809539999999998
Se	37.0943839999999980	11.5644030000000004	5.0874379999999997
Se	47.3663799999999995	-0.0302580000000000	3.2394059999999998
Se	46.0598099999999988	2.9351219999999998	5.2570680000000003
Se	44.6740610000000018	5.9699669999999996	4.7836480000000003
Se	42.9949470000000034	8.8758669999999995	4.7872620000000001
Se	41.0588880000000032	11.5950980000000001	5.2599720000000003
Se	39.1432709999999986	14.2093749999999996	3.2421570000000002
Se	34.1162429999999972	1.8116470000000000	2.2764069999999998
Se	37.9325189999999992	1.9164030000000001	1.7107079999999999

Se	36.115485999999971	5.066643000000000	1.707794000000000
Se	41.131127999999968	1.972888999999999	1.833537999999999
Se	39.493389999999980	4.917932999999997	2.207155000000002
Se	37.763404999999988	7.809255000000003	1.832627999999999
Se	44.318055000000011	1.944458999999999	2.061611000000001
Se	42.896977999999972	4.975756999999998	1.929048000000001
Se	41.246490000000014	7.836691000000001	1.930344000000001
Se	39.332067999999996	10.583498999999998	2.064973000000002

W₁₅Se₃₀; $E_{tot} = -8\,786\,871.085\,215\,88$ eV; $E_{rel} = 162.622\,492\,066\,6$ meV/f.u.

W	-6.534473000000002	3.363008999999999	0.459076000000000
W	-3.839971999999999	4.080822999999996	0.679729000000000
W	-3.968054000000000	1.508750000000000	0.179871000000000
W	-1.306362000000000	2.296181999999999	0.383658000000000
W	-1.442250999999999	-0.364311000000000	-0.115362000000000
W	1.233004999999999	0.448844000000000	0.093425000000000
W	1.150517000000000	-2.267796999999998	-0.417917000000000
W	3.797763000000002	-1.429738000000000	-0.186820000000000
W	3.755946999999999	-4.171044000000002	-0.677675000000000
W	6.373993999999997	-3.298013999999998	-0.462424000000000
W	6.359793999999999	-6.067287000000003	-0.898605000000000
W	8.905620000000008	-5.162077000000000	-0.707037000000000
W	8.906807999999998	-7.916216000000004	-1.123447000000001
W	11.374299000000006	-7.050620000000003	-0.929671000000000
W	11.440124000000008	-9.814488000000008	-1.368211000000001
Se	-8.599854000000006	3.752759999999999	1.341266000000001
Se	-5.580174999999997	5.495479999999997	-0.296872000000000
Se	-5.101847000000002	2.532804000000001	2.255240999999998
Se	-6.339820999999997	1.626989999999999	-1.124109999999999
Se	-1.889102000000001	4.376871000000004	2.028403000000000
Se	-2.893262000000000	3.200457000000001	-1.395996000000000
Se	-2.445780000000001	0.653280000000000	1.966865000000001

Se	-3.722783999999999	-0.497689000000000	-1.274610999999999
Se	0.893220000000000	2.610589000000000	1.444421000000000
Se	-0.335478000000000	1.286575999999999	-1.698132000000000
Se	0.132896000000000	-1.240667000000000	1.650639000000000
Se	-1.140255000000000	-2.491533000000000	-1.449678000000000
Se	3.500687999999998	0.721713000000000	1.113037000000001
Se	2.240516000000000	-0.580584000000000	-1.973301000000000
Se	1.447127000000001	-4.437635000000002	-1.666863000000000
Se	2.715352000000002	-3.128455999999999	1.371285000000001
Se	4.806227999999999	-2.474905000000001	-2.250312000000001
Se	4.066843000000004	-6.326645000000001	-1.941130000000000
Se	6.110750000000003	-1.153939000000000	0.801496000000000
Se	5.324113999999998	-4.985063000000002	1.129367999999999
Se	7.356672999999998	-4.384330000000003	-2.520222000000000
Se	6.721458000000002	-8.185681000000007	-2.288822999999998
Se	8.717885000000008	-3.061466999999999	0.564573000000000
Se	7.925295000000002	-6.862981000000004	0.917927000000000
Se	11.291055999999993	-5.206038000000004	0.588208000000000
Se	9.953428000000006	-6.261890000000002	-2.757342000000000
Se	9.504773000000001	-10.035930000000005	-2.697195999999999
Se	10.516165000000009	-8.833968000000005	0.668488000000000
Se	13.065421999999999	-8.208914000000000	-2.265781000000000
Se	12.532391000000005	-11.730173000000006	-0.789714000000000

W₁₅Se₃₀; $E_{tot} = -8\ 786\ 873.524\ 553\ 26\ \text{eV}$; $E_{rel} = 0\ \text{meV/f.u.}$

W	5.434720999999997	-0.601981000000000	0.949646000000000
Se	5.254713999999999	0.952773000000000	2.718376999999998
Se	7.309391999999999	-1.479754000000000	-0.173244000000000
W	5.332042999999996	-5.970353000000002	-1.705032000000001
Se	6.094661999999996	-8.101839999999993	-1.488348999999999
Se	3.739421999999998	-5.702567000000002	-3.454143999999999
W	5.377848000000002	-3.371770999999999	-0.414605000000000

Se	4.4232370000000003	-2.6406830000000001	1.8350770000000001
Se	7.1822189999999999	-4.4311720000000001	-1.7844650000000000
W	-2.3626700000000000	4.6585010000000002	1.9575970000000000
Se	-4.0221999999999998	6.1899930000000003	1.2822700000000000
Se	-0.4471630000000000	4.7964380000000002	3.3909020000000001
W	0.4167620000000000	2.9714999999999998	1.5877319999999999
Se	-1.0254460000000001	4.2896690000000000	-0.0603440000000000
Se	1.6698569999999999	2.4998269999999998	-0.5187510000000000
W	2.9037839999999999	1.3422959999999999	1.3165110000000000
Se	4.2992689999999998	0.7478920000000000	-0.7359580000000000
Se	2.4499369999999998	3.0586799999999998	3.0186229999999998
W	2.8949660000000002	-4.1757090000000003	-1.5285830000000000
Se	4.1102699999999999	-5.4894740000000004	0.3223070000000000
Se	0.8958280000000000	-4.1516849999999996	-3.1336919999999999
W	-7.6984430000000001	2.8652660000000001	-0.0474190000000000
Se	-9.9020620000000008	2.8050199999999998	0.5133940000000000
Se	-7.2018250000000004	1.6254230000000001	-2.0201199999999999
W	-5.0613770000000002	3.7235140000000002	0.9443340000000000
Se	-6.8995329999999999	5.1192589999999996	-0.1033890000000000
Se	-3.6990720000000001	2.8749340000000001	2.9591440000000002
W	-5.1673210000000003	1.2715669999999999	-0.4588960000000000
Se	-6.4891249999999996	1.7286940000000000	1.7138119999999999
Se	-4.6393199999999997	-0.3267400000000000	-2.4020280000000001
W	-2.5884730000000000	2.3246799999999999	0.6769320000000000
Se	-0.9030560000000000	1.0709860000000000	2.2272490000000000
Se	-3.9869990000000000	3.2695630000000002	-1.2559020000000001
W	-2.6993350000000000	-0.4207970000000000	-0.9890460000000000
Se	-1.2516910000000001	1.3936379999999999	-1.4613039999999999
Se	-3.7926720000000000	-0.0069340000000000	1.2019850000000001
W	0.3984740000000000	-2.5221410000000000	-1.4308970000000001
Se	-1.8715999999999999	-2.2585470000000001	-2.5301279999999999
Se	1.5322220000000000	-3.5769989999999998	0.5029960000000000
W	3.0059429999999998	-1.4513149999999999	-0.0401040000000000

Se	-1.1010620000000000	-1.8088700000000000	0.5062090000000000
Se	4.2095680000000000	-2.2431820000000000	-2.2368549999999998
W	0.5493160000000000	0.3106600000000000	0.2271020000000000
Se	1.8247260000000001	-0.6899670000000000	2.1349459999999998
Se	1.5012570000000001	-0.4682960000000000	-2.0138889999999998

W₁₆Se₃₂; $E_{tot} = -9\,372\,662.617\,667\,02$ eV; $E_{rel} = 201.621\,371\,312\,5$ meV/f.u.

W	-6.5312739999999998	3.3929220000000000	0.4571990000000000
W	-3.8304279999999999	4.1194509999999998	0.6367170000000000
W	-3.9707189999999999	1.5442760000000000	0.1882570000000000
W	-1.2927280000000001	2.3192759999999999	0.3630120000000000
W	-1.4584410000000001	-0.3352040000000000	-0.1090250000000000
W	1.2387319999999999	0.4407500000000000	0.1084750000000000
W	1.1109789999999999	-2.2574299999999998	-0.4262310000000000
W	3.7909750000000000	-1.4812460000000001	-0.1263020000000000
W	3.6902180000000002	-4.1814970000000002	-0.6907510000000000
W	6.3647640000000001	-3.3965869999999998	-0.3636260000000000
W	6.2654280000000000	-6.0868549999999999	-0.9255949999999999
W	8.9525889999999997	-5.2836429999999996	-0.6469020000000000
W	8.8337020000000006	-7.9322759999999999	-1.1525680000000000
W	11.4995229999999999	-7.1154840000000004	-0.9094130000000000
W	11.4126980000000007	-9.6875630000000008	-1.3854550000000001
W	14.0974269999999997	-8.9105360000000005	-1.1412439999999999
Se	-8.5951769999999996	3.7819639999999999	1.3420090000000000
Se	-5.5884169999999997	5.5098269999999996	-0.3493360000000000
Se	-5.0793400000000002	2.6099990000000002	2.2565130000000000
Se	-6.3459580000000004	1.6316320000000000	-1.1000790000000000
Se	-1.8699520000000001	4.4427420000000000	1.9630369999999999
Se	-2.8904890000000001	3.1974119999999999	-1.4253140000000000
Se	-2.4367700000000001	0.7144200000000001	1.9755750000000001
Se	-3.7431260000000002	-0.4902270000000000	-1.2374320000000001
Se	0.9070500000000000	2.6447720000000001	1.4090240000000001

Se	-0.3183130000000000	1.2823800000000001	-1.7012879999999999
Se	0.1007340000000000	-1.2333220000000000	1.6521090000000000
Se	-1.1539310000000000	-2.4546800000000002	-1.4783350000000000
Se	3.4722300000000001	0.6799570000000000	1.1836050000000000
Se	2.2800880000000001	-0.5807690000000000	-1.9390220000000000
Se	1.4296249999999999	-4.4074190000000000	-1.7406090000000001
Se	2.6266120000000002	-3.1826240000000001	1.3674170000000001
Se	4.8613939999999998	-2.4773179999999999	-2.1751860000000001
Se	4.0495200000000002	-6.3151390000000003	-2.0390090000000001
Se	6.0399950000000002	-1.2521929999999999	0.9500860000000000
Se	5.1870779999999996	-5.0973980000000001	1.1199200000000000
Se	7.4202250000000003	-4.3890900000000004	-2.4323359999999998
Se	6.6594449999999998	-8.2662720000000007	-2.2505519999999999
Se	8.6043880000000001	-3.1891340000000001	0.7435610000000000
Se	7.7984530000000003	-6.9365839999999999	0.9017030000000000
Se	11.2111909999999995	-5.1024050000000001	0.5320060000000000
Se	9.9900090000000006	-6.2943740000000004	-2.7222770000000001
Se	9.4838210000000007	-10.0311880000000002	-2.7533099999999999
Se	10.4098140000000008	-8.8011470000000003	0.6618680000000000
Se	13.8473530000000000	-7.1674069999999999	0.4264410000000000
Se	12.6691739999999999	-8.1410830000000001	-2.9649169999999998
Se	13.1766150000000000	-11.0500109999999996	-0.3710810000000000
Se	16.1881670000000000	-9.2508119999999998	-1.9830129999999999

W₁₆Se₃₂; $E_{tot} = -9\,372\,665.843\,608\,96$ eV; $E_{rel} = 0$ meV/f.u.

W	32.8526219999999967	7.0109779999999997	2.8033939999999999
W	31.3669049999999991	9.6860060000000008	3.0797770000000000
W	29.7368349999999992	12.3143969999999996	3.3266890000000000
W	28.1992709999999995	15.1510949999999998	3.4918369999999999
W	34.1783500000000018	9.6440889999999992	2.9555440000000002
W	32.4555069999999972	12.2139460000000000	3.2227739999999998
W	30.7858079999999994	15.0758759999999992	3.4309729999999998

W	29.7920720000000010	18.0861559999999990	3.7021269999999999
W	35.7731319999999968	12.3045810000000007	3.2108940000000001
W	34.7792269999999988	15.3145710000000008	3.4823210000000002
W	33.1088540000000009	18.1764879999999991	3.6903419999999998
W	31.3869320000000016	20.7469199999999994	3.9567510000000001
W	37.3660100000000028	15.2398609999999994	3.4215879999999999
W	35.8284629999999993	18.0765120000000010	3.5859209999999999
W	34.1983239999999995	20.7051710000000000	3.8321630000000000
W	32.7130969999999976	23.3802209999999988	4.1098699999999999
Se	32.7961439999999982	8.3907469999999993	4.7846419999999998
Se	31.0120259999999988	11.1295739999999999	5.1078080000000003
Se	29.3563800000000015	13.9420889999999993	5.3038670000000003
Se	27.3491980000000012	17.2654180000000004	4.2786419999999996
Se	34.3678930000000022	11.2279470000000003	4.9203780000000004
Se	32.8179500000000033	14.1392070000000007	4.8367339999999999
Se	31.2769210000000015	16.9270090000000017	5.1871440000000000
Se	29.0841430000000010	20.0674799999999998	4.8827780000000001
Se	36.1841750000000033	13.9356120000000008	5.1716280000000001
Se	34.5596699999999970	16.9659340000000007	5.3994109999999997
Se	32.8004200000000026	19.7456829999999997	5.6869030000000000
Se	30.7816839999999985	22.7784289999999991	5.3745180000000001
Se	38.2153240000000025	17.1102319999999999	4.5747540000000004
Se	36.5025479999999973	20.0927429999999987	4.8013990000000000
Se	34.6920360000000016	22.8203229999999984	5.2893999999999997
Se	32.6481679999999983	25.5663149999999995	3.4909460000000001
Se	32.9189980000000020	4.8263220000000002	3.4271550000000000
Se	30.8731459999999984	7.5697580000000002	1.6240110000000001
Se	29.0623070000000006	10.2981700000000007	2.1112750000000000
Se	27.3494810000000008	13.2807379999999995	2.3389020000000000
Se	34.7840190000000007	7.6123779999999996	1.5383270000000000
Se	32.7648599999999988	10.6452220000000004	1.2254250000000000
Se	31.0052769999999995	13.4250460000000000	1.5130960000000000
Se	29.3808149999999983	16.4550669999999997	1.7416240000000001

Se	36.4812640000000030	10.3236290000000004	2.0297070000000001
Se	34.2879030000000000	13.4637469999999997	1.7260830000000000
Se	32.7471109999999967	16.2513730000000010	2.0761360000000000
Se	31.1973589999999987	19.1627480000000006	1.9921480000000000
Se	38.2160900000000012	13.1255539999999993	2.6348460000000000
Se	36.2087379999999968	16.4484180000000002	1.6093200000000001
Se	34.5526660000000021	19.2609850000000016	1.8048130000000000
Se	32.7691310000000016	22.0009079999999990	2.1278079999999999

W₃₆Se₇₂; $E_{tot} = -21\,088\,493.176\,152\,86$ eV; $E_{rel} = 302.459\,197\,250\,0$ meV/f.u.

W	33.7871969999999990	25.9560500000000012	3.1119279999999998
W	34.8898659999999978	28.5251470000000005	2.9560919999999999
W	35.2489699999999999	23.2007669999999990	3.2128000000000001
W	36.4007440000000031	25.7356520000000017	3.0883430000000001
W	36.7829219999999992	20.4374889999999994	3.3233269999999999
W	37.9470010000000002	22.9899589999999989	3.2079149999999998
W	38.3691949999999977	17.6504149999999989	3.4416620000000000
W	39.5349799999999973	20.1871790000000004	3.3142049999999998
W	39.9649410000000032	14.8563440000000000	3.5404629999999999
W	41.1311990000000023	17.3871350000000007	3.4293950000000000
W	41.5685160000000025	12.0646199999999997	3.6111030000000000
W	42.7262979999999999	14.5937809999999999	3.5000170000000002
W	43.1798429999999982	9.2716440000000002	3.6498230000000000
W	44.3319150000000022	11.8047489999999993	3.5447839999999999
W	44.7988089999999985	6.4855119999999999	3.6723479999999999
W	45.9443380000000019	9.0188150000000000	3.5716250000000000
W	46.4234489999999980	3.7031360000000002	3.6882990000000002
W	47.5660170000000022	6.2370570000000001	3.5921759999999998
W	48.0479740000000035	0.9213610000000000	3.7036899999999998
W	49.1905270000000030	3.4554130000000001	3.6076229999999998
W	49.6691679999999991	-1.8603140000000000	3.7247100000000000
W	50.8150509999999969	0.6729450000000000	3.6238809999999999

W	51.281081999999978	-4.646404999999997	3.752311999999999
W	52.433723999999980	-2.113579999999998	3.647072999999998
W	52.886091999999979	-7.435855000000001	3.798236000000002
W	54.044449999999977	-4.906939000000004	3.686569000000000
W	54.480637999999990	-10.229321000000006	3.869673000000001
W	55.647576000000008	-7.699347000000004	3.758278999999999
W	56.076889000000013	-13.029614000000005	3.985361000000002
W	57.242288999999995	-10.493062000000001	3.857473999999998
W	57.664537000000028	-15.832466999999994	4.092086000000001
W	58.828386999999993	-13.281183999999997	3.976003000000000
W	59.210832000000035	-18.578765000000006	4.210752000000003
W	60.362174000000031	-16.043753999999998	4.086725000000004
W	60.721415000000004	-21.368078000000006	4.343448999999997
W	61.823371999999991	-18.798891999999986	4.187591000000003
Se	32.998069999999985	24.121348999999986	4.426645999999999
Se	35.183258999999996	27.090379999999997	4.910812000000000
Se	34.465560000000035	21.105070000000013	4.232769000000002
Se	36.711638999999981	24.207084999999993	5.042427000000000
Se	36.054605000000022	18.266452999999985	4.305684000000003
Se	38.285876999999993	21.400676000000007	5.139494000000000
Se	37.665657000000031	15.452429999999997	4.417555000000001
Se	39.879266000000012	18.601071999999985	5.254330000000004
Se	39.283377999999990	12.645125000000002	4.518708000000002
Se	41.490366999999991	15.792733000000001	5.349164000000000
Se	40.898563000000029	9.837668000000007	4.571213000000002
Se	43.111105000000020	12.991951000000002	5.409817999999996
Se	42.516643000000020	7.037344000000000	4.597203999999996
Se	44.729542000000021	10.195847000000005	5.446335999999996
Se	44.140287999999982	4.246058999999998	4.612544999999999
Se	46.349685000000009	7.405298000000002	5.468499999999997
Se	45.765670000000001	1.463066000000000	4.630425999999999
Se	47.973303999999988	4.621076000000004	5.485896000000003
Se	32.821778000000019	27.812031999999985	1.842965000000000

Se	34.6338670000000022	30.6661859999999997	3.6957979999999999
Se	34.8905730000000034	24.8007239999999989	1.2587420000000000
Se	36.8351669999999984	28.0326279999999990	1.7211460000000001
Se	36.4796750000000003	22.0150809999999986	1.3753439999999999
Se	38.5840490000000003	25.1779240000000009	2.0343100000000001
Se	38.0315099999999973	19.2270520000000005	1.5021000000000000
Se	40.2196720000000028	22.3826169999999998	2.2836590000000001
Se	39.6174200000000027	16.4492219999999989	1.6132370000000000
Se	41.8497460000000032	19.6163029999999985	2.4969600000000001
Se	41.1934290000000018	13.6612779999999994	1.6947900000000000
Se	43.4200590000000020	16.8196429999999992	2.5424180000000001
Se	42.7859479999999976	10.8788680000000006	1.7468750000000000
Se	45.0129629999999992	14.0367899999999999	2.5968580000000001
Se	44.3933899999999966	8.0982380000000003	1.7759229999999999
Se	46.6106100000000012	11.2532680000000003	2.6193979999999999
Se	46.0146299999999968	5.3187360000000004	1.7942210000000001
Se	48.2248919999999970	8.4746039999999994	2.6451630000000002
Se	47.3886380000000003	-1.3158989999999999	4.6508409999999998
Se	49.5992260000000016	1.8399410000000000	5.5018539999999998
Se	47.6407510000000016	2.5374330000000000	1.8100499999999999
Se	49.2642560000000032	-0.2470210000000000	1.8277260000000000
Se	49.0024019999999965	-4.0944560000000001	4.6772099999999996
Se	51.2200739999999968	-0.9396210000000000	5.5204399999999998
Se	50.8840569999999985	-3.0378940000000001	1.8503250000000000
Se	49.8481730000000027	5.6954430000000000	2.6654599999999999
Se	51.4737060000000000	2.9121939999999999	2.6834340000000001
Se	53.0972039999999978	0.1204860000000000	2.6992829999999999
Se	50.5994409999999988	-6.8781800000000004	4.7006720000000000
Se	52.8270649999999975	-3.7205659999999998	5.5503119999999999
Se	52.5019789999999986	-5.8343429999999996	1.8877999999999999
Se	54.7149140000000003	-2.6802359999999998	2.7260640000000000
Se	52.1918560000000014	-9.6614369999999994	4.7559790000000000
Se	54.4189679999999996	-6.5033969999999997	5.6033010000000001

Se	54.122160000000009	-8.635616000000006	1.949560000000000
Se	56.3295590000000033	-5.488264000000000	2.779462000000000
Se	53.761580999999996	-12.458337000000002	4.802653000000003
Se	55.994326000000009	-9.291292999999996	5.685957000000001
Se	55.732723999999975	-11.444100999999999	2.044775000000000
Se	57.946891000000008	-8.295572999999992	2.881483999999999
Se	55.392114999999969	-15.225153999999999	5.016142999999996
Se	57.579709999999986	-12.069207000000005	5.797436000000003
Se	57.325535999999996	-14.243304999999994	2.160061999999999
Se	59.557074000000001	-11.109486999999997	2.994031999999998
Se	57.027059000000013	-18.020794999999997	5.265080000000002
Se	59.131669000000023	-14.857939000000000	5.924264000000000
Se	58.899799999999990	-17.049986000000005	2.257016999999998
Se	61.146253999999990	-13.948088999999995	3.067133999999998
Se	58.775655999999979	-20.875341999999998	5.578630000000004
Se	60.720982999999968	-17.643746000000002	6.040550999999998
Se	60.4285970000000034	-19.932957999999993	2.388402000000001
Se	62.612864000000019	-16.965060999999986	2.873580000000000
Se	60.977598999999979	-23.509207000000000	3.603730999999998
Se	62.789512000000020	-20.654512000000004	5.456805000000001

W₃₆Se₇₂; $E_{tot} = -21\,088\,494.614\,603\,22$ eV; $E_{rel} = 262.502\,242\,805\,5$ meV/f.u.

W	14.562459999999997	15.382111999999993	4.512843000000002
W	13.457739000000001	18.267147999999988	3.792689000000002
W	11.917562999999995	20.906566999999990	3.400115000000000
W	9.874193999999992	24.051556000000015	3.033987000000002
W	18.324995999999987	15.417002999999993	4.003839000000001
W	16.224267999999986	18.141103000000011	3.759103999999998
W	15.156295999999993	20.866960999999999	3.522955000000001
W	13.278390999999992	24.145253000000003	3.267957000000000
W	11.761437000000008	26.679368000000002	3.367897999999998
W	21.399188999999998	15.381629000000002	3.576226000000001

W	19.977160000000014	18.142063000000003	3.4223620000000001
W	17.907818999999999	20.402377000000013	3.4344579999999998
W	16.223113000000014	23.720279000000014	3.2282050000000000
W	14.597502000000004	26.637028999999983	3.0121690000000001
W	13.194471000000001	29.211442999999992	3.3398970000000001
W	24.470103999999992	14.856654999999999	2.9704830000000002
W	22.876923000000015	17.704612000000009	3.2669039999999998
W	21.750018000000007	20.317727000000014	3.1520429999999999
W	17.962666999999997	26.722532999999985	3.2869640000000002
W	16.049731999999988	29.125263000000003	3.2396759999999998
W	14.458290999999991	32.100222999999997	2.9636559999999998
W	26.257972999999998	18.198996999999985	3.0332270000000001
W	24.587158999999998	21.026744000000008	3.1947470000000000
W	23.466712999999986	23.525839999999988	3.2126999999999999
W	21.469183000000010	26.967151999999987	3.4746450000000002
W	19.837731999999990	29.204819000000005	3.5151200000000000
W	18.209164999999987	31.942954000000003	3.3772270000000000
W	27.700907999999983	20.766702999999997	3.0621999999999998
W	26.166577000000002	23.691580999999993	3.3152170000000001
W	24.600104999999992	26.213487000000006	3.4487510000000001
W	22.720152999999998	29.519559999999985	3.7668889999999999
W	21.286546999999988	31.891538000000006	3.7770779999999999
W	29.632256999999992	23.991161999999992	3.1119170000000000
W	27.579454999999994	26.435189999999986	3.7035130000000001
W	26.086694999999989	28.987528999999985	3.9686430000000001
W	24.325375000000011	32.312111999999991	4.4556019999999998
Se	16.607206999999989	13.924206999999991	5.0265500000000003
Se	14.751827000000005	17.370132999999992	5.8412059999999997
Se	13.251390999999999	20.209679999999988	5.3723460000000003
Se	11.413401000000004	22.983194000000010	4.8456029999999997
Se	9.669964999999995	25.868306000000005	4.6290670000000000
Se	19.865390000000014	13.869281000000009	4.9884069999999996
Se	18.246338999999990	17.376740999999991	5.3456099999999998

Se	16.5723020000000005	20.0530289999999987	5.4664970000000004
Se	14.7946249999999999	22.9796709999999997	5.0123119999999997
Se	13.2295879999999997	25.7930010000000003	5.1107570000000004
Se	10.9829430000000006	28.7543399999999991	4.4354779999999998
Se	23.0596619999999994	13.9008909999999997	4.7405130000000000
Se	21.4434639999999987	17.1502240000000015	5.2746690000000003
Se	19.9670589999999990	20.4741940000000007	4.8629879999999996
Se	18.2868840000000006	24.5156430000000007	4.2132610000000001
Se	14.6476880000000005	28.3093450000000004	5.0964470000000004
Se	12.7681229999999992	31.3774629999999988	4.5703750000000003
Se	24.8946240000000003	16.7674079999999996	4.6986819999999998
Se	23.2590520000000005	19.6472979999999993	4.9089039999999997
Se	17.8364370000000001	28.3990599999999986	4.9980169999999999
Se	16.1446140000000007	31.3195399999999999	4.8030099999999996
Se	26.3349970000000013	19.8531769999999987	4.9071290000000003
Se	24.7360630000000015	22.6336510000000004	5.1353999999999997
Se	22.4065179999999984	25.0784370000000010	4.8326799999999999
Se	21.1916809999999991	28.3257820000000002	5.4900580000000003
Se	19.4765039999999985	31.1492159999999991	5.3602169999999996
Se	28.1308609999999994	22.6080340000000000	4.7709849999999996
Se	26.1188199999999995	25.3609299999999998	5.3010130000000002
Se	24.3761070000000011	28.0945910000000012	5.3570909999999996
Se	22.6972430000000003	31.2011879999999984	5.8264030000000000
Se	29.6757460000000002	25.6155849999999994	4.9249919999999996
Se	28.2984159999999996	28.4887060000000005	4.8669659999999997
Se	26.5985680000000002	31.2242430000000013	4.9485229999999998
Se	12.8405369999999994	16.0105140000000006	2.8800400000000002
Se	11.2434030000000007	18.7584069999999983	2.5841360000000000
Se	9.6018539999999994	21.5284149999999990	2.7280050000000000
Se	16.2207380000000008	15.7889599999999994	2.5329869999999999
Se	14.7809430000000006	18.9557320000000011	1.8468240000000000
Se	13.3700720000000004	21.8973119999999994	1.7882380000000000
Se	11.4950930000000007	24.8786529999999999	1.4541409999999999

Se	19.5946290000000012	15.9010429999999996	1.9086790000000000
Se	17.9427480000000017	18.5686339999999994	1.8709560000000001
Se	16.8361720000000012	21.8332499999999996	1.7080839999999999
Se	14.8867119999999993	24.7009599999999985	1.3731800000000001
Se	12.9841099999999994	27.6227570000000000	1.3583130000000001
Se	22.8318820000000002	15.7475220000000000	1.4610140000000000
Se	21.3981010000000005	18.6626450000000013	1.3757580000000000
Se	16.4577519999999993	27.4102110000000003	1.4207110000000001
Se	14.6010570000000008	30.2805140000000002	1.3900340000000000
Se	26.7651859999999999	15.8651789999999995	2.3493430000000002
Se	24.5764929999999993	18.9036849999999994	1.5136170000000000
Se	22.6534550000000010	21.9364449999999991	1.4815170000000000
Se	19.7835549999999998	27.2927290000000013	1.6949510000000001
Se	18.0590800000000016	30.1911850000000008	1.7689429999999999
Se	16.4958269999999985	33.6141730000000010	2.6821920000000001
Se	28.5058310000000006	18.6417220000000015	2.1468120000000002
Se	26.3007479999999987	21.8324029999999993	1.4126580000000000
Se	24.6923640000000013	24.6632679999999986	1.4257930000000001
Se	23.1236749999999986	27.7506750000000011	1.9088449999999999
Se	21.3397210000000008	30.4052079999999982	1.8289510000000000
Se	19.7534770000000002	33.5964150000000004	2.5956280000000000
Se	30.0156090000000013	21.5377369999999999	2.4892970000000001
Se	27.9609650000000016	24.9201629999999987	1.6474050000000000
Se	26.2321729999999995	27.5850149999999985	1.9070050000000001
Se	24.7554149999999993	30.6321620000000010	2.4905450000000000
Se	22.9455999999999989	33.5151060000000030	2.8222870000000002
Se	25.0905319999999996	34.0921700000000030	5.6642409999999996
Se	31.6689749999999997	24.3685560000000017	2.1602109999999999
Se	25.2448020000000000	12.9246529999999993	2.0322460000000002
Se	13.3718120000000003	13.8710810000000002	5.7417369999999996
Se	7.8341719999999997	24.1776130000000009	2.0115530000000001
Se	13.2933880000000002	33.7641520000000028	1.9168970000000001

W₃₆Se₇₂; $E_{tot}=-21\,088\,494.778\,584\,56\text{ eV}$; $E_{rel}=257.947\,205\,583\,3\text{ meV/f.u.}$

W	-5.6247680000000004	27.705709999999998	-11.7959270000000007
W	-3.7588729999999999	28.650335999999994	-9.3962620000000001
W	-1.7813369999999999	29.494970999999996	-6.8591949999999997
W	0.2556670000000000	29.913565999999994	-4.3122299999999996
W	2.1832769999999999	30.4586790000000001	-2.0552619999999999
W	4.2274580000000004	30.8992010000000015	0.3615000000000000
W	-5.5932380000000004	24.8620429999999999	-13.1883800000000004
W	-3.8178030000000001	26.0399630000000002	-10.7640170000000008
W	-2.0556100000000002	26.8905679999999982	-8.3514309999999998
W	-0.2604370000000000	27.5115650000000009	-5.8949490000000004
W	1.6106320000000001	27.5906149999999997	-3.5260250000000002
W	4.1503410000000001	28.4075200000000017	-0.6140880000000000
W	5.8651790000000004	28.9779680000000006	1.3415410000000001
W	-5.6371490000000000	22.1769169999999995	-14.5688340000000007
W	-3.6913770000000001	23.0402130000000014	-12.3137360000000005
W	4.0416189999999999	24.7524659999999983	-2.1032210000000000
W	6.0183989999999996	25.9710940000000008	0.1981390000000000
W	-5.5711529999999998	19.1562529999999995	-15.7714079999999992
W	-3.8853100000000000	20.0129240000000017	-13.8163850000000004
W	4.4840159999999996	21.9461629999999985	-3.0705339999999999
W	6.0182060000000002	23.1252199999999988	-0.9373060000000000
W	-5.3925570000000000	16.1727470000000011	-16.6396739999999994
W	-3.7325490000000001	17.1724290000000011	-14.7895500000000002
W	4.5059040000000001	19.0660360000000004	-4.3666960000000001
W	6.2206039999999998	20.1295129999999993	-2.1478229999999998
W	-3.4704999999999999	14.1099669999999993	-15.7159600000000008
W	-1.4290280000000000	14.2354780000000005	-13.2947530000000000
W	0.3508200000000000	14.7804120000000001	-10.7037239999999994
W	2.4288859999999999	15.4654710000000009	-8.2858900000000002
W	4.3843459999999999	16.2463809999999995	-5.8360040000000000
W	6.2145510000000002	17.1763650000000005	-3.5594410000000001

W	-1.544238999999999	11.986207999999995	-14.734030999999999
W	0.455519000000000	12.474926000000000	-12.344929000000000
W	2.286337000000000	12.996950999999993	-9.965488999999998
W	4.133397999999997	13.554306000000004	-7.420153000000000
W	6.042421000000000	14.324213000000003	-4.973653999999998
Se	-7.544454000000000	26.678377999999986	-12.707504999999994
Se	-5.769466000000004	27.077111999999996	-9.414604000000006
Se	-3.867719999999998	27.993151999999985	-6.969350000000004
Se	-1.985270000000001	28.737317999999984	-4.465243000000001
Se	0.131976000000000	28.993341000000009	-1.981643000000000
Se	2.104185999999999	29.678446999999985	0.395699000000000
Se	-7.445534000000003	23.874368000000005	-14.474111999999999
Se	-5.484719000000001	24.030841999999998	-10.876531999999992
Se	-3.120858999999998	24.726669000000011	-8.610963999999992
Se	-0.764587000000000	25.288958999999984	-6.670226999999997
Se	-0.043364000000000	25.912002000000011	-3.724355000000001
Se	2.344875000000000	26.570774000000001	-1.191939000000001
Se	4.274046000000002	27.146027000000001	1.675527999999999
Se	-7.421631999999998	20.811395999999985	-15.804546000000002
Se	-5.607670999999999	21.223589000000005	-12.306908999999992
Se	2.235367999999998	23.239969999999989	-2.341041000000001
Se	4.206110999999999	24.239412000000015	0.410106000000000
Se	-7.410326000000004	17.408315999999992	-16.700409000000005
Se	-5.569223000000000	18.251321000000008	-13.414621000000004
Se	2.779955999999999	21.074107000000015	-4.543504999999997
Se	4.476047000000003	21.148407999999999	-0.641415000000000
Se	-5.368991000000003	15.179565999999994	-14.403679999999996
Se	-2.818636999999998	16.269539999999992	-12.361340999999995
Se	2.492970000000001	17.945600999999999	-5.055155000000001
Se	4.539396000000000	18.216409999999998	-1.984321000000000
Se	-3.520573999999999	12.814014999999995	-13.508518000000005
Se	-1.545642000000000	13.204304000000005	-10.961703000000000
Se	0.473970000000000	13.705225000000004	-8.415654000000000

Se	2.3896820000000001	14.5931599999999992	-5.9717430000000000
Se	4.4316649999999997	15.3408309999999997	-3.4106860000000001
Se	-0.7590479999999999	10.2394610000000004	-13.3420839999999998
Se	1.4468449999999999	10.7900869999999998	-10.8073540000000001
Se	3.4990320000000001	11.3888409999999993	-8.2718209999999992
Se	5.2139810000000004	12.1503080000000008	-5.3378810000000003
Se	-4.9979380000000004	29.9461089999999999	-11.4900319999999994
Se	-3.0475970000000001	30.8679589999999990	-8.7358849999999997
Se	-0.8285940000000001	31.5780940000000001	-6.1256930000000001
Se	1.3241510000000001	32.08102800000000034	-3.6886060000000001
Se	-3.8712830000000000	26.7613510000000012	-13.2481729999999995
Se	-1.8617340000000000	27.6628299999999996	-10.7230010000000000
Se	0.0025900000000000	28.4171920000000000	-8.2466620000000006
Se	1.9369570000000000	28.7274740000000008	-5.7513949999999996
Se	3.8383680000000000	29.1536539999999995	-3.1289180000000001
Se	-3.7647510000000000	23.8731860000000005	-14.6577540000000006
Se	-1.8532180000000000	24.2430090000000007	-11.4449839999999998
Se	3.6236660000000001	26.1448619999999998	-4.2174519999999998
Se	5.7861890000000002	26.8637850000000000	-1.9831240000000001
Se	-3.9906079999999999	21.0534070000000000	-16.1430679999999995
Se	-2.3803730000000001	20.9167270000000016	-12.0204699999999995
Se	6.0618670000000003	23.8843829999999997	-3.3353150000000000
Se	7.8860599999999996	24.3928870000000018	0.1798320000000000
Se	-3.8636010000000001	18.0142850000000010	-17.2427780000000013
Se	-1.8036970000000001	18.8627129999999994	-14.5781340000000004
Se	6.2903019999999996	20.9345150000000011	-4.5204630000000003
Se	7.9751779999999997	21.3410960000000003	-1.0024700000000000
Se	-4.4606789999999998	14.4448760000000007	-18.0453629999999983
Se	-1.6913080000000000	15.6727740000000004	-15.5884350000000005
Se	-0.4019950000000000	16.4696929999999995	-12.5589139999999997
Se	0.5676990000000000	16.8698079999999990	-9.4258080000000000
Se	3.4882659999999999	17.5844239999999985	-8.0237079999999992
Se	6.1960139999999999	18.0709650000000011	-5.8978739999999998

Se	8.0211670000000002	18.1887630000000016	-2.3428710000000001
Se	-2.3816929999999998	12.0981290000000001	-16.9727500000000013
Se	0.5149520000000000	13.3288779999999996	-14.7450039999999998
Se	2.3070400000000002	14.1664549999999991	-12.2000989999999998
Se	4.2697229999999999	14.5320850000000004	-9.7423669999999998
Se	6.1746790000000003	15.0825010000000006	-7.3118540000000003
Se	8.0261189999999996	15.1580739999999992	-4.0442419999999997
Se	6.1690899999999997	30.0034370000000017	-0.9037650000000000
Se	3.6051620000000000	32.5416529999999966	-1.3266490000000000
Se	7.8514759999999999	27.5663519999999984	1.1865120000000000
Se	4.9380980000000001	30.7986119999999985	2.7229800000000002

W₃₆Se₇₂; $E_{tot} = -21\,088\,496.812\,146\,12\text{ eV}$; $E_{rel} = 201.459\,384\,472\,2\text{ meV/f.u.}$

W	11.7186149999999998	15.5107959999999991	3.4604180000000002
W	10.0177899999999998	18.2023709999999994	3.6059040000000002
W	8.4718110000000006	20.9377479999999991	3.6155499999999998
W	6.7802650000000000	23.7180010000000010	3.4023119999999998
W	5.3339470000000002	26.5747919999999986	3.1167300000000000
W	14.9002070000000000	15.3815620000000006	3.3084210000000001
W	13.0401030000000002	17.7942479999999996	3.4514649999999998
W	11.3758780000000002	20.4529059999999987	3.6989730000000001
W	9.4268230000000006	23.7741870000000013	3.6627990000000001
W	7.9887569999999997	26.3428940000000011	3.3668890000000000
W	6.8022809999999998	29.2518209999999996	3.0854810000000001
W	18.0468149999999987	15.4136760000000006	3.2961800000000001
W	16.1704620000000006	17.6835160000000009	3.2024379999999999
W	11.2793460000000003	26.6688830000000010	3.7443450000000000
W	9.9148130000000005	29.6747019999999999	3.3678140000000001
W	8.3884190000000007	31.8586910000000003	3.1153209999999998
W	21.2978950000000005	15.3419790000000003	3.5102699999999998
W	20.0243870000000008	17.6625340000000008	3.2468129999999999
W	12.8582040000000006	29.7107950000000010	3.6662910000000002

W	11.584398999999994	32.031466000000018	3.4029010000000000
W	24.4940210000000000	15.5144020000000005	3.7978070000000002
W	22.9676819999999999	17.6985689999999991	3.5451750000000000
W	21.6031820000000003	20.7043929999999996	3.1687210000000001
W	16.7122369999999982	29.6901359999999990	3.7111619999999998
W	14.8357460000000003	31.9598930000000010	3.6170789999999999
W	26.0803680000000000	18.1215289999999989	3.8273410000000001
W	24.8942650000000008	21.0308129999999984	3.5457679999999998
W	23.4557989999999990	23.5990460000000013	3.2501159999999998
W	21.5067260000000005	26.9201659999999983	3.2141989999999998
W	19.8420519999999989	29.5791359999999983	3.4623029999999999
W	17.9823820000000012	31.9918240000000011	3.6051799999999998
W	27.5484590000000011	20.7982359999999993	3.7958740000000000
W	26.1022829999999999	23.6549930000000010	3.5103119999999999
W	24.4111529999999988	26.4353680000000004	3.2971710000000001
W	22.8650060000000011	29.1709759999999996	3.3072859999999999
W	21.1641680000000001	31.8625669999999985	3.4533659999999999
Se	12.9969239999999999	13.7328829999999993	4.3586999999999998
Se	11.4573470000000004	17.0505819999999986	5.3723089999999996
Se	9.7229510000000001	19.8425769999999986	5.5020369999999996
Se	7.9135759999999999	22.6408430000000003	5.3867260000000003
Se	6.2532230000000002	25.5230940000000004	5.1443810000000001
Se	4.4049449999999997	28.6638149999999996	3.8792550000000001
Se	16.4467449999999999	13.6517280000000003	4.1468259999999999
Se	14.7904079999999993	17.0383470000000017	5.1799580000000001
Se	13.4437090000000001	20.0953060000000008	4.8214290000000002
Se	11.4786929999999998	22.7761840000000007	4.9781139999999997
Se	9.6426149999999993	25.6196880000000000	5.3572490000000004
Se	8.1154740000000007	28.4917349999999985	4.9065120000000002
Se	6.1131279999999997	31.6228179999999988	3.8754339999999998
Se	19.7101240000000004	13.7202249999999992	4.4027029999999998
Se	18.0504919999999984	17.2671449999999993	4.9098420000000003
Se	11.3652580000000007	28.6057470000000009	5.3612750000000000

Se	9.756093999999992	31.587679000000014	5.144487999999999
Se	23.239612000000010	13.743938000000000	4.711541000000004
Se	21.257336999999997	17.052820000000005	5.330898000000004
Se	19.277343999999994	20.236775999999990	3.782696000000001
Se	14.750678999999999	28.437716000000018	4.984218000000003
Se	13.083192000000004	31.591020000000003	5.388397999999996
Se	24.502245999999995	17.180561000000009	5.582063999999999
Se	22.913327999999999	19.952663999999986	5.008602999999999
Se	20.849463000000001	22.958558000000000	3.781534000000002
Se	18.058398000000004	28.095818999999988	4.856988000000003
Se	16.414539000000013	31.438023000000012	5.504251000000000
Se	26.110661000000003	19.958819999999993	5.581724000000004
Se	24.602301000000006	22.834839999999998	5.332385999999996
Se	22.813634000000004	25.503892000000005	4.917066000000002
Se	21.382203000000005	28.446076999999989	5.186748999999998
Se	19.703202000000010	31.333771999999997	5.372499999999996
Se	28.459306999999990	22.768063000000015	4.706977000000002
Se	26.719384999999991	25.841205999999997	4.392057000000003
Se	25.138933000000015	28.700572999999986	4.142944000000000
Se	23.346389999999995	31.647642999999986	4.344655999999996
Se	9.536303000000002	15.725410999999994	2.569232000000000
Se	7.744003000000002	18.672616999999989	2.769746000000000
Se	6.163789999999997	21.531925999999986	2.519833000000002
Se	4.423478000000002	24.604859000000011	2.205003000000000
Se	13.179354999999993	16.039428999999984	1.541293000000000
Se	11.500432000000000	18.926984000000009	1.726197000000000
Se	10.069495999999991	21.869308000000002	1.995703000000000
Se	8.280632999999999	24.538560000000004	1.580411000000000
Se	6.772198000000004	27.414472000000000	1.330985000000001
Se	16.467767999999995	15.935539000000003	1.409262000000000
Se	14.824115000000008	19.277933000000009	2.057065000000001
Se	12.033372000000000	24.414732000000008	3.131764000000000
Se	9.969523999999998	27.420560999999993	1.904301999999999

Se	8.380489000000007	30.192703000000016	1.3307739999999999
Se	19.799088999999986	15.782495000000008	1.5247470000000001
Se	18.131934999999986	18.935860999999992	1.9290980000000000
Se	13.605363999999998	27.136531999999990	3.1306180000000001
Se	11.625313000000002	30.320425000000002	1.5823280000000000
Se	9.642635000000003	33.629330000000031	2.2016119999999999
Se	23.126270999999991	15.785396000000004	1.7686660000000001
Se	21.517264000000008	18.767510999999989	1.5518080000000001
Se	14.832269000000001	30.106391999999996	2.0036060000000000
Se	13.172385000000002	33.653084999999973	2.5103130000000000
Se	26.769196999999984	15.750133999999992	3.0376829999999999
Se	24.766870999999983	18.881367999999984	2.0063800000000001
Se	23.239886999999995	21.753441999999997	1.5556230000000000
Se	21.403915000000014	24.596821999999995	1.9348200000000000
Se	19.438517000000009	27.278106000000011	2.0920850000000000
Se	18.092258999999985	30.335363000000010	1.7335680000000000
Se	16.435997000000004	33.721752000000022	2.7668260000000000
Se	28.477565999999995	18.709177000000004	3.0328240000000002
Se	26.629187000000017	21.849879000000014	1.7680240000000000
Se	24.968939999999999	24.732285000000010	1.5258989999999999
Se	23.159604000000016	27.530864000000011	1.4112790000000000
Se	21.425005999999998	30.322880000000014	1.5414060000000001
Se	19.885888999999988	33.640545000000030	2.5553889999999999

W₃₆Se₇₂; $E_{tot} = -21\,088\,500.923\,118\,43$ eV; $E_{rel} = 87.265\,709\,194\,4$ meV/f.u.

W	20.004286000000005	1.220250000000001	3.5274770000000002
W	22.638431000000006	1.137134000000001	3.7737069999999999
W	21.277501999999984	3.5459939999999999	3.6806930000000002
W	26.398865000000007	1.142578000000001	3.7781080000000000
W	24.606287999999993	3.8394189999999999	3.6593179999999998
W	23.158756000000003	6.791114000000003	3.7110219999999998
W	29.591761000000018	1.139075000000001	3.5421849999999999

W	27.831203999999996	3.436840000000001	3.643886000000002
W	25.876135999999998	6.918225999999998	3.621840000000002
W	24.7264729999999986	9.5546229999999994	3.471560000000002
W	32.8225100000000012	1.0909409999999999	3.440303999999998
W	30.9924870000000006	3.456144000000001	3.566567000000000
W	29.909041999999995	6.738851000000004	3.478680000000002
W	27.427033999999990	9.748305000000002	3.564395000000002
W	26.3092669999999984	12.3062260000000006	3.415565000000000
W	36.0904049999999970	1.195367000000001	3.467601999999999
W	34.2504920000000013	3.396542999999999	3.597394000000000
W	32.7987910000000014	6.993277000000000	3.485437999999998
W	31.4573180000000008	9.386737000000001	3.437358000000001
W	29.0544599999999988	12.4982780000000009	3.585361999999999
W	27.9851640000000010	15.057169999999993	3.515810000000001
W	39.3089239999999975	1.329054000000000	3.684695000000001
W	38.0232469999999978	3.617913000000002	3.679592000000000
W	35.9140969999999982	7.033462000000001	3.623670000000002
W	34.4360029999999995	9.512295999999992	3.640194000000002
W	33.0617179999999991	12.114744000000000	3.569173000000002
W	31.1086010000000002	15.634541000000005	3.668253000000000
W	29.7167640000000013	17.8846719999999983	3.756734999999999
W	42.4536119999999997	1.345947999999999	3.776384999999999
W	40.8402900000000031	3.917253000000001	3.877285000000001
W	39.3950269999999989	6.455268000000002	3.859033999999999
W	37.4811779999999999	9.712521999999999	3.912380000000002
W	36.0532120000000020	12.196256999999992	3.847831999999999
W	34.2532360000000011	15.396053000000002	3.788357000000000
W	32.7616500000000030	17.898863999999997	3.859402999999999
W	31.3337010000000014	20.6155110000000015	3.823861000000000
Se	21.0403170000000017	-0.594500000000000	4.709410000000001
Se	18.9518239999999984	3.115781999999998	4.568031000000004
Se	24.4482689999999998	-0.151153000000000	4.914774000000004
Se	22.8409809999999993	2.897724999999999	5.466870000000001

Se	21.1268080000000005	5.7562840000000000	4.8907340000000001
Se	27.8325530000000008	-0.6170030000000000	4.4978420000000003
Se	26.1545500000000004	2.9059210000000002	5.4869389999999996
Se	24.5610070000000000	5.7177740000000004	5.4399340000000000
Se	22.3335410000000003	8.9303120000000007	4.3889790000000000
Se	31.1163950000000007	-0.5620200000000000	4.4624210000000000
Se	29.4560479999999991	2.7549229999999998	5.4570900000000000
Se	27.8844870000000000	5.7504390000000001	4.9153599999999997
Se	26.0647629999999992	8.6815569999999997	5.4185439999999998
Se	24.0400980000000004	11.7501590000000000	4.4341739999999996
Se	34.4904030000000006	-0.6524280000000000	4.1072189999999997
Se	32.7002120000000005	2.6216110000000001	5.3900399999999999
Se	31.2759520000000002	5.6372380000000000	5.1619760000000001
Se	29.4296280000000010	8.6771840000000005	4.9635509999999998
Se	27.6412690000000012	11.5247449999999994	5.4098259999999998
Se	25.6860560000000007	14.6619960000000003	4.2617469999999997
Se	37.7745740000000012	-0.3969660000000000	4.5631630000000003
Se	36.1099079999999972	2.8191410000000001	5.2857339999999997
Se	34.3959279999999978	5.6376730000000004	5.0824550000000004
Se	32.8184150000000017	8.6108469999999997	5.4210330000000004
Se	31.0644129999999983	11.4400860000000009	5.0164080000000002
Se	29.4893660000000004	14.3527380000000004	5.3055640000000004
Se	27.4937199999999997	17.4319239999999986	4.5984759999999998
Se	41.1021599999999978	-0.1928180000000000	4.9431740000000000
Se	39.4855129999999974	2.8850539999999998	5.6396810000000004
Se	37.6799189999999982	5.7241689999999998	5.3278540000000003
Se	36.0665529999999990	8.6488530000000008	5.5571349999999997
Se	34.4857360000000028	11.4034250000000004	5.5183190000000000
Se	32.7748589999999993	14.2755519999999994	5.2730309999999996
Se	31.2091439999999984	17.2523240000000015	5.6514949999999997
Se	29.3587330000000009	20.2154060000000015	5.0360079999999998
Se	44.3114699999999999	0.3428520000000000	2.9460130000000002
Se	43.0503289999999978	3.2495569999999998	5.0603710000000000

Se	41.5528240000000011	6.0911470000000003	4.8921729999999997
Se	39.8033420000000007	8.8765809999999998	4.5258979999999998
Se	38.1902159999999995	11.7515990000000006	5.0776700000000003
Se	36.5885400000000018	14.5996559999999995	4.4028780000000003
Se	35.0022650000000013	17.4384550000000011	4.8603790000000000
Se	33.3088139999999981	20.1541369999999986	5.0481049999999996
Se	31.3956240000000015	22.7332450000000001	3.0165289999999998
Se	21.3004689999999997	1.8940859999999999	1.6317240000000000
Se	24.5388430000000000	1.7027170000000000	2.1270330000000000
Se	22.7367109999999997	4.8712090000000003	2.0659980000000000
Se	27.8474390000000014	1.6244680000000000	1.7605440000000001
Se	26.1942300000000010	4.7957390000000002	2.0477259999999999
Se	24.3412380000000006	7.7737600000000002	1.7006110000000001
Se	31.1667279999999991	1.6959700000000000	1.6607060000000000
Se	29.4300970000000000	4.6814099999999996	1.9778739999999999
Se	27.8225610000000003	7.6754579999999999	2.0790929999999999
Se	25.9689210000000017	10.6321239999999992	1.5871640000000000
Se	34.4547960000000018	1.7364710000000001	1.6243019999999999
Se	32.7791909999999973	4.7319100000000001	2.0868400000000000
Se	31.2069900000000011	7.6485969999999996	1.5756349999999999
Se	29.4676110000000016	10.5109300000000001	2.0648499999999999
Se	27.6603080000000006	13.4421569999999999	1.6143209999999999
Se	37.7584889999999973	1.8636800000000000	1.7543660000000001
Se	36.1057040000000029	4.7682310000000001	2.3088400000000000
Se	34.5010800000000017	7.7009369999999997	1.7307610000000000
Se	32.9033530000000027	10.5203460000000000	1.7042569999999999
Se	31.1531359999999999	13.3996530000000007	2.2914089999999998
Se	29.3758869999999987	16.2881420000000006	1.8175319999999999
Se	41.0641090000000020	2.0881759999999998	1.9382200000000001
Se	39.4438779999999980	4.8747720000000001	1.9473400000000001
Se	37.9496759999999966	7.8060590000000003	2.1868870000000000
Se	36.1952640000000017	10.5794029999999992	1.9723310000000001
Se	34.6833609999999979	13.4993960000000008	2.0799840000000001

Se	32.8780870000000007	16.2451550000000005	1.9108300000000000
Se	31.2451609999999995	19.0424900000000008	1.9869450000000000

W₃₆Se₇₂; $E_{tot} = -21\,088\,500.984\,693\,52$ eV; $E_{rel} = 85.555\,290\,027\,7$ meV/f.u.

W	21.4119689999999991	-1.1767890000000001	3.1756280000000001
W	19.9441459999999999	1.4648319999999999	3.1759379999999999
W	18.3480010000000000	4.0518429999999999	3.0379700000000001
W	16.4294660000000015	7.3260129999999997	3.0861160000000001
W	15.0098660000000006	9.9000249999999994	3.2402869999999999
W	13.3964409999999994	12.5838850000000004	3.2009989999999999
W	11.4822159999999993	15.8057479999999995	3.2068230000000000
W	10.0523439999999997	18.2374340000000004	3.1624420000000000
W	8.1908960000000004	21.4785989999999991	3.1581570000000001
W	6.8072239999999997	23.9588530000000013	3.0611069999999998
W	4.9511680000000000	27.2393169999999998	3.0220710000000000
W	3.5280740000000002	29.9323639999999997	3.1385600000000000
W	1.9950390000000000	32.5373609999999971	3.1160079999999999
W	22.5580509999999990	1.3108949999999999	4.2757610000000001
W	21.2888739999999999	3.8704149999999999	4.3876920000000004
W	19.3091469999999994	7.1243530000000002	4.3717530000000000
W	17.8966260000000013	9.4004829999999995	4.4478879999999998
W	16.0158029999999982	12.7036379999999998	4.4717450000000003
W	14.6044780000000003	15.1636249999999997	4.4838310000000003
W	12.6109130000000000	18.4777869999999993	4.5158009999999997
W	11.3099489999999996	20.7996349999999985	4.4815459999999998
W	9.3769449999999992	24.1881480000000018	4.4458810000000000
W	8.1056830000000009	26.5258469999999988	4.3683240000000003
W	6.2734759999999996	29.8785370000000015	4.3728740000000004
W	4.7081369999999998	32.2672389999999965	4.2433949999999996
W	23.7717379999999991	3.8111400000000000	5.3896540000000002
W	22.2436819999999997	6.7054530000000003	5.5496010000000000
W	20.7997629999999987	9.1859359999999999	5.7384800000000000

W	18.880483999999992	12.456604999999997	5.7692360000000003
W	17.287621999999998	15.1225020000000008	5.6696600000000004
W	15.7531180000000006	17.7406949999999988	5.7523030000000004
W	13.8745940000000001	21.0291120000000014	5.8372029999999997
W	12.4808810000000001	23.5079829999999994	5.7814490000000003
W	10.6269939999999998	26.7912700000000008	5.7531809999999997
W	9.19858400000000003	29.2742329999999988	5.5606559999999998
W	7.4680369999999998	32.0538200000000018	5.3852240000000000
Se	20.5646529999999998	-0.0688730000000000	5.1545920000000001
Se	18.9527639999999984	2.7605580000000001	5.0801040000000004
Se	17.2169820000000016	5.5672699999999997	4.8104570000000004
Se	15.6444960000000002	8.4168730000000007	5.1986660000000002
Se	13.9843700000000002	11.2233079999999994	5.1848440000000000
Se	12.2606190000000002	14.0520200000000006	4.9609730000000001
Se	10.6505650000000003	16.9833800000000004	5.2614489999999998
Se	8.9318150000000003	19.7705839999999995	4.9511360000000000
Se	7.3929780000000003	22.7281399999999998	5.1746949999999998
Se	5.6984300000000001	25.5092059999999989	4.8057090000000002
Se	4.1290500000000003	28.4240910000000007	5.0505180000000003
Se	2.5012420000000000	31.2497219999999984	5.1038500000000004
Se	23.6887229999999995	-0.5078900000000000	2.9070589999999998
Se	22.0091040000000007	2.5298129999999999	6.4886390000000000
Se	20.2956479999999999	5.4802119999999999	6.1910119999999997
Se	18.7315299999999993	8.2707189999999997	6.5985449999999997
Se	17.0227150000000016	11.1127230000000008	6.3690720000000001
Se	15.3589529999999996	13.9548109999999994	6.6109429999999998
Se	13.6708010000000009	16.7731670000000008	6.3664930000000002
Se	12.0341260000000005	19.7093810000000005	6.6897029999999997
Se	10.3910140000000002	22.5356270000000016	6.3476100000000004
Se	8.7923270000000002	25.4579290000000000	6.6002700000000001
Se	7.1547900000000002	28.2062510000000017	6.1812709999999997
Se	5.4624660000000000	31.1798269999999995	6.4654330000000000
Se	24.2171239999999983	5.5663830000000001	6.9730410000000003

Se	22.6279520000000005	8.5011910000000004	7.2079930000000001
Se	20.7798529999999992	11.3750250000000008	7.0568980000000003
Se	19.1923800000000000	14.3385639999999999	7.2171230000000000
Se	17.5580560000000006	17.0965769999999999	7.2244630000000001
Se	15.7744830000000000	19.8939330000000005	7.1046500000000004
Se	14.2024600000000003	22.8679290000000002	7.4154749999999998
Se	12.5490619999999993	25.7258250000000004	7.0361070000000003
Se	10.9117420000000003	28.7049319999999994	7.2498440000000004
Se	9.2004049999999999	31.5645640000000007	6.9774880000000001
Se	18.1128590000000003	2.1829749999999999	1.5391610000000000
Se	16.4666519999999998	5.1210909999999998	1.7531490000000001
Se	14.6862610000000000	8.0091300000000007	1.5743849999999999
Se	13.1652869999999993	10.7544360000000001	1.6446149999999999
Se	11.4963130000000007	13.6557089999999999	1.8834880000000001
Se	9.7888870000000008	16.4242990000000013	1.5425750000000000
Se	8.0701769999999993	19.2590420000000009	1.9326900000000000
Se	6.5076159999999996	22.1221490000000003	1.4816480000000001
Se	4.8805019999999999	25.0580229999999986	1.7640180000000001
Se	3.2378239999999998	27.9854050000000001	1.5040780000000000
Se	1.9297940000000000	30.9353529999999992	1.3591519999999999
Se	-0.0123250000000000	33.5529340000000005	3.4529519999999998
Se	21.9118700000000004	2.5975690000000000	2.2450770000000002
Se	20.1974310000000017	5.4114990000000001	2.4610390000000000
Se	18.4844700000000017	8.2551249999999996	2.2211370000000001
Se	16.9791209999999992	11.0779540000000001	2.6276730000000001
Se	15.2369339999999998	13.8861860000000004	2.3339080000000001
Se	13.5663350000000005	16.8017690000000002	2.6482679999999998
Se	11.8860390000000002	19.5667580000000001	2.3102399999999998
Se	10.2826319999999996	22.4528430000000014	2.5917150000000002
Se	8.6671499999999995	25.2488290000000006	2.2153040000000002
Se	7.0619719999999999	28.1531139999999986	2.4576750000000001
Se	5.5088369999999998	31.0544440000000002	2.2221030000000002
Se	3.7286450000000002	34.1590089999999975	2.8569460000000002

Se	25.098396999999985	2.1425160000000001	4.3788729999999996
Se	23.2648730000000015	5.3773410000000004	3.5880580000000002
Se	21.5455520000000007	8.1141020000000008	3.5963900000000000
Se	20.0103900000000010	10.9377569999999995	4.0061650000000002
Se	18.303869999999999	13.8266799999999996	3.7585329999999999
Se	16.6449929999999995	16.5953939999999989	3.7209590000000001
Se	14.9821139999999993	19.5154159999999983	4.0395760000000003
Se	13.2730169999999994	22.2864140000000006	3.7429779999999999
Se	11.7558710000000008	25.2231249999999996	3.9996010000000002
Se	10.0765539999999998	27.9710770000000011	3.6081360000000000
Se	8.5765580000000003	30.8249740000000010	3.5925680000000000
Se	6.7091570000000003	34.0388760000000019	4.3609109999999998
Se	19.9962790000000012	-0.4362980000000000	1.4130940000000001
Se	21.2643610000000010	-3.4182610000000002	3.5300240000000001

$\mathbf{W}_{36}\mathbf{Se}_{72}$; $E_{tot} = -21\,088\,501.190\,420\,91$ eV; $E_{rel} = 79.840\,640\,305\,5$ meV/f.u.

W	14.9331099999999992	15.3243620000000007	3.4147340000000002
W	13.1403140000000000	18.1599080000000015	3.5636640000000002
W	11.5758050000000008	20.8719719999999995	3.6070630000000001
W	10.1318160000000006	23.7370079999999994	3.4958860000000000
W	18.1617120000000014	15.2779209999999992	3.3268399999999998
W	16.3459730000000008	17.5196919999999992	3.4531930000000002
W	14.2641279999999995	20.6765420000000013	3.4394610000000001
W	12.7571150000000006	23.4361420000000003	3.4238879999999998
W	11.6718750000000000	26.5626430000000013	3.3886799999999999
W	21.2740040000000015	15.2739469999999997	3.3931979999999999
W	19.4123610000000006	17.7301900000000003	3.4286669999999999
W	18.3418279999999996	20.8198180000000015	3.4464210000000000
W	16.7838540000000016	23.6336469999999998	3.5557370000000001
W	14.7429810000000003	26.9159490000000012	3.4268779999999999
W	13.2124640000000007	29.2171750000000010	3.3384890000000000
W	24.4802129999999991	15.3878760000000003	3.4920610000000001

W	23.4021930000000005	17.7992319999999999	3.4071180000000001
W	21.2078290000000003	21.1568289999999983	3.5316429999999999
W	17.9433100000000003	26.2316259999999986	3.4368289999999999
W	16.1860169999999997	29.6824779999999997	3.4397319999999998
W	14.9001959999999993	31.9877460000000013	3.4334220000000002
W	26.2202120000000001	18.0895900000000012	3.5718990000000002
W	25.0259059999999991	20.5341529999999999	3.3966099999999999
W	22.5985809999999994	23.6962420000000016	3.4625290000000000
W	21.1629719999999999	26.2151710000000016	3.4763320000000002
W	19.5999249999999989	29.8405710000000006	3.4363470000000000
W	18.1787659999999995	32.1628169999999969	3.5453830000000002
W	27.7677760000000013	20.7570709999999998	3.5220229999999999
W	26.6316999999999986	23.9676439999999999	3.4940449999999998
W	25.0824309999999997	26.7848089999999992	3.5346890000000002
W	23.4419480000000000	29.5435359999999996	3.4999229999999999
W	21.2066510000000008	32.1287450000000021	3.5494849999999998
W	29.2843459999999993	23.7204669999999993	3.3938030000000001
W	27.7834959999999995	26.5703659999999999	3.3501509999999999
W	26.2376739999999984	29.2610150000000004	3.3435950000000001
W	24.5097069999999988	31.9789560000000002	3.3943690000000002
Se	16.2207790000000003	13.5799090000000007	4.3378220000000001
Se	14.5707470000000008	16.9312460000000016	5.2828860000000004
Se	12.8719649999999994	19.7860699999999987	5.4398520000000001
Se	11.2574860000000001	22.6379979999999996	5.4022069999999998
Se	9.3122229999999995	25.8060429999999990	4.3740300000000003
Se	19.7065190000000001	13.5418599999999998	4.2353009999999998
Se	17.9738429999999987	16.8070899999999988	5.2881660000000004
Se	16.3270389999999992	19.7632629999999985	4.7992600000000003
Se	14.7042420000000007	22.6870229999999999	4.9768770000000000
Se	13.0752530000000000	25.5854520000000001	5.0313179999999997
Se	10.9176939999999991	28.7974500000000013	4.1758490000000004
Se	23.1096159999999990	13.6414360000000006	4.3909640000000003
Se	21.4064049999999995	16.9989789999999985	5.0227570000000004

Se	19.7482010000000017	19.7435520000000011	5.1595170000000001
Se	18.066324999999991	22.6080150000000017	5.2939990000000003
Se	16.2802630000000015	25.5974010000000014	5.1557420000000000
Se	14.6656420000000001	28.6459389999999985	5.2549229999999998
Se	12.7243650000000006	31.7607940000000006	4.3111439999999996
Se	24.8698090000000001	16.9261119999999998	5.3820759999999996
Se	23.0647829999999985	19.8599050000000013	4.9336110000000000
Se	21.3261509999999994	22.7874109999999988	5.3527839999999998
Se	19.6511209999999998	25.5570929999999983	5.1988469999999998
Se	18.0198150000000012	28.4784779999999991	4.8869879999999997
Se	16.4497609999999987	31.5005810000000004	5.2981199999999999
Se	26.4882060000000017	19.7462069999999983	5.4066440000000000
Se	24.6929109999999987	22.7502320000000005	4.7860699999999996
Se	23.1391440000000017	25.6824310000000011	5.0110489999999999
Se	21.4045120000000004	28.4984329999999986	4.7981460000000000
Se	19.6850659999999991	31.4828520000000012	5.4212470000000001
Se	28.0398969999999998	22.6444890000000001	5.2496359999999997
Se	26.4925899999999999	25.6715139999999984	5.3213559999999998
Se	24.8346440000000008	28.5566400000000016	5.3267620000000004
Se	22.9730799999999995	31.4079170000000012	5.2606299999999999
Se	30.2083900000000014	25.6868519999999982	4.3071289999999998
Se	28.4204280000000011	28.7189450000000015	4.4894910000000001
Se	26.6836319999999994	31.7937869999999982	4.3066490000000002
Se	12.7341909999999991	15.6331299999999995	2.5630839999999999
Se	10.8990770000000001	18.6161910000000006	2.6414010000000001
Se	9.1958289999999998	21.7551220000000001	2.5967419999999999
Se	16.4503079999999997	15.7604009999999999	1.5078830000000001
Se	14.6758120000000005	18.7756280000000011	1.7824460000000000
Se	12.8625729999999994	21.6933690000000006	1.5977220000000001
Se	11.4109339999999992	24.7335889999999985	1.6243810000000001
Se	19.7525559999999984	15.9995390000000004	1.5412969999999999
Se	17.9301430000000011	18.8622809999999994	1.8014220000000001
Se	16.2637129999999992	21.7120989999999985	2.0151960000000000

Se	14.734242000000001	24.611219999999994	2.1743370000000000
Se	13.086088999999994	27.480449000000001	1.5427569999999999
Se	22.968627999999989	15.970658000000002	1.6181559999999999
Se	21.388519999999998	18.898572999999990	2.1421220000000001
Se	19.720945000000004	21.806217000000002	1.6982210000000000
Se	18.100805000000011	24.543033000000012	1.6835970000000000
Se	16.471761000000008	27.615690000000007	1.8054060000000001
Se	14.537663000000002	30.428388000000018	1.5414450000000000
Se	26.654534999999992	15.584027000000007	2.5655239999999999
Se	24.836794999999986	18.775013000000013	1.5791649999999999
Se	23.117528000000001	21.691998000000017	1.9064719999999999
Se	21.293067000000006	24.625198000000010	1.5936729999999999
Se	19.686350999999984	27.621286999999988	1.9665459999999999
Se	17.957152000000007	30.588091999999996	1.6750689999999999
Se	16.188521000000015	33.757849999999977	2.5283180000000001
Se	28.500334999999998	18.614084999999993	2.5798939999999999
Se	26.472829999999983	21.827048000000013	1.7730950000000001
Se	24.644216000000001	24.663955999999989	2.0306090000000001
Se	23.060414999999990	27.486768000000014	2.0241829999999998
Se	21.473631999999985	30.455103999999986	1.8136790000000000
Se	19.714824000000001	33.922581999999985	2.7091020000000001
Se	30.144027000000012	21.694887999999988	2.5216820000000002
Se	28.122294000000001	24.828409000000006	1.5231619999999999
Se	26.535896999999985	27.641087999999999	1.4971969999999999
Se	24.907036000000015	30.432859000000005	1.5190999999999999
Se	23.156121999999999	33.728399000000031	2.5391119999999998

W₃₆Se₇₂; $E_{tot} = -21\,088\,501.284\,784\,41$ eV; $E_{rel} = 77.219\,431\,972\,2$ meV/f.u.

W	20.042995000000012	1.2933660000000000	3.3783080000000001
W	18.254076000000013	4.0407549999999999	3.2988819999999999
W	16.759449000000000	6.485965000000002	3.1475469999999999
W	14.893646999999996	9.748625000000005	3.1185459999999998

W	13.458294999999997	12.197020000000002	3.049554999999998
W	11.585188999999997	15.429273000000002	3.049500999999998
W	10.150022999999999	17.880396999999985	2.976367999999999
W	8.271010000000004	21.116543000000001	2.976810000000000
W	6.845765000000001	23.574210000000008	2.901638999999999
W	4.963371000000004	26.842835000000009	2.913589000000000
W	3.560773999999999	29.548767000000016	3.044173999999999
W	2.013437999999998	32.142521999999996	3.095407999999999
W	23.028414000000015	1.216591999999999	3.595403999999998
W	21.421265999999993	3.580823000000001	3.583734000000002
W	19.579118000000011	6.927994000000000	3.614522000000000
W	18.269026000000002	9.244234000000005	3.546292999999999
W	16.312695999999990	12.621565999999996	3.518470999999999
W	14.975569999999994	14.915801999999993	3.467207999999998
W	13.004542000000007	18.305754000000003	3.446099999999999
W	11.667020000000008	20.599340000000015	3.393571999999998
W	9.711007999999996	23.977139000000011	3.365696999999999
W	8.401486999999995	26.293362999999994	3.298605999999999
W	6.559014999999996	29.640450999999988	3.330121999999998
W	4.952236000000001	32.004671999999993	3.318916000000002
W	25.967099000000010	1.079191999999999	3.818951999999999
W	24.419594000000000	3.672613000000001	3.869454000000002
W	23.016797000000004	6.378731000000002	3.999566000000002
W	21.134320999999999	9.647603999999994	4.010999000000000
W	19.709054999999993	12.104981999999997	3.935013999999998
W	17.829827999999991	15.340733999999994	3.935452999999999
W	16.394300000000012	17.791796999999990	3.863785000000000
W	14.521796999999994	21.024166999999985	3.863487999999998
W	13.086729000000001	23.472595999999993	3.793432000000001
W	11.221002999999996	26.735226999999983	3.765366000000002
W	9.726259999999999	29.180170000000004	3.614669000000001
W	7.937844000000001	31.928063999999991	3.536759000000000
Se	21.155090999999988	-0.504993000000000	4.424059999999999

Se	19.514889000000002	2.828860000000002	5.199009000000002
Se	17.987480999999998	5.674291000000002	5.180404000000002
Se	16.176463999999993	8.356671000000004	4.871561999999999
Se	14.704732999999992	11.329522000000008	5.051787000000000
Se	12.880656999999994	14.039336999999997	4.798835999999997
Se	11.395338999999999	17.012889999999987	4.979269999999996
Se	9.570097000000005	19.723876000000006	4.723935000000000
Se	8.091001000000003	22.705006000000009	4.903399000000003
Se	6.285787000000000	25.415904999999986	4.626267999999996
Se	4.787517000000002	28.359759000000004	4.879653000000002
Se	3.172401999999999	31.189807999999993	4.995620999999999
Se	24.463812999999983	-0.442188000000000	4.880649000000000
Se	22.869012000000014	2.762963000000001	5.540104000000004
Se	21.219621000000001	5.617862999999998	5.340696000000003
Se	19.665354000000007	8.560513999999995	5.592837000000003
Se	17.915206000000013	11.295104000000003	5.266545999999999
Se	16.360942000000014	14.235537000000008	5.512705999999997
Se	14.604062000000008	16.971056999999983	5.189549000000004
Se	13.053979999999993	19.918092999999989	5.440795999999997
Se	11.296504999999998	22.652100999999983	5.119180000000001
Se	9.780950000000007	25.605285999999995	5.351168999999996
Se	8.016358999999996	28.273265999999996	5.013927999999999
Se	6.411079000000000	31.288184000000011	5.329387999999998
Se	27.795878999999993	-0.015675000000000	3.025164999999999
Se	26.534542999999993	2.945879000000001	5.180133999999998
Se	25.146453000000011	5.856565999999999	4.990896000000002
Se	23.401977999999997	8.734597000000008	4.804890999999996
Se	21.847774000000011	11.717314000000000	5.090270000000003
Se	20.111729000000004	14.494737000000006	4.687508000000002
Se	18.515198999999991	17.406712999999999	5.044373000000002
Se	16.809664000000015	20.188307999999993	4.599248000000002
Se	15.205099000000006	23.093303999999998	4.974516999999996
Se	13.483313000000008	25.879177999999996	4.539880000000001

Se	11.8933719999999994	28.8668879999999994	4.7580799999999996
Se	10.1036300000000008	31.6777890000000006	4.5473990000000004
Se	17.8767020000000016	1.5426270000000000	2.3677340000000000
Se	16.0872439999999983	4.3538800000000002	2.1556910000000000
Se	14.4971390000000007	7.3417830000000004	2.3726419999999999
Se	12.7750660000000007	10.1278340000000000	1.9383750000000000
Se	11.1707380000000001	13.0328909999999993	2.3122460000000000
Se	9.4644870000000001	15.8142099999999992	1.8680220000000001
Se	7.8677359999999998	18.7267790000000005	2.2250960000000002
Se	6.1320910000000000	21.5044959999999996	1.8219740000000000
Se	4.5782780000000001	24.4866999999999990	2.1077940000000002
Se	2.8336150000000000	27.3653049999999993	1.9224209999999999
Se	1.4462260000000000	30.2761780000000016	1.7336549999999999
Se	0.1845680000000000	33.2371550000000013	3.8894679999999999
Se	21.5690199999999983	1.9330240000000001	1.5852750000000000
Se	19.9638269999999984	4.9474150000000003	1.8994830000000000
Se	18.1994229999999995	7.6155080000000002	1.5612370000000000
Se	16.6836009999999995	10.5691880000000005	1.7932930000000000
Se	14.9259769999999996	13.3032810000000001	1.4718620000000000
Se	13.3754869999999997	16.2501120000000014	1.7227589999999999
Se	11.6188839999999995	18.9854349999999990	1.3998980000000001
Se	10.0648280000000003	21.9263730000000017	1.6457710000000001
Se	8.3147789999999997	24.6609240000000014	1.3195290000000000
Se	6.7606339999999996	27.6039789999999989	1.5725030000000000
Se	5.1114220000000001	30.4590870000000002	1.3737450000000000
Se	3.5175749999999999	33.6635029999999986	2.0347620000000002
Se	24.8083789999999986	2.0314899999999998	1.9183390000000000
Se	23.1929330000000000	4.8609720000000003	2.0337239999999999
Se	21.6942990000000009	7.8052489999999999	2.2862030000000000
Se	19.8892969999999991	10.5163370000000000	2.0088390000000000
Se	18.4095900000000015	13.4974310000000006	2.1890489999999998
Se	16.5845359999999999	16.2083170000000010	1.9331769999999999
Se	15.0990389999999994	19.1819759999999988	2.1128930000000001

Se	13.2752970000000001	21.8914070000000009	1.8609830000000001
Se	11.8041250000000009	24.8647419999999997	2.0409920000000001
Se	9.9931099999999997	27.5473670000000013	1.7326360000000001
Se	8.4654840000000000	30.3931450000000005	1.7147699999999999
Se	6.8253219999999999	33.7259230000000017	2.4913669999999999

W₃₆Se₇₂; $E_{tot}=-21\,088\,502.714\,441\,44$ eV; $E_{rel}=37.506\,736\,694\,4$ meV/f.u.

W	14.9499279999999999	15.4059320000000000	3.4342959999999998
W	13.3215050000000002	17.8085899999999988	3.4313110000000000
W	11.3077349999999992	20.9826590000000017	3.2737930000000000
W	18.1033890000000000	15.2647709999999996	3.3492970000000000
W	16.4595279999999988	17.5434100000000015	3.4689920000000001
W	14.7232819999999993	21.1420959999999987	3.3763070000000002
W	13.0504090000000001	23.7679949999999991	3.4516279999999999
W	11.3206070000000008	26.3858159999999984	3.7536010000000002
W	21.1946070000000013	15.2909659999999992	3.3780579999999998
W	19.5912089999999992	17.5220580000000012	3.4293170000000002
W	17.9139569999999999	21.2160170000000008	3.2820490000000002
W	16.0460710000000013	23.6499670000000002	3.3937460000000002
W	14.4818390000000008	26.2370739999999998	3.4581870000000001
W	13.3328769999999999	29.5301399999999994	3.4664640000000002
W	24.5142270000000018	15.4057899999999997	3.5018250000000002
W	23.3727890000000009	17.7850129999999993	3.3944860000000001
W	21.1462749999999993	21.1529570000000007	3.4319799999999998
W	19.8677740000000007	23.6236989999999984	3.4197080000000000
W	18.3082220000000007	26.1710269999999987	3.5032310000000000
W	16.5304670000000016	29.7637259999999984	3.4383720000000002
W	14.9850689999999993	31.8995679999999986	3.4632930000000002
W	26.2038089999999997	18.1007640000000016	3.5974650000000001
W	24.9681420000000003	20.4781809999999993	3.4272209999999999
W	22.7158510000000007	23.8337719999999997	3.4847540000000001
W	21.2332369999999990	26.2205270000000006	3.5287869999999999

W	19.728760999999987	29.881259000000000	3.422280000000000
W	18.1709020000000017	32.0946830000000034	3.5219649999999998
W	27.7484900000000003	20.8164690000000014	3.5712429999999999
W	26.7110079999999996	23.9122349999999990	3.4826090000000001
W	25.1236460000000008	26.6245779999999996	3.5068500000000000
W	22.9319650000000017	29.8357850000000013	3.4533330000000002
W	21.2782240000000016	32.1157070000000004	3.5655079999999999
W	29.3155649999999994	23.7252000000000010	3.4142359999999998
W	27.8185299999999991	26.5509939999999993	3.3319510000000001
W	26.2756340000000002	29.2165749999999989	3.3760880000000002
W	24.4933450000000015	31.9885960000000011	3.5331370000000000
Se	16.2403930000000010	13.7578549999999993	4.6125230000000004
Se	14.7351270000000003	17.0247579999999985	5.3224700000000000
Se	12.9235450000000007	19.8229460000000017	4.9705040000000000
Se	11.1813359999999999	22.6421269999999986	5.0058800000000003
Se	9.3734459999999995	26.1396699999999989	4.9405840000000003
Se	19.7282909999999987	13.5882140000000007	4.3620080000000003
Se	18.0314799999999984	16.8496309999999987	5.3098789999999996
Se	16.3635410000000014	19.8305639999999990	4.8209929999999996
Se	14.5778119999999998	22.7424509999999991	5.2710730000000003
Se	12.9232460000000007	25.5327130000000011	5.3673760000000001
Se	10.9752620000000007	28.9134980000000006	4.0261399999999998
Se	23.1720340000000000	13.6662920000000003	4.3876150000000003
Se	21.4363250000000001	16.9877760000000002	5.0994330000000003
Se	19.5646260000000005	19.7906610000000001	4.8344120000000004
Se	17.9308820000000004	22.8394070000000013	5.0680529999999999
Se	16.3164550000000013	25.6140770000000018	5.0941039999999997
Se	14.7573410000000003	28.4776139999999991	5.0458600000000002
Se	12.7471619999999994	31.7783419999999985	4.4083470000000000
Se	24.8307469999999988	16.9535079999999994	5.3958789999999999
Se	22.9986120000000014	19.8733280000000008	4.9274509999999996
Se	21.3881389999999989	22.7189799999999984	5.3395330000000003
Se	19.7786350000000013	25.4356930000000006	5.3951729999999998

Se	18.143744999999991	28.449415999999994	4.9390879999999999
Se	16.490050000000001	31.564633000000006	5.3633350000000002
Se	26.4633809999999983	19.7640269999999987	5.4348169999999998
Se	24.740035999999999	22.7331779999999988	4.7885920000000004
Se	23.1804309999999987	25.6625650000000007	5.1324880000000004
Se	21.3585789999999989	28.4695859999999996	4.9467160000000003
Se	19.7165950000000016	31.5954979999999992	5.4153180000000001
Se	28.0898639999999986	22.6483080000000001	5.3007710000000001
Se	26.5670690000000000	25.6583159999999992	5.3304260000000001
Se	24.7026949999999985	28.5887990000000016	5.1012610000000000
Se	22.9568750000000001	31.5670369999999991	5.4111719999999996
Se	30.2039289999999987	25.6935140000000004	4.3770980000000002
Se	28.5249179999999996	28.7794039999999995	4.2729999999999997
Se	26.6937519999999999	31.6933459999999982	4.3793990000000003
Se	12.7056600000000000	15.5704049999999992	2.4949210000000002
Se	10.9996469999999995	18.4624500000000005	2.8404250000000002
Se	9.2620419999999992	21.1740789999999990	2.2613400000000001
Se	16.4302549999999989	15.7709290000000006	1.5195380000000001
Se	14.7570610000000002	18.8659919999999985	1.8448380000000000
Se	12.8975069999999992	21.8304480000000005	1.6505950000000000
Se	11.0672420000000002	24.7139640000000007	2.0386220000000002
Se	19.6704439999999998	15.8180560000000003	1.4754240000000001
Se	18.0180259999999990	18.8934519999999999	1.9062180000000000
Se	16.2415209999999988	21.8740290000000002	1.5125010000000001
Se	14.5585920000000009	24.6717440000000003	1.5720179999999999
Se	12.8920549999999992	27.5628250000000001	1.9085300000000001
Se	22.9691890000000001	15.9170719999999992	1.6258220000000001
Se	21.3630980000000008	18.8807459999999985	2.0576140000000001
Se	19.6796809999999986	21.8073569999999997	1.5433589999999999
Se	18.0063129999999987	24.5523910000000001	1.7643390000000001
Se	16.4316090000000017	27.4450620000000001	2.1496100000000000
Se	14.7950379999999999	30.2539769999999990	1.5941179999999999
Se	26.6909840000000003	15.6085010000000004	2.6078109999999999

Se	24.845490000000016	18.768816000000011	1.5793390000000000
Se	23.099779999999991	21.685593999999983	1.9566600000000001
Se	21.320215000000010	24.656338999999991	1.5574509999999999
Se	19.728170999999997	27.614004999999988	1.9836450000000001
Se	18.077594000000013	30.468358999999995	1.5992430000000000
Se	16.231853000000010	33.581544000000009	2.3029020000000000
Se	28.489173999999984	18.641743000000017	2.6580580000000000
Se	26.415558000000008	21.850380000000012	1.8182100000000001
Se	24.703158999999994	24.663084999999988	1.9498450000000001
Se	23.047375999999999	27.551653000000017	2.1596560000000000
Se	21.385004999999996	30.528597000000013	1.6096670000000000
Se	19.726321999999997	33.713059000000012	2.3872510000000000
Se	30.130751000000001	21.648444000000014	2.5767050000000000
Se	28.177212000000008	24.811582000000014	1.5123640000000000
Se	26.475643999999991	27.582803999999994	1.5011429999999999
Se	24.757636999999990	30.378267000000010	1.6686700000000001
Se	23.249635999999989	33.769669999999979	2.6002010000000002

W₃₆Se₇₂; $E_{tot} = -21\,088\,503.607\,691\,06$ eV; $E_{rel} = 12.694\,247\,250\,0$ meV/f.u.

W	19.909575000000002	1.4184019999999999	3.5450249999999999
W	18.162786000000005	4.1633490000000002	3.3539620000000001
W	16.607741000000008	6.6764970000000003	3.0873469999999998
W	14.986879999999993	9.224938999999991	2.8536250000000001
W	23.129796999999999	1.2690980000000001	3.5843929999999999
W	21.460288999999995	3.6079699999999999	3.5273780000000001
W	19.408598000000013	6.9161250000000001	3.2265950000000001
W	18.120702999999989	9.218581999999996	2.9229390000000000
W	26.328049000000000	1.2060960000000001	3.6165370000000001
W	24.617829000000004	3.5109629999999998	3.5931310000000001
W	23.187751999999997	7.1825210000000004	3.2572869999999998
W	21.492854000000012	9.4072540000000000	3.1644760000000001
W	29.537950999999996	1.1708680000000000	3.6313510000000000

W	27.8618290000000002	3.4637080000000000	3.5908660000000001
W	26.3351259999999989	7.1738710000000001	3.2894040000000002
W	24.7314949999999989	9.4597180000000005	3.2727930000000001
W	32.7438050000000018	1.1367060000000000	3.6449989999999999
W	31.1177239999999991	3.4344700000000001	3.5942200000000000
W	29.5451529999999991	7.1435810000000002	3.3188439999999999
W	27.9190259999999988	9.4416239999999991	3.2681360000000002
W	35.9313629999999975	1.1186469999999999	3.6404120000000000
W	34.3277050000000017	3.4039199999999998	3.6235510000000000
W	32.8010930000000016	7.1147080000000003	3.3223360000000000
W	31.1249360000000017	9.4070780000000003	3.2816749999999999
W	39.1699690000000018	1.1709799999999999	3.7488130000000002
W	37.4750599999999991	3.3953970000000000	3.6556970000000000
W	36.0451759999999979	7.0674510000000001	3.3200370000000001
W	34.3347309999999979	9.3716050000000006	3.2964310000000001
W	42.5421830000000014	1.3597490000000001	3.9905469999999998
W	41.2543879999999987	3.6619030000000001	3.6867070000000002
W	39.2025349999999975	6.9701019999999998	3.3855870000000001
W	37.5329460000000026	9.3086780000000005	3.3284449999999999
W	45.6760080000000031	1.3530599999999999	4.0593959999999996
W	44.0548670000000016	3.9016060000000001	3.8259349999999999
W	42.4999690000000001	6.4147439999999998	3.5588810000000000
W	40.7532059999999987	9.1598020000000009	3.3677600000000001
Se	21.0555120000000002	-0.3316760000000000	4.5898750000000001
Se	19.5762949999999982	3.1627710000000002	5.2616350000000001
Se	17.9725900000000003	5.9298529999999996	5.1053550000000003
Se	16.3856439999999992	8.7308699999999995	4.7694809999999999
Se	24.4973029999999987	-0.4214460000000000	4.6503560000000004
Se	22.9489079999999994	2.9593110000000000	5.4334009999999999
Se	21.3669839999999986	5.9573619999999998	4.6942719999999998
Se	19.7205100000000009	8.9340290000000007	4.8792299999999997
Se	27.7982879999999994	-0.4729140000000000	4.6471159999999996
Se	26.2280830000000016	2.9238610000000000	5.4529930000000002

Se	24.662804999999988	5.874909999999999	4.8700279999999996
Se	23.055471000000007	8.989865000000000	5.1005529999999997
Se	31.059480000000006	-0.507650000000000	4.6610420000000001
Se	29.479988999999998	2.903686000000000	5.453830000000000
Se	27.891746000000013	5.823312999999997	4.851030999999999
Se	26.308897999999992	9.017464999999996	5.1526430000000003
Se	34.337150999999986	-0.507279000000000	4.7214070000000001
Se	32.710783999999968	2.856525000000000	5.481068999999997
Se	31.149132000000016	5.779689000000003	4.849863000000000
Se	29.519066999999997	9.006942000000004	5.162280000000000
Se	37.678462000000032	-0.558581000000000	4.585176999999998
Se	35.935380999999996	2.786365000000000	5.532168000000004
Se	34.389671999999974	5.746042000000001	4.868242999999997
Se	32.730772000000018	8.964166000000005	5.170715999999996
Se	41.009180999999981	-0.281478000000000	4.973887000000004
Se	39.321016000000002	2.954623999999999	5.382673999999997
Se	37.580741000000033	5.725101000000004	4.947754999999999
Se	35.937381000000020	8.900925000000009	5.189222000000000
Se	44.331972000000004	0.006214000000000	5.441164999999998
Se	42.705243000000030	3.126096000000000	5.736065000000000
Se	40.862295000000031	5.801886999999998	5.170367999999999
Se	39.173347999999972	8.828179999999997	5.228828000000000
Se	47.524051000000000	0.239014000000000	3.353943000000001
Se	46.284032000000034	3.423934000000000	5.050679999999998
Se	44.718567000000002	6.212340000000002	4.539168000000001
Se	42.897089999999986	8.967454000000000	4.360021999999998
Se	17.765668000000016	1.610660000000000	2.552811999999999
Se	15.944193000000003	4.365832000000002	2.373879000000001
Se	14.378792000000007	7.154347999999997	1.862646999999999
Se	13.138600999999995	10.339226000000000	3.559972999999998
Se	21.489491999999985	1.749943999999999	1.684075999999999
Se	19.800565999999999	4.776272999999998	1.742709000000001
Se	17.957408000000009	7.452276000000003	1.177283000000001

Se	16.330870000000009	10.572025999999993	1.4726220000000001
Se	24.725512999999994	1.677168999999999	1.7237730000000000
Se	23.082087999999988	4.8530160000000002	1.9652760000000000
Se	21.341736000000009	7.6236620000000004	1.5305700000000000
Se	19.653621000000011	10.859897999999994	1.939389999999999
Se	27.932110000000015	1.6139150000000000	1.7423660000000001
Se	26.273208000000003	4.8320220000000003	2.0446780000000002
Se	24.727456000000001	7.791871999999997	1.3809950000000000
Se	22.984335000000015	11.136837999999991	2.328056999999998
Se	31.143830999999987	1.5711370000000000	1.7508230000000000
Se	29.513794999999982	4.7984020000000003	2.0631010000000001
Se	27.952048000000013	7.721665999999999	1.4320070000000000
Se	26.325677999999999	11.085492999999996	2.191638999999999
Se	34.354014999999969	1.5605920000000000	1.760486999999999
Se	32.771102999999965	4.754834999999999	2.062021999999998
Se	31.182891999999989	7.674410000000000	1.4591580000000000
Se	29.603421000000009	11.085767000000006	2.252016999999999
Se	37.607363999999969	1.5882140000000000	1.8127030000000000
Se	36.000013000000027	4.703214000000000	2.0431080000000001
Se	34.434744999999995	7.654168999999996	1.4599230000000001
Se	32.864615999999981	11.051038999999994	2.2659210000000001
Se	40.942255000000030	1.6440450000000000	2.034057999999999
Se	39.295744999999966	4.620707999999996	2.2187920000000001
Se	37.713872000000021	7.618682999999999	1.4794600000000000
Se	36.165469999999991	10.999454999999993	2.2625630000000001
Se	44.277282999999971	1.8472180000000000	2.1438370000000000
Se	42.690297999999985	4.648242999999999	1.807874999999999
Se	41.086463000000020	7.4151530000000001	1.651359999999999
Se	39.607174999999980	10.909632000000002	2.3228040000000001

W₃₆Se₇₂; $E_{tot} = -21\,088\,504.064\,683\,96$ eV; $E_{rel} = 0$ meV/f.u.

W	29.633275999999986	1.2652530000000000	3.5064860000000002
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W	27.873190999999985	3.984850999999999	3.4627520000000001
W	26.286042999999994	6.728640999999997	3.4146470000000000
W	24.7688190000000006	9.5482940000000003	3.2512520000000000
W	23.2039480000000005	12.4681940000000004	2.9291969999999998
W	21.5753780000000006	15.130905999999995	2.8212989999999998
W	32.9845720000000000	1.1501370000000000	3.5402950000000000
W	30.7284429999999986	3.6912600000000002	3.3899699999999999
W	29.0822870000000009	6.380315999999997	3.3181479999999999
W	27.5400489999999998	9.1566069999999993	3.2684510000000002
W	25.8732359999999986	12.5709079999999993	3.1589580000000002
W	24.6627289999999988	15.0017289999999992	2.9737890000000000
W	36.1695939999999965	1.1782340000000000	3.5768290000000000
W	34.64646900000000033	3.6307450000000001	3.4980009999999999
W	32.9538340000000005	6.9521559999999996	3.5155940000000001
W	31.4607059999999983	9.7336919999999996	3.5422050000000000
W	29.8030679999999997	12.5504169999999995	3.3691000000000000
W	27.8538150000000009	15.0681469999999997	3.1787359999999998
W	39.3454550000000012	1.1707580000000000	3.7343810000000000
W	37.3963359999999980	3.6884100000000002	3.5436749999999999
W	35.7380039999999966	6.5053549999999998	3.3711679999999999
W	34.24582800000000030	9.28660900000000003	3.3976299999999999
W	32.5528359999999992	12.6077019999999997	3.4156740000000001
W	31.0297319999999992	15.0601590000000005	3.3367089999999999
W	42.5366149999999976	1.2373810000000001	3.9395380000000002
W	41.32608400000000016	3.6676460000000000	3.7537669999999999
W	39.6590899999999991	7.0824710000000000	3.6444690000000000
W	38.1173709999999986	9.8584779999999999	3.5945670000000001
W	36.47070300000000003	12.5473230000000004	3.5233200000000000
W	34.2150389999999973	15.0884879999999999	3.3730069999999999
W	45.6247499999999988	1.1086980000000000	4.0911980000000003
W	43.99520400000000011	3.7709100000000002	3.9837080000000000
W	42.4301019999999980	6.6908740000000000	3.6614689999999999
W	40.91288300000000008	9.5100949999999997	3.4985590000000002

W	39.326214999999977	12.253686999999993	3.450275000000000
W	37.566187999999968	14.973252999999997	3.406778000000000
Se	30.978217000000008	-0.438368000000000	4.472538000000000
Se	29.185240000000003	2.849336000000000	5.341154999999997
Se	27.521176000000005	5.632385000000002	5.292646999999997
Se	25.943363000000015	8.467703000000002	5.191491000000000
Se	24.363120999999996	11.388961000000001	4.922120999999997
Se	22.828223999999987	14.336216999999995	4.741063999999997
Se	34.404437000000015	-0.585350000000000	4.372901999999998
Se	32.687699999999995	2.914975999999998	5.105100000000002
Se	31.028528000000014	5.748705000000002	4.913045000000003
Se	29.437653000000010	8.527850000000008	4.836818000000001
Se	27.760379000000004	11.419904000000007	4.603876999999998
Se	26.143090000000008	14.427369000000006	4.939263000000004
Se	37.709780999999996	-0.546125000000000	4.513798000000004
Se	36.018965999999989	2.752094000000000	5.481595999999997
Se	34.331626000000000	5.630208999999998	5.210014000000001
Se	32.792937999999995	8.611490999999991	5.389980999999997
Se	31.109261000000001	11.518490999999991	5.270160999999999
Se	29.340448999999996	14.406997000000005	5.102428999999999
Se	40.959381999999980	-0.497853000000000	4.729497000000003
Se	39.277594999999980	2.963372000000001	5.297375999999999
Se	37.696711000000005	5.824224000000001	4.991133999999997
Se	36.165948000000002	8.624416000000001	4.943329999999996
Se	34.467553000000023	11.501754999999993	4.817325000000003
Se	32.660044999999967	14.488295000000008	5.219205999999998
Se	44.179063999999968	-0.357894000000000	5.242645000000004
Se	42.598323000000006	2.849202000000000	5.816138999999997
Se	40.989353000000013	5.755238000000003	5.378714000000004
Se	39.503445999999967	8.799974999999999	5.469940000000002
Se	37.856064000000035	11.632853000000008	5.394857000000000
Se	35.931547000000019	14.464140000000004	5.201134999999998
Se	47.495865999999995	0.026098000000000	3.399356000000000

Se	46.155757999999987	3.028959000000000	5.342786000000000
Se	44.690885000000015	5.956889999999996	4.802233000000000
Se	43.207895000000006	8.897012000000001	4.440629999999996
Se	41.508822000000021	11.835786999999998	4.502730999999998
Se	39.705598000000019	14.853481000000004	4.359938999999998
Se	27.494029999999986	1.385119999999999	2.553100999999998
Se	25.690535000000006	4.402960000000002	2.410744999999999
Se	23.991578000000005	7.342190999999997	2.472262000000002
Se	22.508672000000007	10.282346999999997	2.110069000000002
Se	21.043361999999983	13.211308000000007	1.569824000000001
Se	19.704087999999987	16.214203000000013	3.513342000000002
Se	31.268059999999984	1.774502999999999	1.712078999999999
Se	29.343340000000013	4.605904999999999	1.518373999999999
Se	27.695802000000005	7.438979999999999	1.443554999999999
Se	26.209963999999994	10.483985999999998	1.534030999999999
Se	24.601241000000017	13.390295999999993	1.096819999999999
Se	23.020963999999993	16.597645000000000	1.670140000000000
Se	34.539343999999998	1.750292000000000	1.694171000000001
Se	32.731729000000014	4.736870999999998	2.096017999999999
Se	31.033526999999994	7.614599000000001	1.970137000000000
Se	29.502310000000014	10.414320999999993	1.922245000000000
Se	27.921641000000010	13.275434000000006	1.616150999999999
Se	26.240286999999986	16.736869999999997	2.183940000000002
Se	37.858967999999973	1.831863999999999	1.810764000000000
Se	36.089976000000001	4.720461000000002	1.643278999999999
Se	34.406418000000022	7.627456999999997	1.523036000000001
Se	32.867401999999985	10.608302000000001	1.703534000000001
Se	31.180792000000003	13.486594999999994	1.431290000000000
Se	29.489560999999984	16.784637000000000	2.399804000000000
Se	41.055799999999979	1.811375000000000	1.973568999999999
Se	39.438833000000025	4.818992999999999	2.309035999999999
Se	37.761032000000002	7.710880000000004	2.076392999999999
Se	36.170940999999991	10.490017999999992	2.000077000000001

Se	34.5116110000000020	13.3237439999999996	1.8079030000000000
Se	32.7953460000000021	16.8241039999999984	2.5405940000000000
Se	44.3710349999999991	1.9031780000000000	2.1711730000000000
Se	42.8358619999999988	4.8501899999999996	1.9907210000000000
Se	41.2557339999999968	7.7713460000000003	1.7217720000000001
Se	39.6779709999999994	10.6064849999999993	1.6201220000000001
Se	38.0141360000000006	13.3893509999999996	1.5721650000000000
Se	36.2210899999999967	16.6771029999999989	2.4410170000000000

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,239.021\,027\,68$ eV; $E_{rel} = 365.463\,760\,772\,7$ meV/f.u.

W	20.9139739999999996	-0.1989630000000000	3.4086509999999999
W	22.0205430000000000	2.1408480000000001	3.8230590000000002
W	19.2825950000000006	2.4581439999999999	3.4122810000000001
W	17.6765469999999993	5.1815490000000004	3.3982950000000001
W	16.0728159999999995	7.9566340000000002	3.3508969999999998
W	14.4641999999999999	10.7421249999999997	3.2894410000000001
W	12.8553250000000006	13.5348039999999994	3.2257479999999998
W	11.2382650000000002	16.3272280000000016	3.1835670000000000
W	9.6194559999999996	19.1214039999999983	3.1733690000000001
W	8.0023890000000009	21.9178320000000006	3.1904870000000001
W	6.3917760000000001	24.7153579999999984	3.2182070000000000
W	4.7850619999999999	27.5140799999999999	3.2398430000000000
W	3.1765560000000002	30.3105790000000006	3.2476490000000000
W	23.6551110000000016	-0.5816850000000000	3.8375949999999999
W	20.4373019999999990	4.8717530000000000	3.8176960000000002
W	18.8149489999999986	7.6650520000000002	3.8014679999999998
W	17.1994259999999990	10.4641110000000008	3.7305980000000001
W	15.5893429999999995	13.2568719999999995	3.6642800000000002
W	13.9755240000000001	16.0476920000000014	3.6196510000000002
W	12.3548960000000001	18.8357199999999985	3.6096499999999998
W	10.7374860000000005	21.6246259999999992	3.6244670000000001
W	9.1245259999999995	24.4185319999999990	3.6522649999999999

W	7.5165290000000002	27.2181509999999989	3.6778330000000001
W	5.9071730000000002	30.0191060000000007	3.6932209999999999
W	1.5625869999999999	33.1046210000000016	3.2439870000000002
W	2.6760530000000000	35.6141959999999997	3.6893940000000001
W	-0.0554250000000000	35.8980379999999997	3.2364809999999999
W	-1.6734130000000000	38.6931450000000012	3.2305489999999999
W	-3.2897409999999998	41.4896150000000006	3.2298119999999999
W	-4.9040749999999997	44.2861970000000014	3.2323390000000001
W	-6.5182209999999996	47.0819159999999997	3.2337699999999998
W	-8.1347690000000004	49.8768209999999996	3.2312479999999999
W	-9.7536070000000006	52.6704300000000032	3.2247020000000002
W	-11.3716200000000001	55.4668769999999967	3.2177099999999998
W	-12.9866960000000002	58.2661140000000017	3.2198600000000002
W	-14.5958530000000000	61.0680850000000035	3.2338629999999999
W	-16.2060139999999997	63.8689359999999979	3.2600099999999999
W	4.2935619999999997	32.8184510000000031	3.6955320000000000
W	1.0575159999999999	38.4078429999999997	3.6830259999999999
W	-0.5589210000000000	41.2015320000000003	3.6808450000000001
W	-2.1732770000000001	43.9972830000000030	3.6818360000000001
W	-3.7876200000000000	46.7939020000000028	3.6841390000000001
W	-5.4037780000000000	49.5909049999999993	3.6834730000000002
W	-7.0219509999999996	52.3861959999999982	3.6779910000000000
W	-8.6403890000000008	55.1809099999999972	3.6698640000000000
W	-10.2550279999999994	57.9748779999999968	3.6657790000000001
W	-11.8646259999999995	60.7726510000000033	3.6727210000000001
W	-13.4717310000000001	63.5709360000000032	3.6945389999999998
W	-17.8168620000000004	66.6634279999999961	3.2865250000000001
W	-16.7001980000000003	69.1672300000000035	3.7407720000000002
W	-19.4358359999999983	69.4533700000000067	3.3018589999999999
W	-21.0550700000000006	72.2422849999999954	3.2908569999999999
W	-22.6709430000000012	75.0335850000000022	3.2473209999999999
W	-24.2820760000000000	77.8264410000000026	3.1813340000000001
W	-25.8979500000000016	80.6262159999999994	3.1094789999999999

W	-27.520537999999984	83.4189520000000044	3.0931739999999999
W	-29.1046890000000005	86.1500929999999983	3.0862259999999999
W	-30.7387480000000011	88.8727810000000034	3.0714549999999998
W	-15.0831649999999993	66.3696630000000027	3.7227440000000001
W	-18.3205710000000010	71.9610919999999936	3.7332329999999998
W	-19.9368659999999984	74.7553259999999966	3.6905850000000000
W	-21.5477629999999998	77.5479870000000062	3.6271480000000000
W	-23.1560069999999989	80.3327450000000027	3.5652729999999999
W	-24.7614270000000012	83.1094570000000061	3.5166100000000000
W	-26.3657560000000011	85.8325990000000019	3.5015010000000002
W	-27.9995089999999998	88.4902220000000028	3.5030920000000001
Se	21.8857399999999984	-2.1141160000000001	4.5807039999999999
Se	20.2536149999999999	1.1255090000000001	5.3574970000000004
Se	18.6527290000000008	3.9193590000000000	5.3560720000000002
Se	17.0202719999999985	6.6841699999999999	5.3119600000000000
Se	15.4197690000000005	9.4780999999999995	5.2544570000000004
Se	13.8096560000000004	12.2649679999999996	5.1885610000000000
Se	12.1944529999999993	15.0416919999999994	5.1346900000000000
Se	10.5719949999999994	17.8122369999999997	5.1091290000000003
Se	8.9526819999999994	20.5901330000000016	5.1141769999999998
Se	7.3397880000000004	23.3809499999999986	5.1383939999999999
Se	5.7309089999999996	26.1824350000000017	5.1644090000000000
Se	4.1202170000000002	28.9865409999999990	5.1797209999999998
Se	25.4560730000000000	-1.8011640000000000	3.1532290000000001
Se	24.0562819999999995	1.1921100000000000	5.3359259999999997
Se	22.5000889999999991	4.1775929999999999	5.1702110000000001
Se	20.9192539999999987	7.0327390000000003	5.0387089999999999
Se	19.3322390000000013	9.8557830000000006	4.9351870000000000
Se	17.7252919999999996	12.6527519999999996	4.8603079999999999
Se	16.1216979999999985	15.4441179999999996	4.7955180000000004
Se	14.4972139999999996	18.2190989999999999	4.7868839999999997
Se	12.8743289999999995	20.9943519999999992	4.8020060000000004
Se	11.2557630000000000	23.7758970000000005	4.8319270000000003

Se	9.6444910000000004	26.5695949999999996	4.8605830000000001
Se	8.0341889999999996	29.3727049999999998	4.8804720000000001
Se	19.0986469999999997	0.2021540000000000	1.9088050000000001
Se	17.2099790000000006	2.9545460000000001	2.1864599999999998
Se	15.5646400000000007	5.7440759999999997	2.2019959999999998
Se	13.9459289999999996	8.5368399999999998	2.1599320000000000
Se	12.3411229999999996	11.3398190000000003	2.0852970000000002
Se	10.7315179999999994	14.1462140000000005	2.0208309999999998
Se	9.1144940000000005	16.9539709999999992	1.9847820000000000
Se	7.4903180000000003	19.7581449999999990	1.9892550000000000
Se	5.8701809999999996	22.5593530000000015	2.0154909999999999
Se	4.2601310000000003	25.3568800000000003	2.0422039999999999
Se	2.6556660000000001	28.1503100000000011	2.0553680000000001
Se	1.0493930000000000	30.9423400000000015	2.0541040000000002
Se	22.7880070000000003	0.6141510000000000	1.8940319999999999
Se	21.0874179999999996	3.3953199999999999	1.8751640000000001
Se	19.4703720000000011	6.1652220000000000	1.8804860000000001
Se	17.8651969999999984	8.9406440000000007	1.8353630000000001
Se	16.2458880000000008	11.7298539999999996	1.7645720000000000
Se	14.6340900000000005	14.5354430000000008	1.7073380000000000
Se	13.0196470000000009	17.3463920000000016	1.6794929999999999
Se	11.4023970000000006	20.1538229999999992	1.6808799999999999
Se	9.7863769999999999	22.9549880000000002	1.7030860000000001
Se	8.1768959999999993	25.7527380000000008	1.7312710000000000
Se	6.5718699999999997	28.5482699999999987	1.7526430000000000
Se	4.9649660000000004	31.3425860000000007	1.7613129999999999
Se	2.5047269999999999	31.7870600000000003	5.1810369999999999
Se	0.8860040000000000	34.5827269999999984	5.1743829999999997
Se	-0.7327200000000000	37.3755319999999998	5.1672390000000004
Se	-2.3490869999999999	40.1684770000000029	5.1641040000000000
Se	-3.9632890000000001	42.9637760000000029	5.1652990000000001
Se	-5.5772830000000004	45.7608010000000007	5.1676140000000004
Se	-7.1935799999999999	48.5582939999999965	5.1669539999999996

Se	-8.8120940000000001	51.3544940000000025	5.1621610000000002
Se	-10.4302510000000002	54.1490179999999981	5.1547000000000001
Se	-12.0439779999999992	56.9430329999999998	5.1515370000000003
Se	-13.6518949999999997	59.7376000000000005	5.1595079999999998
Se	-15.2578390000000006	62.5339049999999972	5.1801870000000001
Se	6.4207760000000000	32.1787890000000019	4.8870690000000003
Se	4.8033400000000004	34.9808530000000033	4.8844750000000001
Se	3.1850730000000000	37.7766499999999965	4.8787300000000000
Se	1.5682400000000001	40.5689729999999997	4.8750679999999997
Se	-0.0468640000000000	43.3619160000000008	4.8750049999999998
Se	-1.6615810000000000	46.1575369999999978	4.8770540000000002
Se	-3.2778830000000001	48.9555509999999998	4.8777509999999999
Se	-4.8967070000000001	51.7536229999999975	4.8748719999999999
Se	-6.5151459999999997	54.5493510000000015	4.8676259999999996
Se	-8.1283100000000008	57.3432189999999977	4.8596139999999997
Se	-9.7357949999999995	60.1355649999999997	4.8580329999999998
Se	-11.3406199999999995	62.9295180000000016	4.8715669999999998
Se	-0.5632250000000000	33.7352330000000009	2.0460710000000000
Se	-2.1807859999999999	36.5305329999999984	2.0388679999999999
Se	-3.7991549999999998	39.3283050000000003	2.0360200000000002
Se	-5.4155430000000004	42.1263610000000028	2.0371779999999999
Se	-7.0305739999999997	44.9217360000000028	2.0396529999999999
Se	-8.6458990000000000	47.7148520000000005	2.0397590000000001
Se	-10.2625069999999994	50.5076880000000017	2.0353800000000000
Se	-11.8807849999999995	53.3042019999999965	2.0291429999999999
Se	-13.4984289999999998	56.1067370000000025	2.0256710000000000
Se	-15.1125600000000002	58.9136239999999987	2.0316060000000000
Se	-16.7233540000000005	61.7179140000000004	2.0511539999999999
Se	-18.3353240000000000	64.5126450000000062	2.0786340000000001
Se	3.3520020000000001	34.1360480000000024	1.7586649999999999
Se	1.7345029999999999	36.9299820000000025	1.7519270000000000
Se	0.1164630000000000	39.7258369999999985	1.7470520000000000
Se	-1.4996540000000000	42.5228910000000013	1.7467980000000001

Se	-3.1140230000000000	45.3197100000000006	1.7488230000000000
Se	-4.7284910000000000	48.1150620000000018	1.7503040000000001
Se	-6.3447810000000002	50.9085809999999981	1.7469349999999999
Se	-7.9633760000000002	53.7020759999999981	1.7398780000000000
Se	-9.5825390000000006	56.4982010000000017	1.7326250000000001
Se	-11.1987530000000000	59.2994669999999999	1.7339840000000000
Se	-12.8101500000000001	62.1043060000000011	1.7485649999999999
Se	-14.4191680000000009	64.9070980000000048	1.7751429999999999
Se	-16.8682459999999992	65.3317899999999980	5.2086930000000002
Se	-18.4853710000000007	68.1335980000000063	5.2299460000000000
Se	-20.1039889999999986	70.9413229999999970	5.2320679999999999
Se	-21.7196449999999999	73.7518979999999971	5.2030709999999996
Se	-23.3319560000000017	76.5584910000000036	5.1473820000000003
Se	-24.9519790000000015	79.3471049999999991	5.0760610000000002
Se	-26.5573049999999995	82.1246309999999937	5.0302920000000002
Se	-28.1731200000000008	84.8948000000000036	5.0347759999999999
Se	-29.8751500000000014	87.6761290000000031	5.0161490000000004
Se	-12.9515349999999998	65.7272300000000058	4.8981050000000002
Se	-14.5719899999999996	68.5287859999999966	4.9256209999999996
Se	-16.1975550000000013	71.3334310000000045	4.9324409999999999
Se	-17.8157199999999989	74.1414659999999941	4.8981859999999999
Se	-19.4269269999999992	76.9486859999999950	4.8363790000000000
Se	-21.0317529999999984	79.7519810000000007	4.7603549999999997
Se	-22.6509569999999982	82.5462239999999952	4.7175149999999997
Se	-24.2964720000000014	85.3355480000000028	4.7301810000000000
Se	-26.1848209999999995	88.0889190000000042	5.0051550000000002
Se	-19.9531859999999988	67.2952619999999939	2.1082290000000001
Se	-21.5757109999999983	70.0714320000000015	2.1211069999999999
Se	-23.1997940000000007	72.8478439999999949	2.1109909999999998
Se	-24.8045429999999989	75.6388670000000047	2.0475129999999999
Se	-26.4122689999999984	78.4357130000000069	1.9728730000000001
Se	-28.0005980000000001	81.2586780000000033	1.8706520000000000
Se	-29.5824290000000012	84.1132589999999993	1.7371900000000000

Se	-31.139019999999986	87.0989710000000059	1.5720190000000001
Se	-32.542000000000016	90.0904840000000036	3.7541280000000001
Se	-16.0319000000000003	67.6991359999999958	1.7994619999999999
Se	-17.6497379999999993	70.4785020000000060	1.8062199999999999
Se	-19.2724970000000013	73.2504129999999947	1.7817799999999999
Se	-20.8880680000000005	76.0276989999999984	1.7287290000000000
Se	-22.4987969999999997	78.8143519999999995	1.6620600000000001
Se	-24.1010929999999988	81.6083909999999975	1.6038079999999999
Se	-25.7348609999999987	84.3722219999999936	1.5576019999999999
Se	-27.3368080000000013	87.1655580000000043	1.5554159999999999
Se	-28.9707849999999993	90.4060580000000016	2.3303440000000002

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,254.387\,172\,96$ eV; $E_{rel} = 132.643\,377\,742\,4$ meV/f.u.

W	38.319733999999969	3.1185900000000002	3.0885199999999999
W	41.509320999999999	2.9188950000000000	3.4705080000000001
W	39.5584619999999987	6.3027420000000003	3.4576199999999999
W	36.4436109999999971	6.3792640000000000	3.0705070000000001
W	35.0799870000000027	8.9824500000000000	3.1320350000000001
W	33.4495489999999975	11.6381320000000006	3.0672560000000000
W	31.5203759999999988	14.8615499999999994	3.0772900000000001
W	30.0659719999999986	17.2803870000000011	3.0540289999999999
W	28.1968859999999992	20.5168409999999994	3.0563359999999999
W	26.7851199999999992	22.9818929999999995	2.9574340000000001
W	24.9203510000000001	26.2616340000000008	2.9302700000000002
W	23.5254259999999995	28.9729719999999986	3.0387330000000001
W	21.9798480000000005	31.5656849999999984	3.0802839999999998
W	38.2075779999999980	8.6195149999999998	3.4995150000000002
W	36.3246669999999980	11.9340060000000001	3.4585439999999998
W	34.9073110000000000	14.3779249999999994	3.4492509999999998
W	32.9119639999999976	17.6898599999999995	3.4987089999999998
W	31.5881940000000014	19.9969239999999999	3.4595150000000001
W	29.6457610000000003	23.3787790000000015	3.4243990000000002

W	28.352368999999995	25.702203999999983	3.3359510000000001
W	26.525895999999995	29.057849999999984	3.3329170000000001
W	24.9199950000000001	31.4244960000000013	3.3040949999999998
W	44.6243460000000027	2.8820739999999998	3.8588819999999999
W	42.7585940000000022	6.1184180000000001	3.8212109999999999
W	41.3407839999999993	8.5853780000000004	3.8736340000000000
W	39.4644850000000034	11.8450220000000002	3.8470569999999999
W	37.8254820000000009	14.4931260000000002	3.7606350000000002
W	36.3062550000000002	17.1098770000000009	3.8350689999999998
W	34.4389650000000032	20.3971960000000010	3.9093730000000000
W	33.0244209999999967	22.8590429999999998	3.8486630000000002
W	31.1685209999999984	26.1328080000000007	3.8102299999999998
W	29.6896969999999989	28.5859869999999994	3.6335020000000000
W	27.9090330000000009	31.3426639999999992	3.5239370000000001
Se	39.6016139999999979	2.1942339999999998	5.0333880000000004
Se	37.7559979999999982	4.9545740000000000	4.8144460000000002
Se	36.3061700000000016	7.8842879999999997	5.0642199999999997
Se	34.6465889999999987	10.6731029999999993	5.0096930000000004
Se	32.8449430000000007	13.4295329999999993	4.7926570000000002
Se	31.3152469999999994	16.3989159999999998	5.0524750000000003
Se	29.4985770000000009	19.1290179999999985	4.8042069999999999
Se	28.0233390000000000	22.1213890000000006	4.9695660000000004
Se	26.2271110000000007	24.8413480000000000	4.6622000000000003
Se	24.7442489999999999	27.7932729999999992	4.8846140000000000
Se	23.1387569999999982	30.6211659999999988	4.9841049999999996
Se	42.9493429999999989	2.1874729999999998	5.4637729999999998
Se	41.1692409999999995	4.9958109999999998	5.1846800000000002
Se	39.6691029999999998	7.8847560000000003	5.4775510000000001
Se	37.9089110000000034	10.7000779999999995	5.2218249999999999
Se	36.3060970000000012	13.5663380000000000	5.4332549999999999
Se	34.5352010000000007	16.3191839999999999	5.2098890000000004
Se	32.9831349999999972	19.2949850000000005	5.4976510000000003
Se	31.2342779999999998	22.0555720000000015	5.1848400000000003

Se	29.7198630000000001	25.0190389999999994	5.3987980000000002
Se	27.9699430000000007	27.6979110000000013	5.0329860000000002
Se	26.3769840000000002	30.7219650000000009	5.3188899999999997
Se	46.7689909999999998	2.4633639999999999	4.9529509999999997
Se	45.0391860000000008	5.2942609999999997	4.5625830000000001
Se	43.5022540000000006	8.1808680000000003	4.9349429999999996
Se	41.6987650000000016	10.9974299999999996	4.6546550000000000
Se	40.1358030000000028	13.9558710000000001	4.7612249999999996
Se	38.4878590000000003	16.7011180000000010	4.7897809999999996
Se	36.6737859999999998	19.4690249999999985	4.7092760000000000
Se	35.1721780000000024	22.4711409999999994	4.9783869999999997
Se	33.4211060000000018	25.2616620000000012	4.6023690000000004
Se	31.8489889999999995	28.2683970000000002	4.7892450000000002
Se	30.0748819999999988	31.0914119999999983	4.5373729999999997
Se	36.0712139999999977	3.9804849999999998	2.2936980000000000
Se	34.3241829999999979	6.8318740000000000	2.0195159999999999
Se	32.8117579999999975	9.5652709999999992	2.0236040000000002
Se	31.2167829999999995	12.5160719999999994	2.1997860000000000
Se	29.3764770000000013	15.2166329999999999	1.9378430000000000
Se	27.7740049999999989	18.1229820000000004	2.3303579999999999
Se	26.0609810000000017	20.9070329999999984	1.8956189999999999
Se	24.5269399999999997	23.9023520000000005	2.1418560000000002
Se	22.8004740000000012	26.7862359999999988	1.9206770000000000
Se	21.4156529999999989	29.6967520000000000	1.7208079999999999
Se	20.1497239999999991	32.6569390000000013	3.8755799999999998
Se	39.9123450000000020	4.2418350000000000	1.7334510000000001
Se	38.1261700000000019	7.0533330000000003	1.4669719999999999
Se	36.7437839999999980	9.9613390000000006	1.7514230000000000
Se	34.9055990000000023	12.7193140000000007	1.4717410000000000
Se	33.3107809999999986	15.6883169999999996	1.7518020000000001
Se	31.5161270000000009	18.3903689999999997	1.4649330000000000
Se	29.9872850000000000	21.3202619999999996	1.7156070000000001
Se	28.2583240000000018	24.0546620000000004	1.3699939999999999

Se	26.725435999999984	27.006935999999996	1.5915319999999999
Se	25.084095999999988	29.868749000000011	1.3674890000000000
Se	23.486581000000010	33.083232000000024	2.0179380000000000
Se	43.304023999999983	4.273297999999996	2.0980479999999999
Se	41.462637999999983	7.048733999999996	1.8912890000000000
Se	40.033143000000026	9.978533000000005	2.1380580000000000
Se	38.260607000000003	12.844158999999994	1.8963559999999999
Se	36.575372000000015	15.600035000000001	1.8646229999999999
Se	34.995784000000004	18.567875000000008	2.1511140000000002
Se	33.191040000000010	21.279775999999982	1.9122030000000001
Se	31.744659999999997	24.251644999999999	2.0970059999999999
Se	29.953405000000001	26.936928000000018	1.7654099999999999
Se	28.442101000000010	29.789860000000009	1.7186840000000001
Se	26.800959999999999	33.130543000000030	2.4580929999999999
W	56.431767000000007	-27.810618000000016	3.3865820000000002
W	59.421084999999979	-27.892500999999993	3.6073140000000001
W	57.815497000000006	-25.526298000000006	3.5800250000000000
W	54.651105999999986	-25.054200000000016	3.2774890000000001
W	53.172047999999966	-22.601651000000004	3.1013320000000002
W	51.316321999999995	-19.327801000000009	3.0636450000000002
W	49.902445999999976	-16.865030999999983	3.0016129999999999
W	48.034888999999997	-13.578029000000008	3.0767350000000002
W	46.514772999999981	-10.961684000000000	3.1525629999999998
W	44.875754999999981	-8.313337999999999	3.0666699999999998
W	42.999836999999994	-5.053814000000000	3.0399579999999999
W	41.582225999999986	-2.586688000000001	3.0920010000000002
W	39.716586999999970	0.649492000000000	3.0548069999999998
W	55.988872000000006	-22.169662999999999	3.5769050000000000
W	54.694439000000027	-19.847139999999996	3.4881700000000002
W	52.752335999999997	-16.465181000000012	3.4538500000000001
W	51.428970999999971	-14.157498000000004	3.4142589999999999
W	49.433714000000019	-10.846645000000005	3.4639090000000001
W	48.015276000000001	-8.402281999999996	3.4552190000000000

W	46.1331830000000025	-5.0881809999999996	3.4142269999999999
W	44.7821629999999971	-2.7709560000000000	3.4556580000000001
W	42.8314579999999978	0.6127050000000001	3.4430200000000002
W	62.3608380000000011	-28.0338050000000010	3.8327710000000002
W	60.8140640000000019	-25.4416769999999985	3.8751440000000001
W	59.420239999999997	-22.7296380000000013	3.9835609999999999
W	57.5555239999999984	-19.4497880000000016	3.9567999999999999
W	56.1436589999999995	-16.9852489999999996	3.8578530000000000
W	54.2747239999999991	-13.7488200000000003	3.8601740000000002
W	52.8194179999999989	-11.3295499999999993	3.8365019999999999
W	50.8909939999999992	-8.1065290000000001	3.8466670000000001
W	49.2603009999999983	-5.4510860000000001	3.7820450000000001
W	47.8970720000000014	-2.8475720000000000	3.8428879999999999
W	46.0212379999999968	0.4131660000000000	3.8248489999999999
Se	57.5395090000000025	-29.5998559999999991	4.4524699999999999
Se	55.8976040000000012	-26.2585629999999988	5.1926480000000002
Se	54.3868300000000033	-23.4059419999999996	5.1457689999999996
Se	52.5956199999999967	-20.7203289999999996	4.8136299999999999
Se	51.1488990000000001	-17.7484779999999986	4.9994370000000004
Se	49.3444450000000003	-15.0367669999999993	4.7614660000000004
Se	47.7650580000000033	-12.0688709999999997	5.0481480000000003
Se	46.0797910000000002	-9.3128759999999993	5.0169499999999996
Se	44.3074820000000003	-6.4470200000000002	4.7755080000000003
Se	42.8779419999999973	-3.5170689999999998	5.0222850000000001
Se	41.0367749999999987	-0.7415600000000000	4.8157100000000002
Se	60.8540139999999994	-29.5515380000000007	4.8943800000000000
Se	59.2558110000000013	-26.3375629999999994	5.5452019999999997
Se	57.6141780000000026	-23.4756309999999999	5.3211349999999999
Se	56.0813830000000024	-20.5238709999999998	5.5431689999999998
Se	54.3530009999999990	-17.7893459999999983	5.1978450000000000
Se	52.8234619999999993	-14.8589149999999997	5.4483340000000000
Se	51.0292990000000017	-12.1569730000000007	5.1618000000000004
Se	49.4344919999999988	-9.1881839999999997	5.4418490000000004

Se	47.596559999999966	-6.430036999999996	5.162329999999999
Se	46.214506000000001	-3.521805000000001	5.446551000000004
Se	44.4285610000000020	-0.710070000000000	5.1801570000000003
Se	64.1910649999999947	-29.1248170000000002	3.0381510000000000
Se	62.9245420000000024	-26.165268999999986	5.193038999999997
Se	61.5395370000000028	-23.255047999999986	4.9943590000000002
Se	59.8130200000000016	-20.3708360000000006	4.7735810000000001
Se	58.2786120000000025	-17.375941999999984	5.020222999999997
Se	56.565584999999987	-14.591597999999994	4.5857390000000002
Se	54.9633930000000035	-11.6848530000000004	4.9767390000000002
Se	53.123961999999988	-8.984391999999997	4.714262999999999
Se	51.528255999999989	-6.033801999999997	4.890884999999999
Se	50.0161360000000030	-3.3004220000000002	4.894518999999998
Se	48.2695760000000007	-0.448954000000000	4.6199700000000004
Se	54.266489999999975	-27.5595350000000003	2.372478999999998
Se	52.492351999999968	-24.7360620000000004	2.1200700000000001
Se	50.9205370000000030	-21.7293780000000005	2.3081030000000000
Se	49.169541999999999	-18.939112999999990	1.9323450000000000
Se	47.667701999999985	-15.9368610000000004	2.201410999999998
Se	45.853043999999970	-13.1693160000000002	2.1221380000000001
Se	44.204341999999969	-10.424241999999996	2.1522960000000002
Se	42.6414290000000022	-7.4661140000000001	2.2591670000000001
Se	40.8385790000000028	-4.6489750000000001	1.9783800000000000
Se	39.301381999999967	-1.7626150000000000	2.3511920000000002
Se	37.571948999999965	1.068206999999999	1.9606060000000001
Se	57.9641530000000031	-27.189544999999990	1.592530999999999
Se	56.371653999999995	-24.1655070000000016	1.8787950000000000
Se	54.6218640000000022	-21.4865700000000004	1.5134700000000001
Se	53.1071400000000011	-18.523624999999991	1.7276650000000000
Se	51.358384999999984	-15.7624080000000006	1.414979999999999
Se	49.8058890000000005	-12.7868510000000004	1.7029740000000000
Se	48.034723999999971	-10.0345720000000007	1.4801310000000001
Se	46.4313470000000024	-7.168554999999996	1.6917640000000000

Se	44.6716010000000026	-4.3531789999999999	1.4360649999999999
Se	43.1715009999999992	-1.4640280000000001	1.7289250000000000
Se	41.3914510000000035	1.3441749999999999	1.4498450000000001
Se	61.2037199999999970	-27.0889430000000004	1.9291689999999999
Se	59.5970560000000020	-24.2605059999999995	2.0289679999999999
Se	58.1139920000000032	-21.3092900000000007	2.2519819999999999
Se	56.3180090000000035	-18.5889239999999987	1.9445479999999999
Se	54.8427020000000027	-15.5967079999999996	2.1105670000000001
Se	53.0261690000000030	-12.8667470000000002	1.8616569999999999
Se	51.4957860000000025	-9.8975690000000007	2.1211180000000001
Se	49.6939660000000032	-7.1416060000000003	1.9041450000000000
Se	48.0344949999999997	-4.3526850000000001	1.8496159999999999
Se	46.5848289999999992	-1.4230719999999999	2.0994240000000000
Se	44.7392400000000023	1.3374320000000000	1.8802010000000000

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,255.815\,573\,15$ eV; $E_{rel} = 111.000\,950\,621\,2$ meV/f.u.

W	19.9848479999999995	1.0481339999999999	3.5776990000000000
W	18.1588740000000008	4.0164400000000002	3.5393150000000002
W	16.4938620000000000	6.7191869999999998	3.6159469999999998
W	14.9118639999999996	9.4351830000000003	3.5472280000000000
W	13.3266159999999996	12.1678999999999995	3.4585689999999998
W	23.1630180000000010	1.0610050000000000	3.5315279999999998
W	21.3887560000000008	3.3594759999999999	3.5265019999999998
W	19.2347800000000007	6.5218189999999998	3.4099230000000000
W	17.5992449999999998	9.2812210000000004	3.3853920000000000
W	16.0507470000000012	12.0702710000000000	3.4183919999999999
W	14.9834770000000006	15.2627500000000005	3.4458839999999999
W	26.3948259999999983	1.0402220000000000	3.4966740000000001
W	24.5996319999999997	3.3366090000000002	3.5582669999999998
W	23.1312029999999993	6.9584159999999997	3.4094920000000002
W	21.6719429999999988	9.7160159999999998	3.5373150000000000
W	20.0411779999999986	12.3310720000000007	3.4419400000000002

W	17.7124640000000007	15.4852840000000000	3.4832109999999998
W	16.5358389999999993	18.0398800000000001	3.3597139999999999
W	29.6048189999999991	1.0663220000000000	3.4382950000000001
W	27.8303140000000013	3.3504090000000000	3.5119590000000001
W	26.2589520000000007	7.0849529999999996	3.3312840000000001
W	24.3962509999999995	9.2352969999999992	3.4089160000000001
W	22.6542859999999990	12.3577919999999999	3.4316870000000002
W	21.7596470000000011	15.0384580000000003	3.3200829999999999
W	19.2663019999999996	18.2977099999999986	3.4902259999999998
W	18.1089190000000002	20.8224640000000001	3.4109349999999998
W	32.6392009999999999	0.6080200000000000	3.0056929999999999
W	31.0584759999999989	3.3371270000000002	3.4449550000000002
W	29.4166060000000016	6.9555660000000001	3.3994160000000000
W	28.1334559999999989	9.2236250000000002	3.4211950000000000
W	24.4939239999999998	15.3996680000000001	3.4264039999999998
W	23.2770200000000003	17.8371269999999988	3.3603489999999998
W	20.8721209999999999	21.1322769999999984	3.5069420000000000
W	19.6743430000000004	23.6480740000000011	3.3635660000000001
W	18.3709530000000001	26.6968110000000003	3.0714959999999998
W	34.4590729999999965	3.9668920000000001	3.5373199999999998
W	33.3040719999999979	6.5501990000000001	3.4176080000000000
W	30.8497459999999997	9.7032799999999995	3.5619130000000001
W	29.8503299999999996	12.3554890000000004	3.4482740000000001
W	28.0072849999999995	15.3831959999999999	3.4095330000000001
W	26.2324979999999996	18.2930349999999997	3.5894379999999999
W	24.8353679999999990	20.7237630000000017	3.5219680000000002
W	22.6459510000000002	23.9939500000000017	3.5310519999999999
W	21.5109180000000002	26.4535920000000004	3.2773850000000002
W	36.0105969999999971	6.7240169999999999	3.6609550000000000
W	34.9154229999999970	9.3241289999999992	3.4322580000000000
W	32.4639719999999983	12.3407429999999998	3.4710860000000001
W	30.7330770000000015	15.0337859999999992	3.3252799999999998
W	29.1985059999999983	17.8136639999999993	3.3414730000000001

W	27.722197000000013	20.601845999999983	3.499378999999998
W	25.877517000000010	23.986536999999984	3.629051000000000
W	24.513051999999983	26.429950999999991	3.591054999999999
W	37.589028999999965	9.449182000000004	3.600620999999998
W	36.447324000000018	12.104647999999992	3.456843999999998
W	34.774836000000005	15.505200999999996	3.497279999999999
W	33.209147000000015	18.314267000000010	3.488900000000001
W	31.605343000000013	21.139741000000008	3.523442999999999
W	29.969006000000003	23.900529999999998	3.564779000000001
W	28.032609000000008	26.521381999999991	3.625235000000000
W	39.164819000000014	12.190981000000007	3.498352000000001
W	37.501888999999985	15.289692000000005	3.462946000000001
W	35.935586000000007	18.079442000000002	3.368192000000001
W	34.345241000000015	20.875674000000001	3.424878999999998
W	32.773798999999968	23.689664000000005	3.381826000000002
W	30.993683999999982	26.447596999999982	3.359979000000000
W	34.089275000000007	26.727616000000012	3.159972999999999
Se	21.276386999999997	-0.605149000000000	4.624181000000001
Se	19.560584999999997	2.792256000000001	5.289817000000002
Se	17.858695000000009	5.636179000000003	5.431719000000002
Se	16.200141999999996	8.407823999999997	5.418848999999998
Se	14.550859000000009	11.162378999999996	5.366140999999998
Se	12.914431000000004	14.242029000000005	4.889657999999998
Se	24.601535999999994	-0.692968999999999	4.391351000000002
Se	22.970241000000015	2.727223000000000	5.401931000000003
Se	21.296783000000014	5.670951999999998	4.794929999999999
Se	19.664191999999999	8.570347999999992	4.880065000000001
Se	18.029458999999992	11.349512000000007	4.913971000000001
Se	16.314315000000006	14.163197999999995	5.161144000000002
Se	14.131629000000002	17.348084000000001	4.223516000000000
Se	27.905622999999985	-0.599751000000000	4.507342000000004
Se	26.277090999999986	2.671873000000002	5.381511999999999
Se	24.685939000000012	5.646533999999999	4.918927000000000

Se	23.0081510000000016	8.5456590000000006	5.3597039999999998
Se	21.3709290000000003	11.4486539999999994	5.3807720000000003
Se	19.6667610000000010	14.3675560000000004	4.9067020000000001
Se	17.8702660000000009	17.1989340000000013	5.3261979999999998
Se	15.7652149999999995	20.2037620000000011	4.2897910000000001
Se	31.1655970000000018	-0.4582360000000000	4.6793600000000000
Se	29.5489940000000004	2.7107929999999998	5.3126189999999998
Se	27.8365189999999991	5.6340029999999999	4.8903829999999999
Se	26.2591320000000010	9.2155389999999997	5.0791350000000000
Se	23.3734859999999998	14.0304079999999995	5.1763050000000002
Se	21.2616399999999999	17.1197860000000013	4.8371950000000004
Se	19.5305889999999991	20.0156179999999999	5.3291269999999997
Se	17.5610980000000012	22.9303530000000002	4.6320430000000004
Se	32.9611080000000030	2.4953889999999999	4.9713919999999998
Se	31.2346910000000015	5.5988689999999997	4.7733290000000004
Se	29.5150509999999997	8.5171200000000002	5.3712590000000002
Se	24.6547069999999984	17.0702619999999996	5.2828309999999998
Se	22.8131920000000008	19.9646580000000000	4.9084289999999999
Se	21.1335259999999998	22.9015769999999996	5.2845829999999996
Se	34.6102279999999993	5.5742310000000002	5.4370539999999998
Se	32.8513790000000014	8.5499329999999993	4.9133469999999999
Se	31.1297280000000001	11.4413239999999998	5.4019209999999998
Se	29.0989709999999988	14.0124779999999998	5.1790630000000002
Se	27.8025519999999986	17.0361680000000000	5.2578100000000001
Se	26.2606269999999995	19.9852670000000003	5.4575220000000000
Se	24.4179570000000012	22.8085859999999983	5.1794620000000000
Se	36.2916400000000010	8.4048590000000001	5.4723230000000003
Se	34.4717040000000026	11.3647620000000007	4.9568969999999997
Se	32.8214240000000004	14.3836189999999995	4.9199560000000000
Se	31.2021699999999989	17.1271909999999998	4.8281570000000000
Se	29.6543120000000009	19.9575460000000007	4.9414790000000002
Se	27.9032489999999989	22.8501660000000015	4.8606689999999997
Se	37.9381309999999985	11.1853309999999997	5.4101109999999997

Se	36.1746020000000001	14.1887950000000007	5.1833190000000000
Se	34.60657900000000035	17.2149590000000003	5.3307650000000004
Se	32.94516500000000029	20.00546900000000015	5.3349380000000002
Se	31.3547569999999993	22.8487280000000013	5.3598330000000001
Se	39.57106000000000028	14.2770309999999991	4.9153770000000003
Se	38.35312400000000011	17.37874100000000015	4.2231790000000000
Se	36.7203409999999977	20.23257600000000017	4.2750610000000000
Se	34.8864749999999972	22.9238210000000002	4.7023039999999998
Se	17.9816639999999985	1.74040400000000001	2.1041780000000001
Se	15.88929000000000008	4.34552600000000004	2.7523830000000000
Se	14.2037189999999995	7.25413700000000001	2.5982740000000000
Se	12.49928500000000004	10.1511049999999994	2.5627559999999998
Se	21.4977069999999983	1.5208969999999999	1.6677310000000001
Se	19.7538349999999987	4.60919700000000000	1.7849180000000000
Se	17.7839269999999985	7.4699619999999998	1.5817280000000000
Se	16.18365100000000011	10.3638999999999992	1.5791080000000000
Se	14.59721700000000006	13.39129400000000003	1.7178070000000001
Se	24.7325569999999999	1.56382000000000000	1.6489860000000001
Se	23.0416799999999995	4.6860749999999998	2.0089530000000000
Se	21.1794949999999993	7.62681400000000004	1.9453950000000000
Se	19.6029669999999996	10.34224000000000003	1.9625109999999999
Se	17.9723229999999994	13.28222000000000006	2.0851560000000000
Se	16.21656600000000003	16.3155639999999984	1.5272600000000001
Se	27.9437139999999999	1.57505600000000000	1.5952050000000000
Se	26.26512500000000012	4.7408169999999998	2.0537459999999998
Se	24.6110509999999998	7.64244200000000000	1.4813719999999999
Se	23.31008500000000008	10.68484600000000003	1.6661950000000001
Se	21.32897000000000018	13.3012409999999992	1.5129830000000000
Se	19.69919200000000000	16.16251000000000010	2.0159189999999998
Se	17.7732889999999983	19.16884800000000006	1.5178799999999999
Se	31.12657400000000015	1.65438500000000000	1.4440139999999999
Se	29.52272100000000007	4.69877500000000004	1.9825520000000001
Se	27.9203849999999996	7.6430059999999997	1.4859370000000001

Se	23.115376000000013	16.138998000000008	1.4889530000000000
Se	21.273766999999994	18.998394000000011	2.0256120000000002
Se	19.378458999999994	21.936294000000002	1.5534129999999999
Se	34.921061000000017	1.5826610000000001	2.6682630000000001
Se	32.917897000000035	4.5723240000000001	1.7979940000000001
Se	31.366222000000005	7.6393550000000001	1.9439970000000000
Se	29.216352000000005	10.677619999999992	1.6816759999999999
Se	26.228045999999991	14.140319999999991	2.2282850000000001
Se	24.649781999999983	19.046586999999988	1.6528670000000001
Se	22.927658999999985	21.850398999999995	2.0874139999999999
Se	21.134845999999996	24.724806999999984	1.5788690000000001
Se	36.721328999999972	4.3897240000000002	2.7950460000000001
Se	34.766930999999996	7.4978530000000001	1.6169169999999999
Se	32.918030999999992	10.3543740000000000	1.9938300000000000
Se	31.176559999999985	13.289248999999999	1.5280190000000000
Se	29.396197999999983	16.118341999999984	1.4733920000000000
Se	27.771885999999985	18.957660000000006	1.6000840000000001
Se	26.248408999999988	22.023876999999988	1.9000740000000000
Se	24.449252000000013	24.802458999999989	1.7472770000000000
Se	38.322575999999980	7.274468999999999	2.6753369999999999
Se	36.344791999999982	10.381121999999995	1.6249359999999999
Se	34.527270000000015	13.293138000000008	2.1094960000000000
Se	32.792479999999976	16.167224999999984	2.0221540000000000
Se	31.200186999999997	19.010898000000010	2.0254880000000002
Se	29.570353000000008	21.848203999999991	2.0526239999999998
Se	27.915493999999989	24.787009999999987	2.0119560000000001
Se	39.993375000000003	10.176182000000007	2.6020439999999998
Se	37.904975000000003	13.416930999999999	1.7468919999999999
Se	36.265072000000035	16.344485999999998	1.5431889999999999
Se	34.700077000000003	19.214887999999984	1.5294669999999999
Se	33.104737000000001	21.995321000000006	1.5664620000000000
Se	31.320761000000010	24.801247000000000	1.5842030000000000
Se	17.663163000000008	24.855007000000005	1.8150109999999999

Se	19.6132330000000010	25.8506779999999985	4.9724449999999996
Se	19.9187569999999994	28.0461939999999998	1.9067780000000001
Se	22.8875279999999997	25.8710549999999984	5.3505529999999997
Se	23.0730730000000008	28.0098599999999998	2.2340119999999999
Se	26.2589480000000002	25.8563620000000007	5.3675699999999997
Se	26.2285350000000008	28.2366059999999983	3.1985060000000001
Se	29.5717900000000000	25.7146189999999990	5.3694340000000000
Se	32.8466430000000003	25.8354560000000006	5.0510890000000002
Se	32.5476310000000026	28.0840859999999992	1.9947360000000001
Se	34.8187849999999983	24.8981260000000013	1.9003000000000001
Se	29.4496660000000006	28.2431589999999986	2.6115200000000001
Se	35.8300490000000025	28.0057730000000014	3.8328940000000000
Se	16.6213659999999983	27.9728549999999991	3.7225359999999998
Se	11.3161170000000002	13.6789749999999994	3.1918690000000001
Se	41.1776910000000029	13.6974920000000004	3.2310669999999999
Se	33.2980400000000003	-1.2790159999999999	1.9000600000000001
Se	17.6460709999999992	0.1106570000000000	3.8257029999999999

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,257.361\,483\,67$ eV; $E_{rel} = 87.578\,063\,954\,5$ meV/f.u.

W	19.8554649999999988	1.0675049999999999	3.4091450000000001
W	18.0904589999999992	3.8928729999999998	3.5586080000000000
W	16.4716020000000007	6.6223190000000001	3.6222840000000001
W	14.9341720000000002	9.3764140000000005	3.5628449999999998
W	13.4629600000000007	12.2388560000000002	3.5019600000000000
W	23.0779069999999997	0.8940890000000000	3.3474819999999998
W	21.3713340000000009	3.2275239999999998	3.4809690000000000
W	19.2059099999999994	6.4319819999999996	3.4381789999999999
W	17.6004649999999998	9.2169690000000006	3.4169170000000002
W	16.1165079999999996	12.0225030000000004	3.4345159999999999
W	15.0002929999999992	15.2071159999999992	3.3733430000000002
W	26.2462330000000001	0.8331140000000000	3.3282029999999998
W	24.6030370000000005	3.1045259999999999	3.4543629999999999

W	23.1166990000000006	6.8533450000000000	3.3827140000000000
W	21.6645679999999992	9.6128590000000003	3.5292080000000001
W	20.1271489999999993	12.2285249999999994	3.4799600000000002
W	17.7201850000000007	15.4756540000000005	3.4984649999999999
W	16.5163739999999990	17.9649870000000007	3.3442740000000000
W	29.4146840000000012	0.8945689999999999	3.3475570000000001
W	27.8891920000000013	3.1050900000000001	3.4545910000000002
W	26.2458120000000008	6.7211790000000002	3.3259550000000000
W	24.7692149999999991	9.0983330000000002	3.4401850000000000
W	22.8836100000000009	12.5438050000000008	3.5122640000000001
W	21.6032890000000002	14.9990170000000003	3.4341699999999999
W	19.2879719999999999	18.3086769999999994	3.5140319999999998
W	18.0133830000000010	20.7434879999999993	3.5973760000000001
W	32.6369210000000010	1.0687590000000000	3.4095529999999998
W	31.1208190000000009	3.2287840000000001	3.4814140000000000
W	29.3749010000000013	6.8538139999999999	3.3830490000000002
W	27.7218930000000015	9.0986399999999996	3.4404230000000000
W	24.3530349999999984	15.1900350000000000	3.5230340000000000
W	23.1546769999999995	18.4420810000000017	3.4437739999999999
W	21.3313910000000000	20.7476190000000003	3.5572189999999999
W	19.5846729999999987	24.3831920000000011	3.2817270000000001
W	18.4522779999999997	26.6907570000000014	3.1233430000000002
W	34.4011500000000012	3.8943599999999998	3.5593919999999999
W	33.2851649999999992	6.4334629999999997	3.4387799999999999
W	30.8263339999999992	9.6136230000000005	3.5298080000000001
W	29.6065709999999989	12.5443219999999993	3.5128910000000002
W	28.1365170000000013	15.1899789999999992	3.5236120000000000
W	26.2446009999999994	18.5597430000000010	3.4320909999999998
W	24.6030130000000007	20.8270780000000002	3.5502850000000001
W	22.9359989999999989	24.4391350000000003	3.3759670000000002
W	21.4641869999999990	26.6790009999999995	3.3429579999999999
W	36.0197100000000034	6.6240810000000003	3.6235409999999999
W	34.8899720000000002	9.2187970000000004	3.4178839999999999

W	32.3631870000000035	12.2296239999999994	3.4810449999999999
W	30.8864020000000004	14.9999459999999996	3.4353940000000001
W	29.3348389999999988	18.4430839999999989	3.4446750000000002
W	27.8859229999999982	20.8275189999999988	3.5511100000000000
W	26.2441589999999998	24.4646960000000000	3.4174069999999999
W	24.6435479999999991	26.7156039999999990	3.4559720000000000
W	37.5565080000000009	9.3785819999999998	3.5645289999999998
W	36.3735980000000012	12.0244979999999995	3.4362040000000000
W	34.7694990000000033	15.4772169999999996	3.5003929999999999
W	33.2012280000000004	18.3100909999999999	3.5161539999999998
W	31.1574589999999993	20.7485509999999991	3.5593569999999999
W	29.5523109999999996	24.4402399999999993	3.3783370000000001
W	27.8444609999999990	26.7157659999999986	3.4572349999999998
W	39.0271079999999984	12.2413170000000004	3.5040950000000000
W	37.4893459999999976	15.2092089999999995	3.3756990000000000
W	35.9728410000000025	17.9667589999999997	3.3469159999999998
W	34.4754209999999972	20.7450119999999991	3.6004160000000001
W	32.9035069999999976	24.3846090000000011	3.2857630000000002
W	31.0238879999999995	26.6797709999999988	3.3467030000000002
W	34.0361570000000029	26.6923829999999995	3.1296689999999998
Se	21.0548690000000001	-0.7339000000000000	4.3281720000000004
Se	19.5517180000000010	2.6882510000000002	5.2746519999999997
Se	17.8204360000000008	5.5177050000000003	5.4348280000000004
Se	16.1957279999999990	8.3192389999999996	5.4329340000000004
Se	14.6123189999999994	11.1366259999999997	5.3850129999999998
Se	12.6022200000000009	14.2530370000000008	4.3776690000000000
Se	24.5432680000000012	-0.8133740000000000	4.3535870000000001
Se	22.9509420000000013	2.4972029999999998	5.2886340000000001
Se	21.2917890000000014	5.5334620000000001	4.7805419999999996
Se	19.6543630000000000	8.4569729999999996	4.8989870000000000
Se	18.0838479999999997	11.2732240000000008	4.9318929999999996
Se	16.2924650000000000	14.1440230000000007	5.1294800000000000
Se	14.1671809999999994	17.3079700000000010	4.2310260000000000

Se	27.9494450000000008	-0.8130380000000000	4.3535750000000002
Se	26.2461050000000000	2.4455350000000000	5.2663479999999998
Se	24.6037590000000002	5.3773549999999997	4.8537569999999999
Se	23.0664820000000006	8.4581370000000007	5.3022010000000002
Se	21.5562749999999994	11.3685299999999998	5.3685130000000001
Se	19.6135200000000012	14.2643090000000008	4.9752090000000004
Se	17.8799460000000003	17.2085310000000007	5.3313769999999998
Se	15.7146109999999997	20.2694399999999995	4.2216350000000000
Se	31.4376619999999996	-0.7328370000000000	4.3283769999999997
Se	29.5411810000000017	2.4978769999999999	5.2887789999999999
Se	27.8878750000000011	5.3776799999999998	4.8539040000000000
Se	26.2454800000000006	8.3032769999999996	5.3118740000000004
Se	24.9207339999999995	11.3110739999999996	4.8179850000000002
Se	23.0040849999999999	14.2336690000000008	5.4064629999999996
Se	21.2745970000000000	17.1854900000000015	4.8267360000000004
Se	19.6104470000000006	20.0735910000000004	5.3443949999999996
Se	17.9147999999999996	22.9624290000000002	4.7580470000000004
Se	32.9401110000000017	2.6895539999999998	5.2752489999999996
Se	31.1997239999999998	5.5344210000000000	4.7811029999999999
Se	29.4244200000000014	8.4585480000000004	5.3025890000000002
Se	27.5697450000000011	11.3111700000000006	4.8182590000000003
Se	26.2447519999999983	14.3816690000000005	5.0345399999999998
Se	24.6522509999999997	17.2956429999999983	5.0862749999999997
Se	22.9345619999999997	20.1416959999999996	5.3590910000000003
Se	21.2152220000000007	23.0993490000000001	4.8278420000000004
Se	34.6706250000000011	5.5192430000000003	5.4356429999999998
Se	32.8363900000000015	8.4580939999999991	4.8999370000000004
Se	30.9338879999999996	11.3692170000000008	5.3692469999999997
Se	29.4854330000000004	14.2339889999999993	5.4072519999999997
Se	27.8368989999999989	17.2959220000000009	5.0864960000000004
Se	26.2441269999999989	20.2607700000000008	5.3874820000000003
Se	24.5659419999999997	23.1198119999999996	4.9012169999999999
Se	36.2946730000000031	8.3210440000000006	5.4342059999999996

Se	34.4062920000000005	11.2746359999999992	4.9332659999999997
Se	32.8761510000000001	14.2653409999999994	4.9766120000000003
Se	31.2144730000000017	17.1863150000000005	4.8282689999999997
Se	29.5536980000000007	20.1422489999999996	5.3605159999999996
Se	27.9218229999999998	23.1200609999999998	4.9020500000000000
Se	37.8775449999999978	11.1387190000000000	5.3868380000000000
Se	36.1971180000000032	14.1456579999999992	5.1314690000000001
Se	34.6090459999999993	17.2097750000000005	5.3335640000000000
Se	32.8779910000000015	20.0745420000000010	5.3468859999999996
Se	31.2725089999999994	23.0999139999999983	4.8305400000000001
Se	39.8873180000000005	14.2555589999999999	4.3801550000000002
Se	38.3219870000000000	17.3101419999999990	4.2337879999999997
Se	36.7741389999999981	20.2712970000000006	4.2248109999999999
Se	34.5733859999999993	22.9636800000000001	4.7618440000000000
Se	17.6667389999999997	1.3831720000000001	2.5542220000000002
Se	15.8265069999999994	4.2733010000000000	2.7622770000000001
Se	14.1789860000000001	7.2462840000000002	2.5910690000000001
Se	12.5027399999999993	10.2964409999999997	2.5998399999999999
Se	21.3872000000000000	1.4951340000000000	1.5257730000000000
Se	19.6662689999999998	4.5116209999999999	1.8151820000000001
Se	17.7731430000000010	7.4016140000000004	1.6105510000000001
Se	16.2117420000000010	10.3047389999999996	1.6041319999999999
Se	14.7124450000000007	13.3289899999999992	1.6506230000000000
Se	24.6384550000000004	1.3849790000000000	1.4771330000000000
Se	22.9862690000000001	4.5704669999999998	1.9867030000000001
Se	21.1630520000000004	7.5297530000000004	1.9637309999999999
Se	19.6142609999999991	10.2827999999999999	1.9915620000000001
Se	18.0535020000000017	13.2350030000000007	2.1415560000000000
Se	16.2636220000000016	16.2867519999999999	1.5033470000000000
Se	27.8539980000000007	1.3853670000000000	1.4772850000000000
Se	26.2459780000000009	4.4800760000000004	1.9532849999999999
Se	24.6258440000000007	7.3941600000000003	1.4886919999999999
Se	23.1246270000000003	10.4868380000000005	1.8075300000000001

Se	21.3484710000000000	13.2880929999999999	1.5792759999999999
Se	19.6743750000000013	16.1864530000000002	2.0044580000000001
Se	17.8006029999999988	19.2162310000000005	1.5859559999999999
Se	31.1052110000000006	1.4963670000000000	1.5261100000000001
Se	29.5056219999999989	4.5711800000000000	1.9868720000000000
Se	27.8657550000000001	7.3944739999999998	1.4888690000000000
Se	26.2455269999999992	10.1620450000000009	1.6864589999999999
Se	24.7717039999999997	13.3831070000000008	1.9222729999999999
Se	22.9602870000000010	16.3135270000000006	1.7535620000000001
Se	21.2158599999999993	19.0661230000000010	1.7865789999999999
Se	19.4952180000000013	22.0533299999999990	1.9987459999999999
Se	34.8255120000000034	1.3851150000000001	2.5547960000000001
Se	32.8255180000000024	4.5130670000000004	1.8157420000000000
Se	31.3283139999999989	7.5308289999999998	1.9642660000000001
Se	29.3663279999999993	10.4874440000000000	1.8079719999999999
Se	27.7186589999999988	13.3833219999999997	1.9224559999999999
Se	26.2449919999999999	16.3459590000000006	2.0949230000000001
Se	24.6226799999999990	19.2335209999999996	1.5711800000000000
Se	22.8816619999999986	22.1312989999999985	2.0530450000000000
Se	21.2638630000000006	24.9587590000000006	1.5021370000000001
Se	36.6650309999999990	4.2754510000000003	2.7632129999999999
Se	34.7181339999999992	7.4034279999999999	1.6116690000000000
Se	32.8765319999999974	10.2842000000000002	1.9925480000000000
Se	31.1419919999999983	13.2892700000000001	1.5803330000000000
Se	29.5295740000000002	16.3142829999999996	1.7547130000000000
Se	27.8670009999999984	19.2340459999999993	1.5718019999999999
Se	26.2446379999999984	22.2028640000000017	2.0650860000000000
Se	24.5982990000000008	25.0475369999999984	1.5658730000000001
Se	38.3120380000000011	7.2487950000000003	2.5925650000000000
Se	36.2789169999999999	10.3069210000000009	1.6056919999999999
Se	34.4366899999999987	13.2367849999999994	2.1431119999999999
Se	32.8154049999999984	16.1879729999999995	2.0062489999999999
Se	31.2738019999999999	19.0675279999999994	1.7882050000000000

Se	29.6076230000000002	22.1323860000000003	2.0546989999999998
Se	27.8910950000000000	25.0481400000000001	1.5669430000000000
Se	39.9877120000000019	10.2992410000000003	2.6018720000000002
Se	37.77766900000000031	13.3314400000000006	1.6527060000000000
Se	36.2261189999999971	16.2889760000000017	1.5056740000000000
Se	34.6888009999999980	19.2183369999999982	1.5886320000000000
Se	32.9938879999999983	22.0552239999999991	2.0018620000000000
Se	31.2255029999999998	24.9607230000000015	1.5053500000000000
Se	17.35103900000000001	24.9601909999999982	1.9912510000000001
Se	19.6966089999999987	26.2702419999999996	5.1825229999999998
Se	19.7647520000000014	28.2026930000000000	1.9061340000000000
Se	22.9905539999999995	26.2273829999999997	5.2813949999999998
Se	22.9825890000000008	28.3833249999999992	2.4302079999999999
Se	26.2433019999999999	26.2503689999999992	5.3325290000000001
Se	26.2441269999999989	28.4355140000000013	2.5342699999999998
Se	29.4961559999999992	26.2277050000000003	5.2840189999999998
Se	32.7902899999999988	26.2703820000000015	5.1876660000000001
Se	32.7242839999999973	28.2052760000000013	1.9130970000000000
Se	35.1372679999999988	24.9628310000000013	1.9958890000000000
Se	29.5057189999999991	28.3840930000000000	2.4330900000000000

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,258.432\,320\,26$ eV; $E_{rel} = 71.353\,267\,136\,3$ meV/f.u.

W	33.0744240000000005	1.0749040000000001	3.2659919999999998
W	31.3411100000000005	3.9046289999999999	3.2991320000000002
W	34.6705520000000007	3.2152110000000000	3.4277790000000001
W	29.7502679999999984	6.5708719999999996	3.3730389999999999
W	28.0602260000000001	9.3859340000000007	3.3723200000000002
W	26.4445380000000014	12.1448549999999997	3.1504720000000002
W	24.5475910000000006	15.4345079999999992	3.1821720000000000
W	23.0108099999999993	18.1380160000000004	3.2734200000000002
W	21.4519990000000007	20.9186860000000010	3.2035350000000000
W	19.8245049999999985	23.6942629999999994	3.0955509999999999

W	17.937190000000011	26.996372000000009	3.1013530000000000
W	16.460518000000004	29.559478999999996	3.2880170000000000
W	14.893271999999996	32.351576000000014	3.2906209999999998
W	36.264479000000015	0.9140620000000000	3.2907790000000001
W	32.705482000000035	6.6149920000000000	3.3844509999999999
W	31.1901750000000000	8.9387640000000008	3.4582099999999998
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W	25.763210000000008	18.049841000000007	3.3056980000000000
W	24.253450000000008	20.952973000000001	3.3540350000000001
W	22.991422000000000	23.419201000000010	3.3534540000000002
W	21.210350999999993	26.987352999999988	3.2609530000000002
W	19.795923999999994	29.313257000000001	3.3215780000000001
W	17.472829999999983	32.397680999999986	3.4311690000000001
W	39.351931000000004	0.9151060000000000	3.4307859999999999
W	37.844785000000017	3.1442470000000000	3.5246140000000001
W	36.401266999999972	6.7961250000000000	3.3974859999999998
W	34.444895000000025	8.9294300000000000	3.5742490000000000
W	33.049903000000005	12.609296999999998	3.4071699999999998
W	30.823730999999987	15.034221000000005	3.4373840000000002
W	29.848314999999995	17.815381999999996	3.3142849999999999
W	27.992318000000009	21.307992999999997	3.4874689999999999
W	26.226157000000006	23.495421000000003	3.5581399999999999
W	24.408115999999997	27.097348000000002	3.3879009999999998
W	22.724153000000012	29.411128000000015	3.4428150000000000
W	21.385324000000007	32.051887000000007	3.4774370000000001
W	42.496169999999993	1.0642160000000001	3.5753879999999998
W	41.206263999999973	3.2889360000000001	3.6512560000000001
W	39.514995999999965	6.7976450000000002	3.4910679999999998
W	37.931142999999987	9.071690999999995	3.5873409999999999
W	36.185917000000034	12.626067000000008	3.4816110000000000
W	34.663882000000010	14.896919000000005	3.5769880000000001
W	32.668466999999997	18.254213000000000	3.5848480000000000

W	31.3798740000000009	20.5894359999999992	3.5400740000000002
W	29.2978850000000008	23.9122950000000003	3.6189230000000001
W	28.2494090000000000	26.8856380000000001	3.5888749999999998
W	26.6192379999999993	29.4676180000000016	3.5028370000000000
W	24.6302459999999996	32.8546440000000004	3.5075889999999998
W	44.5044639999999987	3.2695599999999998	4.1169710000000004
W	42.5500520000000009	6.5325610000000003	3.7040430000000000
W	41.0195050000000023	9.0932160000000000	3.6370990000000001
W	39.4929079999999999	11.9603699999999993	3.6725159999999999
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W	34.2617789999999971	20.9477089999999997	3.8391929999999999
W	32.8372120000000010	23.4412839999999996	3.8546770000000001
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W	27.7223089999999992	32.3536140000000003	3.4526590000000001
Se	34.2719730000000027	-0.7407940000000000	4.1767519999999996
Se	32.7542929999999970	2.6984870000000001	5.1038519999999998
Se	31.1421029999999988	5.5128459999999997	5.1940299999999997
Se	29.3676640000000013	8.3157759999999996	5.2094279999999999
Se	27.7132150000000017	11.1500920000000008	5.1213129999999998
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Se	37.7809809999999970	-0.7973519999999999	4.3468489999999997
Se	36.1580110000000019	2.4437250000000001	5.2931569999999999
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Se	19.4471460000000000	31.398710999999987	4.8885319999999997
Se	41.221023000000024	-0.7089690000000000	4.5386780000000000
Se	39.473936000000019	2.4973220000000000	5.3580649999999999
Se	37.847358999999973	5.4121160000000001	4.9699899999999996
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Se	34.505386000000014	11.226043999999999	4.9407649999999999
Se	32.786344999999972	14.209255000000006	5.2055470000000001
Se	31.173801000000010	16.933225000000002	5.2203280000000003
Se	29.453426000000003	19.797868999999986	5.0168210000000002
Se	27.836434000000006	22.915510999999986	5.4332779999999996
Se	26.196176999999987	25.798479000000004	4.8308049999999998
Se	24.613215000000003	28.730782000000014	5.1588260000000004
Se	23.002169999999996	31.449414000000009	5.1677000000000000
Se	42.775354000000001	2.5070649999999999	5.6428779999999996
Se	41.053731999999966	5.4795590000000001	5.2365300000000001
Se	39.525182000000009	8.4606040000000000	5.4730559999999997
Se	37.782628000000025	11.2413770000000000	5.1684419999999998
Se	36.224156999999982	14.206210000000004	5.4996720000000003
Se	34.436698999999973	16.988340999999984	5.2583359999999999
Se	32.876941000000022	19.914259000000013	5.5378710000000000
Se	31.1067380000000000	22.657686000000018	5.2648299999999999
Se	29.569483999999992	25.712669000000018	5.4421730000000004
Se	28.021383000000002	28.642423999999983	5.4332339999999997
Se	26.243410000000008	31.518333999999994	5.1319010000000000
Se	46.541575999999992	2.7891780000000002	5.0220019999999996
Se	44.798065000000011	5.6946180000000002	4.5921580000000004
Se	43.246920000000029	8.6054130000000004	4.7411880000000002

Se	41.678182999999971	11.443626999999993	4.5451370000000004
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Se	38.311143999999988	17.204277999999986	4.712418999999997
Se	36.5814620000000019	20.0732140000000001	4.4560680000000001
Se	35.0580750000000023	23.0514820000000000	4.822569999999998
Se	33.0731650000000030	25.7391250000000014	4.8119740000000002
Se	31.701938999999994	28.9497810000000015	4.5528890000000004
Se	29.9994680000000002	31.8040540000000007	4.3306810000000002
Se	30.9161560000000009	1.4021740000000000	2.3284150000000001
Se	29.113438999999996	4.264262999999997	2.4576810000000000
Se	27.403507999999986	7.104309999999999	2.622949999999999
Se	25.7199540000000013	9.9230540000000005	2.5010900000000000
Se	24.2947710000000008	13.1222370000000002	2.1610170000000002
Se	22.2825090000000010	15.8665160000000007	2.4172630000000002
Se	20.7268730000000012	18.763142999999995	2.274265999999999
Se	19.089372999999984	21.573070999999988	2.3014230000000002
Se	17.5579910000000012	24.586656999999989	2.3874960000000001
Se	15.6890540000000005	27.410087999999982	2.2716020000000001
Se	14.073171999999996	30.311441999999996	2.3493840000000001
Se	34.641503999999976	1.531760999999999	1.4246120000000000
Se	33.002583999999988	4.5627380000000004	1.741965999999999
Se	31.1575880000000005	7.317447999999997	1.4718050000000000
Se	29.6149440000000013	10.276450999999998	1.783606999999999
Se	27.748927999999994	13.174960000000004	1.3720090000000000
Se	26.225557999999995	16.1458240000000011	1.602584999999999
Se	24.415217999999994	19.0603270000000009	1.475314999999999
Se	22.8499230000000004	21.8479950000000009	1.389545999999999
Se	21.3613360000000014	24.7672330000000009	1.6388840000000000
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Se	32.9155129999999971	10.2918920000000007	2.0232290000000002
Se	31.1550219999999989	13.1584749999999993	1.7675820000000000
Se	29.5314410000000009	16.0651809999999990	1.5061950000000000
Se	27.8800360000000005	19.0688339999999990	2.0402179999999999
Se	26.2137269999999987	21.7942460000000011	1.7494680000000000
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Se	19.5245810000000013	33.4363000000000028	2.1526329999999998
Se	41.0624559999999974	1.5871500000000001	1.6676839999999999
Se	39.5519139999999965	4.5578700000000003	2.1158260000000002
Se	37.9699349999999995	7.4672570000000000	1.5832329999999999
Se	36.2028079999999974	10.3479679999999998	2.1634470000000001
Se	34.6470130000000012	13.2646130000000007	1.5876980000000001
Se	32.8592519999999979	16.0952640000000002	2.1477119999999998
Se	31.2543490000000013	18.9790500000000009	1.5950850000000001
Se	29.7212800000000001	22.0059840000000015	1.9143829999999999
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Se	24.6626230000000000	30.5974189999999986	2.1804299999999999
Se	22.8704999999999998	33.4811479999999975	1.8765410000000000
Se	44.6155469999999994	1.3138140000000000	2.4635440000000002
Se	43.0947379999999995	4.4970999999999997	2.2191130000000001
Se	41.3096269999999990	7.3972629999999997	1.7449150000000000
Se	39.6075209999999984	10.2603890000000000	1.8474330000000001
Se	38.1443650000000005	13.2249160000000003	1.8758670000000000
Se	36.2697659999999971	16.0774429999999988	1.8398960000000000
Se	34.6876660000000001	19.0458609999999986	2.1022979999999998
Se	32.9540399999999991	21.8656509999999997	1.9035230000000001
Se	31.4157790000000006	24.8574680000000008	2.1883260000000000
Se	29.8304660000000013	27.7983179999999983	1.7230639999999999
Se	28.0098389999999995	30.6200249999999983	1.6515150000000001

Se	26.328365999999990	33.455750999999994	1.6530480000000001
W	16.5451410000000010	35.1852129999999974	3.3547449999999999
W	19.4424279999999996	35.6445470000000029	3.5962900000000002
W	17.9252800000000008	38.0399329999999978	3.8914260000000001
W	23.1561710000000005	35.482999999999970	3.6022170000000000
W	20.9696330000000017	37.8648159999999976	3.7091740000000000
W	26.0271700000000017	35.1441980000000029	3.4884860000000000
W	24.3024619999999985	37.8339530000000011	3.6262870000000000
Se	13.9919720000000005	34.315069999999986	4.2062510000000000
Se	17.8468310000000017	34.260480999999986	5.2080270000000004
Se	15.4514709999999997	37.1852110000000025	4.1134779999999997
Se	21.2382199999999983	34.2745620000000031	4.9237940000000000
Se	19.4215000000000018	37.2351019999999977	5.6295089999999997
Se	16.8793299999999995	39.755327999999987	5.0652379999999999
Se	24.6183729999999983	34.4702950000000001	5.4368220000000003
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Se	28.3157989999999984	34.6887049999999988	4.3064190000000000
Se	26.4630229999999997	37.6555579999999992	4.5437649999999996
Se	17.8634459999999997	36.5160440000000008	1.7252030000000000
Se	21.2535540000000012	36.2503669999999971	1.9190790000000000
Se	19.5317860000000003	39.5282190000000000	2.6547510000000001
Se	24.7333710000000018	36.3667960000000008	1.6791760000000000
Se	22.9384839999999990	39.5512439999999970	2.7340819999999999

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,258.687\,202\,18$ eV; $E_{rel} = 67.491\,419\,863\,6$ meV/f.u.

W	-0.3684040000000000	56.6934860000000000	10.4667510000000004
W	0.7561860000000000	59.1307070000000010	10.4733339999999995
W	-2.1124480000000001	59.4020340000000004	10.3879959999999993
W	-3.7810920000000001	62.1585189999999983	10.3283629999999995
W	-5.4134690000000001	64.9557010000000048	10.3181270000000005
W	-7.0398980000000000	67.7474859999999950	10.3244790000000002
W	-8.6631909999999994	70.5370510000000053	10.3337389999999996

W	-10.281625999999993	73.329206999999967	10.342124999999993
W	-11.896108999999992	76.122294999999940	10.345252999999996
W	-13.509382999999997	78.917150000000066	10.340550999999996
W	-15.119718999999999	81.715693000000017	10.331405999999994
W	-16.725681999999991	84.518234000000067	10.323632999999992
W	-18.330787000000008	87.325041999999963	10.318801000000006
W	2.880838999999999	56.558590999999998	10.669278000000003
W	-0.896966000000000	61.806215000000017	10.387164000000003
W	-2.551822000000000	64.586414000000049	10.374418999999996
W	-4.203700999999997	67.404938000000014	10.375973000000001
W	-5.848410000000003	70.218869999999955	10.384392999999993
W	-7.485698000000002	73.031645999999950	10.394090000000003
W	-9.118339000000006	75.849093999999938	10.399499999999997
W	-10.747600999999995	78.670222999999929	10.398690999999995
W	-12.371427999999999	81.492699999999992	10.392512999999992
W	-13.989115000000000	84.316288000000001	10.383238000000004
W	-15.603462999999996	87.147651999999937	10.376027999999998
W	5.823035000000000	56.465434000000019	10.934630000000003
W	4.648436000000002	59.016216999999975	10.779189000000006
W	2.979852000000002	62.422932000000030	10.735433000000004
W	1.405267000000000	65.138450000000060	10.702863999999999
W	-0.218379000000000	67.891932999999945	10.671768999999994
W	-1.853799999999999	70.684842000000033	10.673519999999999
W	-3.486399000000000	73.485549000000060	10.687775999999995
W	-5.113012999999996	76.292923999999993	10.699923000000001
W	-6.739683999999996	79.100646999999950	10.704461000000002
W	-8.358686999999998	81.912825999999955	10.699804000000003
W	-9.977439000000004	84.725033999999937	10.687839999999996
W	-11.587116999999992	87.539226999999968	10.673883000000000
W	8.849774999999993	56.341994999999972	11.153012000000004
W	7.283496999999997	59.059085000000032	11.078041999999999
W	5.759769000000004	62.054132000000027	10.825741000000007
W	4.193674999999998	64.889210000000056	10.727569000000008

W	2.5801280000000002	67.6509920000000022	10.7502969999999998
W	0.9433490000000000	70.4283879999999982	10.7560219999999997
W	-0.6938900000000000	73.2172079999999994	10.7645959999999992
W	-2.3220950000000000	76.0193050000000028	10.7803380000000004
W	-3.9523299999999999	78.8345470000000006	10.7931729999999995
W	-5.5794280000000001	81.6514949999999970	10.7931290000000004
W	-7.2030269999999996	84.4700950000000006	10.7804760000000002
W	-8.8158750000000001	87.2800280000000015	10.7645250000000008
Se	0.8687910000000000	54.9482179999999971	11.4912469999999995
Se	-0.8851740000000000	58.2438799999999972	12.3103920000000002
Se	-2.5663360000000002	61.0086609999999965	12.2326899999999998
Se	-4.2203650000000001	63.7610790000000023	12.1999440000000003
Se	-5.8549400000000000	66.5447640000000007	12.2039559999999998
Se	-7.4909090000000003	69.3325190000000049	12.2135320000000007
Se	-9.1196479999999998	72.1247149999999948	12.2231769999999997
Se	-10.7419060000000002	74.9223669999999942	12.2288720000000009
Se	-12.3593820000000001	77.7241640000000018	12.2280689999999996
Se	-13.9723910000000000	80.5276219999999938	12.2206960000000002
Se	-15.5767439999999997	83.3348040000000054	12.2115440000000000
Se	-17.1737819999999992	86.1468679999999978	12.2032840000000000
Se	4.1631229999999997	54.7396049999999974	11.6622199999999996
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Se	1.0111889999999999	61.1693229999999986	12.0286019999999994
Se	-0.5985290000000000	63.9105830000000026	11.9351050000000001
Se	-2.2371660000000002	66.6908080000000041	11.9084430000000001
Se	-3.8796879999999998	69.4897169999999988	11.9145400000000006
Se	-5.5170820000000003	72.2953219999999988	11.9265080000000001
Se	-7.1492199999999997	75.1080699999999979	11.9345610000000004
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Se	-12.0248279999999994	83.5631539999999973	11.9259339999999998
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Se	7.3655059999999999	54.7822450000000032	12.1563079999999992

Se	5.8414460000000004	58.0356730000000027	12.8307839999999995
Se	4.2855639999999999	61.0458610000000022	12.4635599999999993
Se	2.7448549999999998	64.0545510000000036	12.6145119999999995
Se	1.0684890000000000	66.7951029999999975	12.5680230000000002
Se	-0.5813400000000000	69.5499310000000008	12.5485589999999991
Se	-2.2189209999999999	72.3366520000000008	12.5570670000000000
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Se	-8.7275039999999997	83.5828549999999950	12.5702569999999998
Se	-10.3392990000000005	86.3972689999999943	12.5572309999999998
Se	10.7358750000000001	55.2984429999999989	10.4410039999999995
Se	9.3535670000000000	58.1863770000000002	12.5222320000000007
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Se	3.1726730000000001	69.8974319999999949	11.7860090000000000
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Se	-0.1072660000000000	75.4550090000000040	11.8251469999999994
Se	-1.7143830000000000	78.2612479999999948	11.8019259999999999
Se	-3.3632279999999999	81.0494810000000001	11.8569150000000008
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Se	-6.5815549999999998	86.6655930000000012	11.8251950000000008
Se	-2.4479329999999999	56.7833010000000016	9.4092330000000004
Se	-4.2708680000000001	59.7090079999999972	9.3581029999999998
Se	-5.9481909999999996	62.5751980000000003	9.3066960000000005
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Se	-15.7617729999999998	79.5468390000000056	9.2904640000000001
Se	-17.3943049999999992	82.3764780000000059	9.2907130000000002

Se	-19.0289810000000017	85.2083310000000012	9.3018310000000000
Se	-20.6632910000000010	88.0544680000000000	9.3141770000000008
Se	1.3097920000000001	57.2658419999999992	8.7506290000000000
Se	-0.5501120000000000	60.0802189999999996	8.5497099999999993
Se	-2.2170410000000000	62.9008949999999984	8.5124800000000000
Se	-3.8492449999999998	65.7252210000000048	8.5118679999999998
Se	-5.4921650000000000	68.5461169999999953	8.5143559999999994
Se	-7.1296819999999999	71.3631259999999941	8.5221020000000003
Se	-8.7600750000000005	74.1794069999999977	8.5304529999999996
Se	-10.3879040000000007	76.9961160000000007	8.5334389999999996
Se	-12.0146210000000000	79.8139520000000005	8.5292230000000000
Se	-13.6391600000000004	82.6341249999999974	8.5205870000000008
Se	-15.2610949999999992	85.4607490000000070	8.5139510000000005
Se	-16.8819750000000006	88.2944540000000018	8.5126810000000006
Se	4.4995719999999997	57.2730990000000020	8.9126600000000007
Se	2.8363380000000000	60.2254000000000005	9.3078420000000008
Se	1.1234900000000001	63.0367710000000017	9.1139600000000005
Se	-0.5237130000000000	65.8007520000000028	9.1269460000000002
Se	-2.1758890000000002	68.6063180000000017	9.1275739999999992
Se	-3.8182820000000000	71.4159760000000006	9.1379439999999992
Se	-5.4497299999999997	74.2244180000000000	9.1512709999999995
Se	-7.0757770000000004	77.0337470000000053	9.1586040000000004
Se	-8.6988990000000008	79.8442679999999996	9.1583570000000005
Se	-10.3194809999999997	82.6569080000000014	9.1506609999999995
Se	-11.9367339999999995	85.4737339999999932	9.1377740000000003
Se	-13.5489920000000001	88.3010649999999941	9.1280870000000007
Se	7.7104860000000004	57.2972279999999969	9.2398679999999995
Se	6.2331130000000003	60.2857150000000033	9.1118520000000007
Se	4.6208679999999998	63.2093879999999970	8.8947040000000008
Se	3.0271249999999998	66.0534600000000012	8.8550179999999994
Se	1.4263459999999999	68.8498570000000001	8.8613870000000006
Se	-0.2082280000000000	71.6379940000000062	8.8684740000000009
Se	-1.8401040000000000	74.4392969999999963	8.8839220000000001

Se	-3.4686230000000000	77.2446809999999999	8.8987250000000007
Se	-5.0891830000000002	80.0558479999999975	8.9071339999999992
Se	-6.7143569999999997	82.8641420000000011	8.8986870000000007
Se	-8.3301300000000005	85.6762449999999944	8.8838930000000005
Se	-9.9406289999999995	88.4890029999999967	8.8682239999999997
W	-19.9357909999999983	90.1399909999999949	10.3295069999999996
W	-18.7958590000000001	92.8130390000000034	10.3870819999999995
W	-21.4853929999999984	92.9655779999999936	10.3848559999999992
W	-22.9569350000000014	95.8319299999999998	10.4556509999999996
W	-17.2173470000000002	89.9881680000000017	10.3753150000000005
W	-20.2849600000000017	95.5852620000000002	10.4693830000000005
W	-21.4465040000000009	98.7143020000000035	10.6614950000000004
W	-13.1878229999999999	90.3527339999999981	10.6724130000000006
W	-14.7587980000000005	93.1371419999999972	10.7036719999999992
W	-16.3219759999999994	95.8610189999999989	10.7352129999999999
W	-18.4350430000000003	99.0112680000000012	10.7805859999999996
W	-20.0534350000000003	101.3063240000000036	10.9358780000000007
W	-10.4117219999999993	90.0914099999999962	10.7557200000000002
W	-11.9970789999999994	92.8971540000000005	10.7499939999999992
W	-13.5794910000000009	95.6759339999999980	10.7284780000000008
W	-15.2488430000000008	98.4509390000000053	10.8300000000000001
W	-17.0776420000000009	101.2691729999999950	11.0883129999999994
W	-18.6443219999999990	103.9858559999999983	11.1675430000000002
Se	-18.7676200000000009	88.9567689999999942	12.2005060000000007
Se	-20.3241639999999997	91.7687279999999959	12.2318870000000004
Se	-21.8786500000000004	94.6096260000000058	12.3035420000000002
Se	-23.8517399999999995	97.7788160000000062	11.4735750000000003
Se	-15.2380709999999997	89.2064749999999975	11.9093610000000005
Se	-16.8254049999999999	92.0175270000000012	11.9360820000000007
Se	-18.3941270000000010	94.7849319999999977	12.0278589999999994
Se	-20.0939669999999992	97.5944889999999958	12.2642129999999998
Se	-22.3822930000000007	100.7335539999999980	11.6542680000000001
Se	-11.9336140000000004	89.2091309999999993	12.5488560000000007

Se	-13.493394999999996	92.016180000000056	12.568500999999995
Se	-15.028007999999998	94.839460000000025	12.614848000000003
Se	-16.862214000000016	97.678201000000014	12.465102999999992
Se	-18.691265999999988	100.530882000000054	12.834390000000009
Se	-20.740899999999999	103.480532999999941	12.163531000000008
Se	-8.158913999999993	89.478768999999998	11.777340000000006
Se	-9.754004000000001	92.284356000000025	11.785830000000007
Se	-11.376144000000000	95.111356000000007	11.814503000000002
Se	-12.998694000000004	98.022136000000033	11.665606999999996
Se	-14.893252999999996	100.756652000000025	12.068986000000007
Se	-16.798646000000015	103.493351000000041	12.539265000000003
Se	-18.601071999999985	106.143366999999978	10.462763000000007
Se	-22.302959000000013	90.941689999999941	9.361271999999996
Se	-23.916962999999991	93.985449000000027	9.398735000000003
Se	-18.509294000000006	91.121162999999957	8.513458000000000
Se	-20.113558999999986	93.977339999999981	8.547520999999997
Se	-21.616219000000010	96.999522999999964	8.743254000000003
Se	-15.151579999999992	91.135706999999965	9.128102000000002
Se	-16.719160999999997	93.945899999999946	9.114395999999993
Se	-18.293890000000011	96.838639000000006	9.307251000000008
Se	-20.012246999999986	99.759787000000029	8.910935000000003
Se	-11.537088999999999	91.298276999999988	8.861102000000007
Se	-13.156501000000004	94.083675999999970	8.855389000000006
Se	-14.818669999999991	96.888823999999996	8.896909000000008
Se	-16.539089000000006	99.750589000000051	9.118164999999994
Se	-18.383722999999998	102.527787000000036	9.250495000000008

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,260.821\,285\,15$ eV; $E_{rel} = 35.156\,829\,409\,0$ meV/f.u.

W	19.896695000000011	1.930533000000001	4.073156000000000
W	17.954108000000015	3.958958000000000	2.889910000000000
W	16.382169999999986	6.696227000000004	3.034253000000001
W	14.775693000000004	9.512755999999995	3.249083999999999

W	13.194426000000000	12.294748999999995	3.388863000000000
W	11.633350999999999	15.056853000000000	3.451896000000000
W	10.043480999999999	17.834588000000000	3.290665999999999
W	8.142222000000000	21.227568000000000	3.048366999999999
W	6.662817999999997	23.991617000000000	3.149706999999999
W	5.169321000000000	26.689371999999998	3.066349999999999
W	3.539574000000000	29.300648999999999	3.016763999999999
W	21.000040999999995	3.871549999999999	2.892386999999999
W	19.364992999999983	6.322473999999997	3.018256000000000
W	17.680778000000000	9.048866000000000	3.137516000000000
W	16.009896999999987	11.933118999999996	3.289076000000000
W	14.379462000000000	14.753088999999992	3.358353000000000
W	12.817743999999994	17.564737000000000	3.364884000000000
W	11.420109000000000	21.152868000000000	3.277288000000000
W	9.940830999999993	23.452056999999999	3.340208000000000
W	7.912402000000000	26.846243999999987	3.200670000000000
W	6.667085000000000	29.201726000000000	3.046231999999998
W	22.593906000000000	6.311576999999998	2.981186000000000
W	21.579482999999997	9.543894999999991	3.290144000000000
W	20.072898999999996	12.304135999999997	3.510584000000000
W	18.413340000000000	15.131605000000000	3.538284000000000
W	16.828065999999997	17.898261999999990	3.495973999999999
W	14.672309999999995	21.166599000000000	3.390946000000000
W	13.129906999999993	23.416658999999992	3.485148000000000
W	11.688190000000000	27.083176999999992	3.255732000000000
W	10.031418999999996	29.314536000000000	3.267882000000000
W	24.654699000000000	9.425893000000000	3.028500000000000
W	23.011770999999995	11.800549000000000	3.368136999999999
W	21.150984999999986	15.154662999999993	3.510161000000000
W	19.719453000000000	17.650158000000000	3.492357999999999
W	17.820579999999996	21.068706999999999	3.486422999999998
W	16.363773999999994	23.396557000000000	3.558786000000000
W	14.860058999999997	27.085831999999999	3.320592000000000

W	13.2731530000000006	29.3615010000000005	3.3606799999999999
W	26.3338859999999997	12.4053269999999998	3.4083429999999999
W	25.1872480000000003	14.8921869999999998	3.4223759999999999
W	22.7242080000000009	18.0325960000000016	3.6005120000000002
W	21.6443800000000017	20.9672179999999990	3.5247760000000001
W	19.6855989999999998	23.3390909999999998	3.6124869999999998
W	18.0827379999999991	27.0584840000000000	3.3777800000000000
W	16.4870130000000010	29.3548989999999996	3.3541870000000000
W	27.9134360000000008	15.1448380000000000	3.5415420000000002
W	26.7268070000000009	17.6263299999999994	3.4037190000000002
W	24.4061640000000004	20.9452950000000016	3.4986700000000002
W	23.0591159999999995	23.3749450000000003	3.5117140000000000
W	21.3364300000000000	27.0378380000000007	3.3828330000000002
W	19.7173769999999990	29.3360750000000010	3.3616690000000000
W	29.4744069999999994	17.8960059999999999	3.3578679999999999
W	28.1767250000000011	21.1676399999999987	3.3457759999999999
W	26.3960380000000008	23.3785179999999997	3.5203110000000000
W	24.5748889999999989	27.0616130000000013	3.3232610000000000
W	22.9407689999999995	29.3305439999999997	3.3539610000000000
W	31.3361529999999995	21.2856090000000009	3.0584820000000001
W	29.5387729999999991	23.5156279999999995	3.3569390000000001
W	27.7406299999999995	27.1020879999999984	3.2563770000000001
W	26.1395669999999996	29.3598759999999999	3.3569900000000001
W	32.7666979999999981	24.0684080000000016	3.1428280000000002
W	31.5084090000000003	26.9175930000000001	3.2010160000000001
W	29.3742710000000002	29.3548119999999990	3.2607879999999998
W	34.2538539999999969	26.7669740000000012	3.0607530000000001
W	32.7349809999999977	29.2797990000000006	3.0424709999999999
W	35.8643310000000000	29.3955769999999994	3.0180020000000001
Se	20.4000449999999987	2.0173580000000002	6.2923970000000002
Se	17.6934569999999987	5.4420690000000000	4.8242820000000002
Se	16.0826649999999987	8.2369719999999997	5.0102719999999996
Se	14.4523480000000006	11.0621799999999997	5.1879710000000001

Se	12.8388240000000007	13.8974689999999992	5.2963120000000004
Se	11.2232810000000001	16.7999469999999995	5.2623749999999996
Se	9.5602780000000003	19.8986289999999997	4.7784620000000002
Se	8.0340889999999998	22.8688439999999993	4.9803949999999997
Se	6.4727810000000003	25.6926519999999989	4.9990059999999996
Se	4.9197259999999998	28.6031540000000000	4.8852820000000001
Se	21.0810069999999996	5.4367340000000004	4.7815190000000003
Se	19.6573460000000004	8.3422090000000004	4.6274569999999997
Se	18.0255919999999996	11.1370400000000007	4.7072909999999997
Se	16.3875230000000016	14.0086429999999993	4.8451480000000000
Se	14.7432239999999997	16.8667259999999999	4.8865170000000004
Se	12.9674619999999994	19.7830650000000006	4.8109520000000003
Se	11.4150170000000006	22.8003539999999987	5.2429839999999999
Se	9.8582190000000001	25.7701379999999993	4.6137750000000004
Se	8.2583479999999998	28.7371550000000013	4.9708019999999999
Se	23.1705299999999994	8.0966600000000000	4.7557710000000002
Se	21.4573070000000001	11.1015499999999996	5.2529599999999999
Se	19.7862779999999994	13.9904960000000003	5.3507009999999999
Se	18.1123590000000014	16.8958049999999993	5.3758010000000001
Se	16.2815709999999996	19.8430970000000002	5.0767119999999997
Se	14.6984440000000003	22.8150529999999989	5.3622470000000000
Se	13.1579540000000001	25.7380369999999985	4.8288029999999997
Se	11.5967289999999998	28.8158420000000000	5.1747610000000002
Se	24.8892880000000005	11.0251730000000006	5.0197050000000001
Se	23.1539089999999987	14.0039540000000002	4.8028579999999996
Se	21.3644660000000002	16.9073500000000010	5.3645980000000000
Se	19.7054070000000010	19.8696899999999985	4.8558269999999997
Se	18.0111589999999993	22.7546689999999998	5.3918559999999998
Se	16.4062589999999986	25.7182659999999998	4.8730370000000001
Se	14.8612450000000003	28.8987830000000017	5.2253740000000004
Se	26.6365559999999988	13.9637750000000000	5.3597149999999996
Se	24.7856209999999990	16.9327329999999989	4.9561109999999999
Se	23.0687950000000015	19.8330960000000012	5.3448460000000004

Se	21.402560999999986	22.7660230000000006	5.3633670000000002
Se	19.701847999999983	25.695962999999990	4.8865590000000001
Se	18.0940280000000016	28.9142790000000005	5.2372100000000001
Se	28.2713810000000016	16.8922370000000015	5.3345200000000004
Se	26.460990999999999	19.842535999999991	4.7931130000000000
Se	24.757446999999991	22.7312130000000003	5.3188700000000004
Se	23.0274970000000003	25.6855820000000001	4.8585469999999997
Se	21.3345820000000010	28.8992390000000015	5.2390549999999996
Se	29.951133999999997	19.9344469999999987	4.8674410000000004
Se	28.098534999999983	22.8006990000000016	5.2835710000000002
Se	26.293559999999994	25.729251999999989	4.826509999999999
Se	24.562729999999984	28.879402999999999	5.225724999999997
Se	31.449846999999983	22.9217340000000007	4.9900969999999996
Se	29.5849550000000008	25.8202840000000009	4.6284039999999997
Se	27.8221460000000000	28.842446999999999	5.1726890000000001
Se	32.9535600000000031	25.769719999999995	4.9943770000000001
Se	31.1515860000000018	28.806582999999998	4.9697009999999997
Se	17.4969050000000017	1.6760310000000000	3.658034999999999
Se	16.0152040000000007	4.392231999999999	1.6135050000000000
Se	14.1132510000000000	7.089364999999999	2.3306670000000000
Se	12.573817999999993	10.010313999999993	2.3018160000000001
Se	10.9531530000000004	12.8836440000000003	2.3786630000000000
Se	9.262527999999997	15.7139720000000001	2.5198200000000002
Se	7.915181999999997	18.8667830000000016	2.2244500000000000
Se	5.9113360000000004	21.679770999999988	2.2979330000000000
Se	4.425514999999999	24.495820999999994	2.1866420000000000
Se	2.932052999999998	27.3349200000000003	1.8557910000000000
Se	1.700917999999999	30.387530999999992	3.786459999999999
Se	21.637982999999984	1.3569760000000000	2.5524870000000002
Se	19.5428050000000013	4.573979999999997	1.0672180000000000
Se	17.891279999999983	7.4308170000000002	1.218121999999999
Se	16.2812820000000009	10.277666999999992	1.3948240000000001
Se	14.6443130000000004	13.0817540000000001	1.487020999999999

Se	13.020305999999997	15.897126999999993	1.5103070000000001
Se	11.4533810000000003	18.912216999999983	1.6527609999999999
Se	9.7844960000000007	21.8058440000000004	1.3661500000000000
Se	8.2954690000000006	24.7600020000000001	1.6118900000000000
Se	6.5071139999999996	27.566044999999990	1.1827810000000001
Se	4.9049750000000003	30.718274999999984	1.7337350000000000
Se	23.2755219999999987	4.2819190000000003	1.8487009999999999
Se	21.2104309999999998	7.5273490000000001	1.4866230000000000
Se	19.657357999999986	10.330735999999999	1.8283229999999999
Se	18.035153999999986	13.096080999999999	2.0001380000000002
Se	16.367986999999994	15.9141790000000007	2.0303990000000001
Se	14.777855999999999	18.8335140000000010	2.0921599999999998
Se	13.0912590000000009	21.7687700000000000	1.5121659999999999
Se	11.5755940000000006	24.794340999999993	1.8769480000000001
Se	9.858656999999991	27.6170720000000003	1.5427329999999999
Se	8.1970740000000006	30.8971130000000009	2.1869380000000000
Se	24.9649700000000010	7.0476340000000004	2.3573520000000001
Se	23.1203579999999995	10.2245030000000003	1.3280559999999999
Se	21.5395040000000009	13.2178760000000004	1.7507820000000001
Se	19.7758579999999995	16.000029999999989	1.5641540000000000
Se	18.174914999999986	18.9310140000000011	1.7931310000000000
Se	16.3522950000000016	21.756599999999988	1.5786169999999999
Se	14.8073820000000005	24.7921380000000013	2.0048400000000002
Se	13.2559810000000002	27.7487490000000001	1.4210039999999999
Se	11.5125060000000001	31.077649999999984	2.4956170000000002
Se	26.8452790000000014	9.994809999999993	2.3131460000000001
Se	24.772073999999999	13.079717999999997	1.6926460000000001
Se	23.197238999999997	16.014556999999999	2.0789840000000002
Se	21.341532999999983	18.9392780000000016	1.8343970000000001
Se	19.7347110000000008	21.691942999999984	1.8194330000000001
Se	18.0917800000000000	24.741807999999989	2.0931419999999998
Se	16.490684999999991	27.6678710000000017	1.4897899999999999
Se	14.8394750000000002	31.0190710000000003	2.3254410000000001

Se	28.574690000000004	12.843420000000001	2.5795979999999998
Se	26.5609810000000017	15.9273199999999999	1.5424199999999999
Se	24.7746969999999997	18.8260919999999992	2.0651739999999998
Se	23.0326290000000000	21.8015079999999983	1.5571880000000000
Se	21.3405650000000016	24.7352789999999985	2.0761980000000002
Se	19.7153129999999983	27.6277110000000015	1.5241279999999999
Se	18.1056409999999985	31.0255369999999999	2.3732270000000000
Se	30.2452170000000002	15.7509209999999999	2.5763010000000000
Se	28.1043349999999990	18.9575500000000012	1.6845209999999999
Se	26.2974180000000004	21.7091409999999989	1.7138679999999999
Se	24.6434369999999987	24.7620970000000007	2.0148020000000000
Se	22.9367640000000002	27.6330519999999993	1.4970770000000000
Se	21.3311180000000000	31.0152530000000013	2.3731979999999999
Se	31.6196529999999996	18.9184389999999993	2.2997600000000000
Se	29.6962620000000008	21.8768729999999998	1.3676429999999999
Se	27.8370320000000007	24.8087219999999995	1.8969090000000000
Se	26.1665279999999996	27.7436700000000016	1.4207580000000000
Se	24.5686350000000004	30.9994769999999988	2.3055539999999999
Se	33.5293720000000022	21.7750410000000016	2.2276189999999998
Se	31.1272300000000008	24.8315039999999989	1.6078859999999999
Se	29.5582889999999985	27.6547230000000006	1.5389230000000000
Se	27.8766239999999996	31.0967139999999986	2.4788239999999999
Se	31.1905010000000011	30.9540329999999990	2.1716780000000000
Se	34.4857859999999974	28.6860579999999992	4.8814669999999998
Se	32.9116270000000029	27.6416870000000010	1.1818470000000001
Se	35.0134290000000021	24.5834040000000016	2.1870080000000001
Se	36.4873550000000009	27.4350759999999987	1.8561160000000001
Se	34.4905339999999967	30.8062439999999995	1.7348110000000001
Se	37.6930419999999984	30.4955239999999996	3.7909679999999999

$W_{66}Se_{132}$; $E_{tot} = -38\,662\,261.457\,186\,48\text{ eV}$; $E_{rel} = 25.521\,960\,772\,7\text{ meV/f.u.}$

W	22.8944019999999995	1.1193730000000000	3.1502610000000000
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W	21.245976999999999	3.935867000000000	3.194210000000000
W	17.659376000000017	14.800527999999999	3.366134000000002
W	19.733508000000005	6.765009000000001	3.332269999999998
W	18.139317999999994	9.532771000000003	3.386531999999999
W	16.510882999999998	12.284620999999996	3.429876000000001
W	14.897161000000005	15.044620999999994	3.503250000000000
W	13.302514000000004	17.835822000000003	3.493367000000001
W	11.741801999999999	20.819489000000008	3.400641999999999
W	26.097864000000013	0.859979000000000	3.708644000000001
W	24.296143000000007	3.435058999999999	3.310136000000000
W	22.701574999999983	6.201024999999996	3.259278000000001
W	20.972923000000015	9.180296000000002	3.307639000000000
W	19.323333000000016	12.006195000000000	3.345108000000002
W	16.034964999999997	17.599239000000007	3.402476000000001
W	14.393205000000000	21.034348000000014	3.478486999999999
W	13.212377999999993	23.691337999999982	3.382930000000000
W	27.166408000000006	3.506373000000000	3.680388999999999
W	26.496567999999999	6.811731000000000	3.314109999999999
W	24.977843000000000	9.565182999999993	3.439279000000000
W	23.373719999999987	12.384154999999998	3.484785000000000
W	21.700053000000005	15.247348999999998	3.510574999999998
W	20.018518000000003	18.048111999999997	3.509672000000001
W	18.372628999999999	20.801331000000011	3.423311000000000
W	15.880399000000006	23.851130999999987	3.500627999999999
W	14.758475000000007	26.453706000000004	3.382394999999998
W	27.769915999999985	9.293499000000006	3.202503999999998
W	26.161079999999983	12.092423999999994	3.332058000000000
W	24.481076000000016	14.933816999999995	3.349476000000001
W	22.815241000000003	17.827811000000005	3.356746999999999
W	21.081485000000007	20.632775999999998	3.343140000000000
W	19.958756000000011	23.558683999999995	3.302340000000001
W	17.483595999999986	26.643364999999993	3.519750000000002
W	16.361861000000011	29.174448999999992	3.554752000000001

W	29.723199000000010	12.591573999999996	3.4019610000000000
W	28.573425000000003	15.176790999999997	3.3941720000000002
W	26.184810999999998	18.356463999999990	3.4742570000000002
W	25.020852000000014	20.887184000000013	3.3942190000000001
W	22.914003000000010	24.002476000000015	3.4174240000000000
W	21.528055999999994	26.403963999999984	3.4111560000000001
W	19.692183000000000	29.789070999999999	3.5932050000000002
W	18.010691000000013	32.119075000000023	3.9734180000000001
W	31.299856999999994	15.368330999999995	3.5797129999999999
W	30.183149000000002	17.956866000000015	3.4132669999999998
W	27.704152000000006	21.033525000000009	3.4455510000000000
W	25.997219999999987	23.678013000000000	3.3394469999999998
W	24.310289999999984	26.526939999999997	3.4246610000000000
W	22.638802999999993	29.313292000000006	3.4268000000000001
W	21.131630000000012	32.067870999999967	3.6471010000000001
W	19.965554999999984	35.364541000000027	3.9133010000000001
W	32.844338999999980	18.114851000000016	3.5579719999999999
W	31.666122000000014	20.777774999999983	3.4144350000000001
W	30.006517999999998	24.164646000000012	3.4972930000000000
W	28.357794999999994	26.951406999999997	3.5342080000000000
W	26.705038999999993	29.716626000000015	3.6068840000000000
W	25.072938000000006	32.458934999999968	3.6980490000000001
W	23.041750000000004	35.547908999999971	3.7781389999999999
W	21.442603999999993	37.887557000000010	3.9403779999999999
W	34.315224999999981	20.985845000000012	3.5127169999999999
W	32.741202999999987	23.964332999999999	3.4258980000000001
W	31.121126000000003	26.743048000000017	3.4228719999999999
W	29.483388999999990	29.494776000000017	3.5095670000000001
W	27.844377999999990	32.232979999999977	3.5500330000000000
W	26.177111000000000	34.999138000000021	3.6753390000000001
W	24.395222000000004	37.824585999999965	3.8834110000000002
W	22.861207000000003	40.561484999999976	3.9325580000000002
Se	23.841242999999986	-0.830828000000000	3.9789059999999998

Se	22.439302999999989	2.6710440000000002	5.0235510000000003
Se	21.033500000000001	5.5351850000000002	5.1284910000000004
Se	19.421527999999986	8.3671380000000006	5.2245920000000003
Se	17.7732640000000011	11.1397180000000002	5.2714639999999999
Se	16.159649999999992	13.9130470000000006	5.3230919999999999
Se	14.5505540000000000	16.7378900000000002	5.3592579999999996
Se	12.984603999999991	19.693844999999996	5.2357170000000002
Se	10.7817640000000008	22.7459370000000014	4.3332600000000001
Se	27.0843950000000007	-0.8331050000000000	4.9095089999999999
Se	25.6537010000000016	2.5796820000000000	5.3828709999999997
Se	24.613576999999994	5.581839999999997	4.8115949999999996
Se	22.9756670000000014	8.4015590000000007	4.7279939999999998
Se	21.340341999999997	11.2691130000000008	4.8096399999999999
Se	19.681291999999991	14.108995999999994	4.8397639999999997
Se	18.014825999999993	16.9263109999999983	4.8707330000000004
Se	16.3191300000000012	19.8195230000000002	4.7890569999999997
Se	14.5054820000000007	22.7344690000000007	5.3166219999999997
Se	12.457335999999997	25.7944749999999985	4.3961660000000000
Se	28.382274999999999	5.2327579999999996	4.7376009999999997
Se	26.4562330000000010	8.406219999999994	5.2010490000000003
Se	24.7390720000000002	11.2641880000000008	5.2869830000000002
Se	23.052500999999995	14.106645999999996	5.3100759999999996
Se	21.376478999999998	16.998312999999996	5.3181360000000000
Se	19.655598999999987	19.8276550000000000	5.3178060000000000
Se	17.9053350000000009	22.7954660000000011	4.8701119999999998
Se	16.0932420000000000	25.6044330000000002	5.3500750000000004
Se	14.093714999999995	28.7308430000000001	4.3450470000000001
Se	28.1776090000000003	11.212201999999996	4.9126589999999997
Se	26.5354090000000014	14.1796100000000003	4.7842310000000001
Se	24.7233640000000001	16.998996999999992	4.9890819999999998
Se	23.0645600000000002	19.908872999999998	4.8622790000000000
Se	21.390164999999997	22.6582760000000007	5.0637460000000001
Se	19.517735999999993	25.5624879999999983	4.8736980000000001

Se	17.939175999999998	28.469961000000014	5.245060999999998
Se	15.821213000000002	31.534530000000002	4.694354999999998
Se	29.945482999999994	14.165414000000002	5.349846999999996
Se	28.148838000000014	17.160019999999994	4.914579999999999
Se	26.412686999999982	20.032617999999994	5.361539999999998
Se	24.607208000000000	22.801315999999999	5.139822999999998
Se	22.965711999999999	25.637965000000012	5.367568999999996
Se	21.202000999999992	28.384022999999991	5.190299999999997
Se	19.613058999999998	31.371957999999993	5.634157000000001
Se	31.584130999999993	17.023464000000006	5.421032000000003
Se	29.714506000000001	20.023734000000010	4.911929999999999
Se	28.072798999999998	23.017175000000017	4.929524999999999
Se	26.386424000000017	25.738015000000008	4.862377000000004
Se	24.696041999999985	28.574048000000012	4.933392999999997
Se	23.067205000000013	31.306938999999999	5.090435000000003
Se	33.145260999999979	19.872406000000016	5.379747000000001
Se	31.437315000000017	22.860430000000009	5.147451000000002
Se	29.776343000000007	25.851373999999999	5.354010999999999
Se	28.080217999999986	28.617013000000000	5.415658999999998
Se	26.470897000000008	31.425322999999988	5.505212000000002
Se	35.153190999999996	22.986916000000008	4.433772000000003
Se	33.549962000000007	26.052649999999999	4.256079999999999
Se	31.807566000000013	28.890090000000007	4.454766000000002
Se	30.093842999999997	31.708259999999992	4.568817000000001
Se	20.907554999999986	1.434990999999999	1.963244999999999
Se	19.017580999999998	4.298607999999998	2.473994999999999
Se	17.509820000000013	7.189833000000001	2.428631000000002
Se	15.891398000000006	10.037971999999999	2.406743000000001
Se	14.200808999999996	12.877561999999993	2.491689000000000
Se	12.477188999999992	15.744770000000008	2.676129000000000
Se	10.895305999999997	18.814699000000010	2.494387999999998
Se	24.760235999999990	1.531436999999999	1.564381000000000
Se	22.844411999999984	4.478608999999996	1.406811000000000

Se	21.274105999999997	7.4238020000000002	1.4886150000000000
Se	19.604981999999997	10.2952860000000008	1.4875270000000000
Se	17.936016999999997	13.1001460000000005	1.5193530000000000
Se	16.2351810000000008	15.9027960000000004	1.5473370000000000
Se	14.6039870000000001	18.9298000000000002	1.7624130000000000
Se	12.893143999999995	21.9532530000000001	1.5372170000000001
Se	28.161553999999989	1.6655210000000000	2.5424820000000001
Se	26.1651670000000003	4.606969999999996	1.8088620000000000
Se	24.628685999999983	7.470177999999998	1.8508370000000001
Se	22.971575999999989	10.302094999999996	1.9477670000000000
Se	21.314133999999992	13.1497630000000001	2.0114060000000000
Se	19.6368180000000017	15.9764920000000004	2.0093800000000002
Se	17.9455360000000006	18.7732500000000009	1.9754689999999999
Se	16.3446700000000007	21.796534999999987	1.9733590000000001
Se	14.451719999999999	24.803035999999988	1.5248050000000000
Se	28.4353400000000001	7.3249290000000000	1.9134690000000001
Se	26.4485920000000014	10.3560750000000006	1.4674130000000001
Se	24.797709999999986	13.209797999999993	1.5278760000000000
Se	23.1195410000000017	16.054791999999991	1.5521090000000000
Se	21.3706910000000008	18.8870450000000005	1.5390260000000000
Se	19.6993420000000015	21.762668999999989	1.5071440000000000
Se	17.9027560000000001	24.651151999999997	1.9925160000000000
Se	16.0657280000000000	27.648326999999983	1.5909930000000001
Se	30.0013210000000008	10.255385999999997	2.4003280000000000
Se	28.119586999999992	13.2622380000000000	1.7302029999999999
Se	26.4942700000000002	16.164740999999994	2.0419320000000001
Se	24.677098999999983	19.0114440000000009	1.6711890000000000
Se	23.0075940000000010	21.8249530000000007	2.0086949999999999
Se	21.300115999999992	24.701046999999991	1.5343220000000000
Se	19.530485999999998	27.583666999999984	2.1622140000000001
Se	17.794212999999992	30.556267999999993	1.9560420000000001
Se	31.9994410000000009	13.032982999999998	2.7153290000000001
Se	29.9838570000000004	16.1604710000000011	1.5783840000000000

Se	28.203877999999996	18.983945999999995	1.995366999999999
Se	26.379025999999996	21.917611999999983	1.507382000000000
Se	24.589069999999995	24.746023999999985	1.581194000000000
Se	22.879759000000000	27.602302000000017	1.598222000000000
Se	21.220731000000007	30.502452999999992	1.694564000000000
Se	19.448601000000000	33.472526000000020	2.234576000000001
Se	33.594053999999999	15.989511999999995	2.563435000000001
Se	31.589455000000010	19.043098000000005	1.597039000000001
Se	29.740076999999994	21.967126000000004	2.068225000000000
Se	28.016026000000001	24.843506999999989	2.032278999999999
Se	26.315785000000018	27.660506000000016	2.078726000000001
Se	24.662389000000010	30.472643999999990	2.142421000000001
Se	23.007197000000015	33.334184000000005	2.329587000000001
Se	35.275171000000003	19.047167000000017	2.604931999999998
Se	33.087059000000036	22.120547999999994	1.672661000000000
Se	31.493451000000003	25.061450000000007	1.559469000000000
Se	29.869600999999994	27.888026000000000	1.602570000000001
Se	28.216833999999986	30.640784000000000	1.669049000000000
Se	26.492781999999983	33.394184000000028	1.758129000000001
Se	17.669955000000016	34.477392999999993	4.676651999999998
Se	21.398695000000000	34.187835999999972	5.391760999999998
Se	19.182808999999989	37.403027999999991	4.935268999999999
Se	24.655170999999993	34.279409000000011	5.438818999999996
Se	22.919049999999986	37.156424999999987	5.770226000000001
Se	20.858361999999996	40.121896999999970	5.123833000000003
Se	28.461787999999985	34.594200999999982	4.423128000000002
Se	26.629836999999984	37.359099999999980	4.766759000000004
Se	24.796113999999993	40.125293999999967	5.193520999999996
Se	22.856808999999984	42.679707000000005	3.113141000000002
Se	21.309411000000008	36.211433999999970	2.005177999999999
Se	24.798648000000000	36.224541999999996	1.961792000000000
Se	22.977221000000001	39.007165000000005	2.076016000000001

$W_{66}Se_{132}$; $E_{tot} = -38\,662\,261.656\,231\,80$ eV; $E_{rel} = 22.506\,122\,590\,9$ meV/f.u.

W	27.427662999999990	-0.965450000000000	3.151406999999998
W	25.777277999999990	1.900293999999999	3.307455000000000
W	24.205562000000000	4.685800999999997	3.351954999999998
W	22.633520000000000	7.459772000000000	3.338965000000000
W	21.045573999999984	10.260303999999996	3.345432000000000
W	19.426970000000000	13.060003000000000	3.375535000000000
W	17.795334000000000	15.850491999999991	3.415875000000000
W	16.222083999999988	18.671815999999997	3.403929000000000
W	14.661134999999998	21.644569000000000	3.351757000000000
W	28.981062999999989	1.200682999999999	3.395026000000000
W	30.601019999999983	-1.223105000000000	3.629451000000000
W	26.986433000000000	4.350298000000000	3.305171000000000
W	25.424492000000000	7.142198999999997	3.299897000000000
W	23.826844999999987	9.951254000000000	3.309928999999999
W	22.199898000000000	12.829043000000000	3.330843000000000
W	20.509274999999988	15.653297000000000	3.316698999999998
W	18.953875000000000	18.438497999999992	3.339798000000000
W	17.316565000000000	21.891958999999999	3.459960999999998
W	16.114119999999998	24.516999999999995	3.409303000000000
W	31.988948000000000	1.408844999999999	3.516470000000000
W	30.962084000000000	4.603867000000000	3.514997999999998
W	29.521000999999983	7.429890999999996	3.512824999999999
W	27.957364999999994	10.309706000000000	3.530370000000000
W	26.289866000000000	13.030336999999994	3.398220999999999
W	24.423514999999983	16.250150000000000	3.404790999999999
W	22.926058000000000	18.952888000000000	3.502848000000000
W	21.316223000000000	21.650299000000000	3.384367000000000
W	18.793693000000000	24.720078000000000	3.534964000000000
W	17.627175000000000	27.337792000000000	3.476799000000000
W	33.601120999999991	4.112928000000000	3.523080999999999
W	32.273038999999971	7.091116000000000	3.374124000000000

W	30.787579999999984	9.8552090000000003	3.3912550000000001
W	29.0217090000000013	13.127599999999993	3.4160770000000000
W	27.5599530000000001	15.9359040000000007	3.3750670000000000
W	25.9816460000000014	18.6251360000000012	3.4164260000000000
W	24.075838999999984	21.926075999999983	3.4884750000000002
W	22.847533999999996	24.452667999999992	3.3931890000000000
W	20.3507810000000013	27.557390999999991	3.5998090000000000
W	19.202291999999999	30.1191770000000005	3.510829999999999
W	34.169697999999968	10.338789999999995	3.3735560000000002
W	33.065272999999977	13.076306999999999	3.376606999999999
W	30.478065999999983	15.939569999999998	3.4001190000000001
W	28.911629999999988	18.6351510000000005	3.323933999999999
W	27.414660999999988	21.2881880000000017	3.437418999999998
W	25.602088999999994	24.758420999999985	3.5646550000000001
W	24.427348999999995	27.2601720000000007	3.4803020000000000
W	21.936894999999998	30.3190500000000007	3.6812870000000002
W	35.714936999999990	13.1206730000000000	3.5299140000000002
W	34.5290910000000011	15.7729440000000007	3.3803990000000002
W	32.8900250000000014	19.1370180000000012	3.4487030000000001
W	31.332001999999992	21.9161970000000004	3.5099770000000001
W	29.6675080000000015	24.6344500000000011	3.574491999999998
W	27.225906999999994	27.612671999999999	3.7144990000000000
W	25.973338999999993	30.055393999999997	3.6571310000000001
W	37.160404999999972	15.941686999999999	3.4745520000000001
W	35.606845999999973	18.885661999999999	3.3696690000000000
W	34.049948999999980	21.675052999999983	3.3448050000000000
W	32.4525640000000024	24.4086140000000000	3.4400640000000000
W	30.8137790000000003	27.1687690000000011	3.7065600000000001
W	28.7870190000000008	30.5000630000000008	3.994505999999999
W	20.8457970000000010	32.8919160000000019	3.6388750000000001
W	24.0214900000000000	33.4944330000000008	3.767342999999999
W	22.5955580000000005	35.740954999999996	3.884809999999999
W	27.101773999999989	33.1914360000000030	3.875961999999999

W	25.531752999999984	35.8039190000000005	3.9265020000000002
W	24.063690999999986	38.5048170000000027	3.9255409999999999
Se	28.340523999999985	-2.9730150000000002	3.8640200000000000
Se	27.0706890000000016	0.5767830000000000	5.0743479999999996
Se	25.4462690000000009	3.4944600000000001	5.2115489999999998
Se	23.8371470000000016	6.2981129999999999	5.2145780000000004
Se	22.2359630000000017	9.0869400000000002	5.2107310000000000
Se	20.6479390000000009	11.8925739999999998	5.2241030000000004
Se	19.029039999999984	14.6974970000000003	5.2527260000000000
Se	17.4518440000000012	17.5536899999999996	5.2709929999999998
Se	15.9069900000000004	20.5082689999999985	5.1755529999999998
Se	13.6583020000000008	23.5372440000000012	4.2936290000000001
Se	31.4289290000000001	-2.9401730000000001	4.9331740000000002
Se	30.4998620000000003	0.5105150000000001	5.3397100000000002
Se	28.9391220000000011	3.4522889999999999	4.7619220000000002
Se	27.4270880000000012	6.3649690000000003	4.8231609999999998
Se	25.8528300000000009	9.1991829999999997	4.7928189999999997
Se	24.222979999999997	12.0381830000000001	4.7834649999999996
Se	22.524354999999999	14.9742149999999992	4.7807170000000001
Se	20.904196999999999	17.7752799999999986	4.8258919999999996
Se	19.2559250000000013	20.6512369999999983	4.7414129999999997
Se	17.414941999999999	23.557992999999997	5.3304419999999997
Se	15.277528999999995	26.5740459999999992	4.4030760000000004
Se	32.189884999999968	3.2233660000000000	5.3379380000000003
Se	30.8426380000000009	6.2913699999999997	5.3496930000000003
Se	29.271280999999983	9.1823440000000005	5.3355020000000000
Se	27.6309560000000012	12.0777610000000006	5.3048929999999999
Se	25.8229390000000016	14.9037500000000005	5.0573639999999997
Se	24.3232140000000001	17.8478160000000017	5.3015429999999997
Se	22.6337560000000018	20.7399829999999987	5.2943270000000000
Se	20.8050730000000001	23.6121850000000002	4.8968290000000003
Se	18.9777510000000014	26.4377609999999983	5.3977380000000004
Se	16.9140949999999997	29.5008219999999994	4.4828299999999999

Se	34.6210319999999996	5.9623039999999996	4.5244470000000003
Se	32.7066480000000013	9.0815760000000001	5.0280849999999999
Se	31.0231560000000002	12.0736539999999994	4.7352049999999997
Se	29.1561149999999998	14.9441059999999997	5.2196040000000004
Se	27.5715749999999993	17.7726630000000014	5.2191280000000004
Se	25.8442749999999997	20.6532190000000000	5.1337479999999998
Se	24.2668560000000006	23.6076380000000015	5.3603399999999999
Se	22.3769740000000006	26.4660800000000016	4.9428099999999997
Se	20.5368020000000016	29.2973070000000000	5.4873459999999996
Se	34.3864329999999967	11.9505189999999999	5.3178679999999998
Se	32.5588830000000016	14.9899579999999997	4.9261059999999999
Se	30.9542290000000015	17.9444249999999990	4.8546269999999998
Se	29.3742640000000002	20.7095230000000008	4.8647770000000001
Se	27.6013890000000011	23.5305089999999986	4.8407220000000004
Se	25.8569460000000007	26.4410500000000006	5.4554190000000000
Se	23.9711549999999995	29.2789800000000007	5.0872460000000004
Se	35.9717679999999973	14.8524060000000002	5.3576969999999999
Se	34.2904789999999977	17.7980580000000010	5.1027170000000002
Se	32.7381430000000009	20.8086990000000007	5.3220660000000004
Se	31.0519980000000011	23.6122000000000014	5.3963520000000003
Se	29.1607769999999995	26.4481679999999990	5.3193760000000001
Se	27.4457099999999983	29.3402199999999986	5.6455679999999999
Se	38.0015530000000012	17.9327040000000011	4.4212249999999997
Se	36.4245000000000019	20.9750750000000004	4.2371730000000003
Se	34.6940290000000005	23.8621370000000006	4.4448949999999998
Se	33.0465269999999975	26.7748640000000009	4.4432309999999999
Se	30.9310820000000000	29.5027690000000007	4.8331549999999996
Se	25.3697909999999993	-0.5649000000000000	2.0904099999999999
Se	23.5766039999999997	2.2873720000000000	2.4388120000000000
Se	22.0165289999999985	5.2054809999999998	2.2828390000000001
Se	20.3768230000000017	8.0512440000000005	2.3388330000000002
Se	18.7352990000000013	10.8729920000000000	2.4053320000000000
Se	17.0762970000000003	13.7101319999999998	2.4370210000000001

Se	15.3794350000000009	16.6034690000000005	2.5762459999999998
Se	13.8336629999999996	19.6665039999999998	2.3804910000000001
Se	29.2267830000000011	-0.5854150000000000	1.5008940000000000
Se	27.4327019999999990	2.4742150000000001	1.6231420000000001
Se	25.6924220000000005	5.4103630000000003	1.4361660000000001
Se	24.1071109999999997	8.2519060000000000	1.4536290000000001
Se	22.5121180000000010	11.1270930000000003	1.4882830000000000
Se	20.8573559999999993	13.9439480000000007	1.4905740000000001
Se	19.1226340000000015	16.7615869999999987	1.4750589999999999
Se	17.5422370000000001	19.8081269999999989	1.7162890000000000
Se	15.8250370000000000	22.8194249999999990	1.5230079999999999
Se	32.5998310000000018	-0.6628270000000001	2.3352400000000002
Se	30.6576039999999992	2.4824489999999999	1.8591670000000000
Se	29.0548089999999988	5.3745380000000003	1.9530430000000001
Se	27.4855620000000016	8.2564779999999995	2.0122220000000000
Se	25.8541750000000015	11.0450529999999993	1.9545509999999999
Se	24.2374499999999991	14.0054979999999993	2.0265200000000001
Se	22.4754879999999986	16.8683559999999986	1.9520780000000000
Se	20.8965950000000014	19.6282719999999991	1.9397570000000000
Se	19.2699199999999990	22.6661539999999988	1.9840240000000000
Se	17.3318820000000002	25.6897379999999984	1.5864460000000000
Se	34.4275719999999978	2.0426899999999999	2.6901850000000000
Se	32.5999120000000033	5.2825639999999998	1.6049240000000000
Se	30.9971379999999996	8.1672309999999992	1.5254500000000000
Se	29.3796910000000011	11.1685250000000007	1.6949500000000000
Se	27.5931269999999991	14.0130060000000007	1.5383190000000000
Se	25.8868140000000011	16.8819340000000011	1.5448370000000000
Se	24.3423480000000012	19.8938309999999987	1.7752720000000000
Se	22.5990600000000015	22.7033050000000003	1.5414610000000000
Se	20.8131880000000002	25.5387169999999983	2.0646550000000001
Se	18.8866990000000001	28.4937560000000012	1.6437630000000001
Se	34.5259890000000027	8.1812629999999995	2.2793809999999999
Se	32.6081190000000021	11.0956229999999998	1.7349500000000000

Se	31.0455550000000002	14.0197120000000002	1.9061269999999999
Se	29.1732750000000003	16.8697160000000004	1.5205620000000000
Se	27.4994979999999991	19.7032389999999999	1.5304819999999999
Se	25.9764319999999991	22.7780260000000006	1.9136100000000000
Se	24.1825609999999998	25.6054710000000014	1.5979120000000000
Se	22.4023380000000003	28.3790419999999983	2.1231710000000001
Se	20.5442110000000007	31.2834059999999994	1.7282270000000000
Se	36.5346959999999967	10.8969869999999993	2.7587940000000000
Se	34.4912020000000012	13.9995720000000006	1.5321659999999999
Se	32.5666760000000011	16.9292450000000017	2.0684680000000002
Se	30.9076799999999992	19.8255279999999985	1.9788250000000001
Se	29.3008370000000014	22.6418959999999991	2.0202160000000000
Se	27.6680549999999990	25.6253409999999988	2.1680100000000002
Se	25.8229350000000011	28.4629200000000004	1.7449250000000001
Se	24.0124950000000013	31.2714029999999994	2.3620800000000002
Se	38.1259999999999977	13.9826029999999992	2.5984280000000002
Se	35.9607000000000028	17.0591949999999990	1.6064929999999999
Se	34.3717680000000030	19.9855419999999988	1.4915950000000000
Se	32.7807540000000017	22.8374179999999996	1.5306700000000000
Se	31.1122620000000012	25.6834670000000003	1.6900340000000000
Se	29.2526410000000006	28.6364850000000004	2.2425700000000002
Se	27.4526299999999992	31.4360129999999991	2.0529030000000001
Se	18.5485210000000009	32.4490559999999988	4.3773619999999998
Se	22.3646129999999985	32.1785959999999989	5.3915519999999999
Se	20.3521420000000006	35.2395160000000018	4.7269709999999998
Se	25.6157269999999997	32.1288630000000026	5.3875770000000003
Se	24.0677500000000002	35.0832669999999993	5.7785010000000003
Se	22.1299489999999999	38.0262430000000009	5.1754009999999999
Se	29.4766109999999983	32.6602699999999970	4.7637939999999999
Se	27.7780340000000017	35.3559180000000026	4.8727039999999997
Se	26.0548310000000001	38.0734489999999965	5.1264349999999999
Se	24.0352169999999994	40.6332570000000004	3.1343030000000001
Se	22.2454719999999995	34.1303529999999995	1.9545319999999999

Se	25.7561180000000007	34.1721110000000010	1.9956460000000000
Se	24.0129309999999982	36.9513609999999986	2.0683569999999998

$\mathbf{W}_{66}\mathbf{Se}_{132}$; $E_{tot} = -38\,662\,262.737\,404\,66$ eV; $E_{rel} = 6.124\,715\,621\,2$ meV/f.u.

W	28.0058310000000006	4.1222490000000001	3.4420999999999999
W	26.2151810000000012	6.8279790000000000	3.3797229999999998
W	24.5276350000000001	9.6018279999999994	3.3114789999999998
W	22.8938549999999985	12.4191830000000003	3.2756090000000002
W	21.2704139999999988	15.2295949999999998	3.2712880000000002
W	19.6523220000000016	18.0369840000000003	3.2898149999999999
W	18.0563700000000011	20.8507409999999993	3.3278249999999998
W	16.5073960000000000	23.6660980000000016	3.3517589999999999
W	14.9802190000000000	26.5089019999999991	3.2248420000000002
W	13.4038989999999991	29.4519300000000008	2.9156659999999999
W	11.7572639999999993	32.1034369999999996	2.8458049999999999
W	31.3317750000000004	4.0257680000000002	3.5137149999999999
W	29.0974649999999997	6.5496990000000004	3.3529320000000000
W	27.4101420000000005	9.2337769999999999	3.2872309999999998
W	25.7459869999999995	12.0453189999999992	3.2656849999999999
W	24.0983429999999998	14.8874849999999999	3.2606370000000000
W	22.4664399999999986	17.7149970000000003	3.2745769999999998
W	20.8455219999999990	20.5384869999999999	3.2976909999999999
W	19.2511000000000010	23.3578940000000017	3.3102230000000001
W	17.7310769999999991	26.1716119999999997	3.2719779999999998
W	16.0900350000000003	29.5718789999999991	3.1714509999999998
W	14.8529780000000002	31.9671179999999993	3.0145940000000002
W	34.4975730000000027	4.0224419999999999	3.5741730000000000
W	33.0291580000000025	6.5624870000000000	3.5010770000000000
W	31.3089210000000016	9.8429359999999999	3.5096550000000000
W	29.7188690000000015	12.5817359999999994	3.5035280000000002
W	28.1015230000000003	15.3562550000000009	3.4863700000000000
W	26.4872039999999984	18.1631500000000017	3.4913919999999998

W	24.8718010000000014	20.9596939999999989	3.4985770000000000
W	23.2539569999999998	23.7515619999999998	3.5152040000000002
W	21.6665670000000006	26.6569879999999984	3.5399140000000000
W	20.0158600000000000	29.5265860000000018	3.3800780000000001
W	18.1086759999999991	32.0560059999999964	3.2131390000000000
W	37.6514840000000035	3.9959050000000000	3.7004510000000002
W	35.7445439999999977	6.5249240000000004	3.5334129999999999
W	34.0936599999999999	9.3948359999999997	3.3735170000000001
W	32.5065659999999994	12.3001240000000003	3.3980969999999999
W	30.8887679999999989	15.0921029999999998	3.4144489999999998
W	29.2733770000000000	17.8887180000000008	3.4214940000000000
W	27.6590880000000006	20.6955479999999987	3.4264380000000001
W	26.0416290000000004	23.4701020000000007	3.4095309999999999
W	24.4516060000000017	26.2087159999999990	3.4037419999999998
W	22.7310979999999994	29.4892189999999985	3.4123999999999999
W	21.2626239999999989	32.0292900000000031	3.3396810000000001
W	40.9073750000000018	4.0845750000000001	3.8983850000000002
W	39.6701490000000021	6.4799199999999999	3.7413820000000002
W	38.0294310000000024	9.8801179999999995	3.6415929999999999
W	36.5094289999999972	12.6939279999999997	3.6032169999999999
W	34.9150440000000017	15.5130490000000005	3.6155070000000000
W	33.2941270000000031	18.3367700000000013	3.6383320000000001
W	31.6621559999999995	21.1643690000000007	3.6522670000000002
W	30.0145179999999989	24.0064430000000009	3.6472680000000000
W	28.3502189999999992	26.8180030000000009	3.6258840000000001
W	26.6631309999999999	29.5019419999999997	3.5602659999999999
W	24.4283989999999989	32.0260450000000034	3.3998539999999999
W	44.0024560000000022	3.9483169999999999	4.0668080000000000
W	42.3564950000000024	6.5994529999999996	3.9971869999999998
W	40.7798149999999993	9.5428599999999992	3.6882799999999998
W	39.2532769999999971	12.3854290000000002	3.5614040000000000
W	37.7043299999999988	15.2007530000000006	3.5853519999999999
W	36.1083569999999980	18.0147650000000006	3.6233930000000001

W	34.490059999999997	20.822289999999989	3.641767999999999
W	32.866667999999971	23.632549999999984	3.637197000000000
W	31.232738999999987	26.450109000000012	3.601305000000000
W	29.545307999999986	29.223675000000001	3.533183000000002
W	27.754483000000005	31.929463999999994	3.470966999999999
Se	29.353260999999998	2.406231000000000	4.393690000000003
Se	27.524392999999999	5.703740999999999	5.272255000000004
Se	25.793717999999984	8.476402999999995	5.198389999999998
Se	24.124257000000001	11.248936999999997	5.150192999999998
Se	22.487456000000017	14.043450999999992	5.138650000000002
Se	20.859518000000013	16.839724000000004	5.149930000000003
Se	19.248972999999994	19.644045999999995	5.179630000000004
Se	17.674160000000005	22.480245000000000	5.212003000000002
Se	16.139126999999984	25.392963999999992	5.160960000000002
Se	14.570577000000001	28.363399999999986	4.902904000000004
Se	13.014087000000000	31.300429000000012	4.760818999999997
Se	32.748913999999992	2.265223000000002	4.329063999999998
Se	31.044136000000017	5.785490000000002	5.077547000000000
Se	29.369972000000006	8.616595999999995	4.871140999999997
Se	27.727374999999986	11.376455000000000	4.786232000000000
Se	26.091706999999995	14.177708000000009	4.762444999999996
Se	24.467175999999985	16.990069999999993	4.770889999999996
Se	22.846439000000002	19.804639999999991	4.789053000000000
Se	21.221744000000011	22.630887999999988	4.822631000000003
Se	19.622357999999984	25.484673000000008	4.829548000000000
Se	17.959351999999991	28.411753999999984	4.621929999999999
Se	16.366192999999991	31.439312000000010	4.959711000000004
Se	36.047901000000031	2.284046000000000	4.496660000000003
Se	34.355198000000015	5.599192000000004	5.469494000000001
Se	32.686075999999999	8.521124000000004	5.217710000000003
Se	31.079567000000008	11.486948999999992	5.371405000000002
Se	29.420284999999998	14.263242000000000	5.347866999999999
Se	27.793258000000016	17.044959999999997	5.339073000000000

Se	26.1778620000000011	19.8481230000000011	5.3478300000000001
Se	24.5708179999999992	22.6558050000000009	5.3542779999999999
Se	22.9720270000000006	25.5009550000000011	5.3527600000000000
Se	21.2848709999999990	28.4353809999999996	5.2733949999999998
Se	19.5738419999999991	31.3726599999999998	5.1256389999999996
Se	39.3193249999999992	2.3387639999999998	4.6604169999999998
Se	37.6169319999999985	5.7802410000000002	5.2802829999999998
Se	36.0604680000000002	8.6478880000000000	4.9812390000000004
Se	34.5153669999999977	11.4949969999999997	4.8740459999999999
Se	32.9058890000000019	14.3688070000000003	4.9329900000000002
Se	31.2832860000000004	17.1826140000000009	4.9470900000000002
Se	29.6575759999999988	19.9932200000000009	4.9525880000000004
Se	28.0186390000000003	22.8136140000000012	4.9516970000000002
Se	26.3787489999999991	25.6011519999999990	4.9620480000000002
Se	24.6541460000000008	28.4164619999999992	4.8292359999999999
Se	22.8693770000000001	31.3703329999999987	5.2203520000000001
Se	42.5484000000000009	2.4751949999999998	5.1978410000000004
Se	40.9485839999999968	5.6662850000000002	5.8062760000000004
Se	39.3496269999999981	8.5590159999999997	5.3874529999999998
Se	37.8342140000000029	11.5661679999999993	5.4845689999999996
Se	36.2335720000000023	14.3784949999999991	5.4595719999999996
Se	34.6185509999999965	17.2015600000000006	5.4770640000000004
Se	32.9893829999999966	20.0336970000000001	5.4952959999999997
Se	31.3536380000000001	22.8794760000000004	5.4919900000000004
Se	29.7261309999999987	25.7359410000000004	5.4746319999999997
Se	28.0508710000000008	28.5776590000000006	5.4399709999999999
Se	26.1152939999999987	31.4017109999999988	5.2515980000000004
Se	45.8737849999999980	2.8606549999999999	3.3809079999999998
Se	44.5245329999999981	5.8445749999999999	5.3527620000000002
Se	43.0774460000000019	8.7577719999999992	4.8070659999999998
Se	41.5937860000000015	11.6842419999999994	4.4775999999999998
Se	39.9617059999999995	14.5632199999999994	4.5834900000000003
Se	38.3457539999999995	17.4408570000000012	4.6106499999999997

Se	36.7105570000000014	20.2999319999999983	4.6350480000000003
Se	35.0663839999999993	23.1540180000000007	4.6369140000000000
Se	33.4244739999999965	26.0263719999999985	4.5853409999999997
Se	31.7363919999999986	28.9212039999999995	4.5026900000000003
Se	29.8697389999999992	31.8605130000000010	4.4578650000000000
Se	25.8905059999999985	4.1910090000000002	2.4549409999999998
Se	24.0239939999999983	7.1304650000000001	2.4101780000000002
Se	22.3358489999999996	10.0253110000000003	2.3275530000000000
Se	20.6940880000000007	12.8977559999999993	2.2761390000000001
Se	19.0499450000000010	15.7519010000000002	2.2781760000000002
Se	17.4147829999999999	18.6107669999999992	2.3026369999999998
Se	15.7987310000000001	21.4882489999999997	2.3298549999999998
Se	14.1666249999999998	24.3673740000000016	2.4354800000000001
Se	12.6833299999999998	27.2935370000000006	2.1056720000000002
Se	11.2360460000000000	30.2071199999999997	1.5596650000000001
Se	9.8867650000000005	33.1906180000000006	3.5311849999999998
Se	29.6451190000000011	4.6500069999999996	1.6615409999999999
Se	27.7096640000000001	7.4740589999999996	1.4731790000000000
Se	26.0343529999999994	10.3157999999999994	1.4383600000000001
Se	24.4068959999999997	13.1722579999999994	1.4209560000000001
Se	22.7711299999999994	16.0181359999999984	1.4176299999999999
Se	21.1419910000000009	18.8501970000000014	1.4359409999999999
Se	19.5269520000000014	21.6732340000000008	1.4536730000000000
Se	17.9262920000000001	24.4854100000000017	1.4286520000000000
Se	16.4108449999999984	27.4924870000000006	1.5257970000000001
Se	14.8119490000000003	30.3851469999999999	1.1067330000000000
Se	13.2118099999999998	33.5762330000000020	1.7148939999999999
Se	32.8909349999999989	4.6813310000000001	1.6930339999999999
Se	31.1063510000000001	7.6353249999999999	2.0839569999999998
Se	29.3820060000000005	10.4505820000000007	1.9509730000000001
Se	27.7419939999999983	13.2381609999999998	1.9612480000000001
Se	26.1029429999999998	16.0585670000000000	1.9603200000000001
Se	24.4771099999999997	18.8691369999999985	1.9658599999999999

Se	22.8545319999999990	21.6829740000000015	1.9801650000000000
Se	21.2454140000000002	24.5568939999999998	2.0390250000000001
Se	19.7002130000000015	27.4038670000000018	1.9318949999999999
Se	18.1434460000000009	30.2714260000000017	1.6331410000000000
Se	16.4412160000000007	33.7126450000000020	2.2532429999999999
Se	36.1861460000000008	4.6788350000000003	1.7879550000000000
Se	34.4755579999999995	7.6162099999999997	1.6400840000000001
Se	32.7884850000000014	10.5507819999999999	1.5603370000000001
Se	31.1897480000000016	13.3958860000000008	1.5588409999999999
Se	29.5826990000000016	16.2036119999999997	1.5651219999999999
Se	27.9672120000000000	19.0068659999999987	1.5738319999999999
Se	26.3401969999999999	21.7886090000000010	1.5650729999999999
Se	24.6809100000000008	24.5648529999999994	1.5416209999999999
Se	23.0741849999999999	27.5306980000000010	1.6956389999999999
Se	21.4051229999999997	30.4526280000000007	1.4440759999999999
Se	19.7121840000000006	33.7677869999999984	2.4170129999999999
Se	39.3936869999999999	4.6122389999999998	1.9536230000000001
Se	37.8008459999999999	7.6402049999999999	2.2915540000000001
Se	36.1381250000000023	10.5670470000000005	2.0839569999999998
Se	34.5388949999999966	13.4206900000000005	2.0905640000000001
Se	32.9142140000000012	16.2470360000000014	2.1239870000000001
Se	31.2933489999999992	19.0616790000000016	2.1419959999999998
Se	29.6687629999999984	21.8740689999999987	2.1505350000000001
Se	28.0330289999999991	24.6753579999999992	2.1268490000000000
Se	26.3903509999999990	27.4351009999999995	2.0419489999999998
Se	24.7160900000000012	30.2662849999999999	1.8357239999999999
Se	23.0112859999999984	33.7864209999999972	2.5846520000000002
Se	42.7462560000000025	4.7508480000000004	2.1513320000000000
Se	41.1894029999999987	7.6881700000000004	2.0100020000000001
Se	39.6215860000000006	10.6586870000000005	1.7521629999999999
Se	38.0865050000000025	13.5714539999999992	1.7010959999999999
Se	36.5116909999999990	16.4075780000000009	1.7336170000000000
Se	34.9010970000000000	19.2120190000000015	1.7631429999999999

Se	33.273119999999987	22.0083030000000015	1.7742150000000001
Se	31.6362150000000000	24.8028259999999996	1.7626329999999999
Se	29.9666589999999999	27.5753020000000006	1.7143569999999999
Se	28.2358340000000005	30.3480379999999990	1.6406790000000000
Se	26.4069520000000004	33.6453630000000032	2.5197250000000002

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,263.141\,635\,89$ eV; $E_{rel} = 0$ meV/f.u.

W	19.809145999999984	1.1377610000000000	3.4219140000000001
W	18.0116399999999999	3.9625080000000001	3.5785019999999998
W	16.4084630000000011	6.6903969999999999	3.6908690000000002
W	14.8427360000000004	9.4435499999999999	3.6184710000000000
W	13.2858219999999996	12.4243989999999993	3.4931130000000001
W	23.0093010000000007	1.0039469999999999	3.2904529999999999
W	21.244855999999986	3.3444389999999999	3.4742320000000002
W	19.156023999999986	6.4227990000000004	3.4836399999999998
W	17.5601750000000010	9.1983890000000006	3.5020570000000002
W	15.930203999999998	12.6477920000000008	3.5538289999999999
W	14.7558779999999992	15.3036999999999992	3.4200970000000002
W	26.246448999999984	1.0248500000000000	3.2082240000000000
W	24.2943140000000000	3.3143479999999998	3.4292750000000001
W	23.1600770000000011	6.8447209999999998	3.4382530000000000
W	21.5786380000000015	9.6343920000000001	3.5906950000000002
W	19.917405999999997	12.4118659999999998	3.4420570000000001
W	17.4242670000000004	15.4325250000000000	3.5190139999999999
W	16.3337490000000010	18.0914830000000002	3.3361000000000001
W	29.4937630000000013	1.0099030000000000	3.3133859999999999
W	28.1966350000000006	3.3125710000000002	3.4387919999999998
W	26.2544350000000009	6.8711630000000001	3.3395950000000001
W	24.424575999999983	9.2499179999999992	3.4310510000000001
W	22.6924370000000017	12.5324559999999998	3.4480590000000002
W	21.462765999999985	15.1483170000000005	3.3451890000000000
W	19.0413220000000010	18.1954290000000007	3.4821700000000000

W	18.032783999999995	20.849872999999998	3.3270179999999998
W	32.689658999999998	1.1394299999999999	3.4562029999999999
W	31.258355999999991	3.3446899999999999	3.4927139999999999
W	29.3663200000000018	6.8678390000000000	3.4709850000000002
W	28.269415999999997	9.3752230000000001	3.3537089999999998
W	25.710015999999995	12.347239999999993	3.4221949999999999
W	24.2296340000000008	15.097272999999995	3.3858750000000000
W	23.1143590000000003	17.8949500000000015	3.3489900000000001
W	21.1238980000000005	21.4169650000000011	3.5091489999999999
W	19.7455019999999983	23.6851969999999987	3.4722840000000001
W	34.4834620000000029	3.9581209999999998	3.6040920000000001
W	33.3745770000000022	6.4576630000000002	3.4893960000000002
W	30.9862940000000009	9.6394690000000001	3.5721370000000001
W	29.801214999999991	12.2674240000000001	3.4205880000000000
W	28.2732859999999988	15.2473060000000000	3.4640409999999999
W	26.2127109999999988	18.4101709999999983	3.4218690000000000
W	24.6176950000000012	20.6397879999999994	3.5044460000000002
W	22.6240340000000018	24.0768939999999994	3.5494479999999999
W	21.4732720000000015	26.5127200000000016	3.4693360000000002
W	36.1197179999999989	6.6809560000000001	3.6618629999999999
W	35.0126100000000022	9.2533499999999993	3.4545129999999999
W	32.5455460000000016	12.3786149999999999	3.5021100000000001
W	30.9997399999999992	15.1343560000000004	3.3708680000000002
W	29.3931649999999998	17.8484830000000017	3.3280110000000001
W	27.8078210000000006	20.6582650000000001	3.5351309999999998
W	26.3728699999999989	24.2960889999999985	3.4977680000000002
W	24.7851640000000017	26.5180250000000015	3.6118899999999998
W	37.6861969999999999	9.4094080000000009	3.6070570000000002
W	36.5409140000000008	12.0546659999999992	3.4486110000000001
W	34.9503180000000029	15.5273889999999994	3.4990410000000001
W	33.4055359999999979	18.3444550000000000	3.5027110000000001
W	31.7796319999999994	21.1247499999999988	3.4959050000000000
W	29.5725429999999996	24.3033460000000012	3.4762870000000001

W	27.933550000000003	26.549512000000000	3.6356090000000001
W	39.1963459999999984	12.2496340000000004	3.5447419999999998
W	37.6858209999999971	15.2500110000000006	3.4322339999999998
W	36.1459230000000034	18.0660230000000013	3.3831859999999998
W	34.5527689999999978	20.8298950000000005	3.3965800000000002
W	33.0555930000000018	23.6485920000000007	3.4312920000000000
W	31.0223149999999990	26.6101269999999985	3.4124669999999999
W	34.2105540000000019	26.7098149999999990	3.1175489999999999
Se	21.0687269999999991	-0.6583720000000000	4.2789409999999997
Se	19.4651320000000005	2.7352710000000000	5.2953049999999999
Se	17.7567969999999988	5.5709559999999998	5.4862109999999999
Se	16.1253400000000013	8.4059489999999997	5.5035369999999997
Se	14.5439670000000003	11.3314330000000005	5.3387070000000003
Se	12.3201839999999994	14.3678550000000005	4.3804740000000004
Se	24.5920220000000000	-0.7299780000000000	4.0709920000000004
Se	22.8377219999999994	2.4999500000000001	5.2873409999999996
Se	21.2494459999999989	5.5943949999999996	4.8230760000000004
Se	19.5709640000000000	8.5089500000000005	4.9683940000000000
Se	17.8778560000000013	11.4339969999999997	4.8478930000000000
Se	16.0434850000000004	14.3864900000000002	5.3664170000000002
Se	14.0030750000000008	17.4386119999999991	4.3468689999999999
Se	27.9082270000000001	-0.7275779999999999	4.0778960000000000
Se	26.2427729999999997	2.6161070000000000	5.0386480000000002
Se	24.6092380000000013	5.5089370000000004	4.9519390000000003
Se	22.9313210000000005	8.4316680000000002	5.3613689999999998
Se	21.2029339999999991	11.4380260000000007	5.3259650000000001
Se	19.4334840000000000	14.3864269999999994	4.9139070000000000
Se	17.6291809999999991	17.2630000000000017	5.3255840000000001
Se	15.7067650000000008	20.3978649999999995	4.1464059999999998
Se	31.4266809999999985	-0.6465490000000000	4.3272990000000000
Se	29.6515869999999993	2.5190329999999999	5.3058829999999997
Se	27.8969400000000007	5.5162839999999997	4.9464940000000004
Se	26.2972420000000007	8.5823260000000001	5.1084690000000004

Se	24.3643420000000006	11.3383289999999999	5.1425549999999998
Se	22.8264670000000010	14.2815700000000003	5.3120940000000001
Se	21.0971800000000016	17.1831700000000005	4.8708340000000003
Se	19.4869449999999986	20.1224249999999998	5.1369829999999999
Se	17.4610869999999991	23.2152969999999996	4.2554360000000004
Se	33.0307889999999986	2.7455650000000000	5.3252720000000000
Se	31.2701099999999990	5.6096370000000002	4.8275249999999996
Se	29.6088629999999995	8.4879300000000004	5.3565160000000001
Se	27.7673920000000010	11.4183450000000004	4.8542639999999997
Se	26.2460659999999990	14.2856529999999999	4.8932349999999998
Se	24.6331379999999989	17.0704250000000002	5.0918109999999999
Se	22.8165230000000001	19.9922250000000012	5.0469600000000003
Se	21.2157470000000004	23.0520950000000013	5.4125819999999996
Se	34.7822019999999981	5.5737209999999999	5.4860860000000002
Se	32.9645319999999984	8.5217919999999996	4.9584320000000002
Se	31.2231220000000000	11.3877109999999995	5.3827449999999999
Se	29.6348069999999986	14.1984290000000009	5.2686279999999996
Se	27.8905299999999983	17.1467959999999984	5.1469240000000003
Se	26.2445680000000010	20.0675980000000003	5.3795900000000003
Se	24.5976199999999992	22.9300210000000000	4.8531129999999996
Se	36.4201869999999985	8.3660309999999996	5.4776590000000001
Se	34.5640819999999991	11.3547419999999999	4.9435159999999998
Se	33.0088009999999983	14.3920270000000006	4.9430660000000000
Se	31.3924440000000011	17.2174739999999993	4.8518829999999999
Se	29.7951240000000013	20.0021139999999988	4.9038000000000004
Se	27.9766109999999983	22.9175220000000017	4.9862719999999996
Se	38.0160490000000024	11.1726019999999995	5.4211749999999999
Se	36.3497180000000029	14.1817100000000007	5.1498189999999999
Se	34.7883640000000014	17.2380749999999985	5.3439329999999998
Se	33.1390540000000016	20.0901400000000017	5.3462350000000001
Se	31.3362049999999996	23.0080880000000008	5.1097219999999997
Se	40.0718900000000033	14.2456169999999993	4.4407300000000003
Se	38.5379709999999989	17.3314599999999999	4.2465159999999997

Se	36.851742999999990	20.2330240000000003	4.3807890000000000
Se	35.1011260000000007	23.0267799999999987	4.6032620000000000
Se	17.6321559999999984	1.4188769999999999	2.5413160000000001
Se	15.7552090000000007	4.3462519999999998	2.7791120000000000
Se	14.0408700000000000	7.3095270000000001	2.8121939999999999
Se	12.4510780000000008	10.3961679999999994	2.6134800000000000
Se	21.3050950000000014	1.6126450000000001	1.5050559999999999
Se	19.5564250000000008	4.5698030000000003	1.7943460000000000
Se	17.7092820000000017	7.4532559999999997	1.6627760000000000
Se	16.1312749999999987	10.5129020000000004	1.8642490000000000
Se	14.4229160000000007	13.5345119999999994	1.6048680000000000
Se	24.5936659999999989	1.6555460000000000	1.4438650000000000
Se	22.8669189999999993	4.6639739999999996	1.8807990000000001
Se	21.1009110000000000	7.5608849999999999	2.0608499999999998
Se	19.5007190000000001	10.3412400000000009	2.0525060000000002
Se	17.8633430000000004	13.3739539999999995	2.0145200000000001
Se	15.9980910000000005	16.3772710000000004	1.5366599999999999
Se	27.9180039999999998	1.6468050000000001	1.4555709999999999
Se	26.2476090000000006	4.5553540000000003	2.1454029999999999
Se	24.5707479999999983	7.5680829999999997	1.5184260000000001
Se	22.9383669999999995	10.4885549999999999	1.7373120000000000
Se	21.1586290000000012	13.3512909999999998	1.5301659999999999
Se	19.4487249999999996	16.2207149999999984	1.9682990000000000
Se	17.6798870000000008	19.1692730000000005	1.5042120000000001
Se	31.2026000000000003	1.6072190000000000	1.5305780000000000
Se	29.6280409999999996	4.6736149999999999	1.9073570000000000
Se	27.9242699999999999	7.5977660000000000	1.5435490000000001
Se	26.2896779999999985	10.3843920000000001	1.9346840000000001
Se	24.4061610000000009	13.3339719999999993	1.5709050000000000
Se	22.8632470000000012	16.2090350000000001	1.5173049999999999
Se	21.1229849999999999	19.1471049999999998	2.1713600000000000
Se	19.4559280000000001	21.9917499999999997	1.5969949999999999
Se	34.8727269999999976	1.4083270000000001	2.5868630000000001

Se	32.9412170000000017	4.5747229999999997	1.8242620000000001
Se	31.4175100000000000	7.5475190000000003	2.0506709999999999
Se	29.6512519999999995	10.4800789999999999	1.5852530000000000
Se	27.8018800000000006	13.2527059999999999	1.9774529999999999
Se	26.2346320000000013	16.1688229999999997	2.0743190000000000
Se	24.5533530000000013	19.0407919999999997	1.5776859999999999
Se	22.9494800000000012	22.0142060000000015	1.9312270000000000
Se	21.0202460000000002	24.9034820000000003	1.6547069999999999
Se	36.7375129999999999	4.3081800000000001	2.7874310000000002
Se	34.7918000000000021	7.4556860000000000	1.6571860000000000
Se	33.0302470000000028	10.3642380000000003	2.0383369999999998
Se	31.2465219999999988	13.3232119999999998	1.5841149999999999
Se	29.6068779999999983	16.1382159999999999	1.4992920000000001
Se	27.9241039999999998	19.0526939999999989	1.6085220000000000
Se	26.3181720000000006	22.0680830000000014	2.0614949999999999
Se	24.5141090000000013	24.8765210000000003	1.8376500000000000
Se	38.4026330000000016	7.2635009999999998	2.6179600000000001
Se	36.4178659999999965	10.3290880000000005	1.6359790000000001
Se	34.6286569999999969	13.3049750000000007	2.1324160000000001
Se	33.0082540000000009	16.2394570000000016	1.9973920000000001
Se	31.3874980000000008	19.0627390000000005	2.0006240000000002
Se	29.6884200000000007	21.9868859999999984	2.1578580000000001
Se	27.9573159999999987	24.9766830000000013	1.6459600000000001
Se	40.1284109999999998	10.2885050000000007	2.6507489999999998
Se	37.9685339999999982	13.3699320000000004	1.6982770000000000
Se	36.4665570000000017	16.3445770000000010	1.5496570000000001
Se	34.9197330000000008	19.1907309999999995	1.5282199999999999
Se	33.2519920000000013	21.9630089999999996	1.5653390000000000
Se	31.3577049999999993	24.8405510000000014	1.7420420000000001
Se	19.4949450000000013	25.8868240000000007	4.9705560000000002
Se	23.0239310000000010	25.9275820000000010	5.3515980000000001
Se	22.8774450000000016	28.1672030000000007	2.5395569999999998
Se	26.3441469999999995	25.9541080000000015	5.4920030000000004

Se	26.2119460000000011	28.2825969999999991	2.7628270000000001
Se	29.6154539999999997	26.0600050000000003	5.4192039999999997
Se	32.9583060000000003	25.8597919999999988	5.0110869999999998
Se	32.6873300000000029	28.2101900000000008	2.1172740000000001
Se	34.7973270000000028	24.9671389999999995	1.6685470000000000
Se	29.4861269999999998	28.2759730000000005	2.5542400000000001
Se	36.0260450000000034	27.8667909999999992	3.8123010000000002
Se	19.1613830000000007	27.5240259999999992	3.2586260000000000

$W_{105}Se_{210}$; $E_{tot} = -61\,508\,146.516\,497\,63$ eV; $E_{rel} = 41.505\,328\,485\,7$ meV/f.u.

W	21.3106919999999995	-1.1064980000000000	3.3699330000000001
W	19.4448380000000007	1.7124820000000001	3.4306299999999998
W	17.7876800000000017	4.4993119999999998	3.4466640000000002
W	16.1358619999999995	7.2587590000000004	3.3906969999999998
W	14.4590519999999998	10.0176920000000003	3.3454410000000001
W	12.8326630000000002	12.7964230000000008	3.3029620000000000
W	11.1786949999999994	15.5890299999999993	3.1460129999999999
W	9.2037479999999992	18.9401609999999998	3.0735749999999999
W	7.6332769999999996	21.9101670000000013	3.3830909999999998
W	6.1352219999999997	24.7211369999999988	3.5319880000000001
W	4.5862449999999999	27.4966860000000004	3.5136949999999998
W	3.0253030000000001	30.4410789999999984	3.4616609999999999
W	24.5360399999999998	-1.2264320000000000	3.4423550000000001
W	22.8291569999999986	1.0808240000000000	3.4778970000000000
W	20.5809390000000008	4.2000609999999998	3.3331330000000001
W	18.9392819999999986	7.0024009999999999	3.3516629999999998
W	17.2129699999999985	9.8109160000000006	3.3017249999999998
W	15.5570450000000005	12.5903360000000006	3.2475200000000002
W	13.9706279999999996	15.3590280000000003	3.2089590000000001
W	12.4340550000000007	18.9221590000000006	3.1886880000000000
W	10.8547390000000004	21.1986729999999994	3.3406110000000000
W	8.8981499999999993	24.6025230000000015	3.4002379999999999

W	7.4614770000000004	27.1828250000000011	3.4397470000000001
W	5.6457030000000001	30.5813519999999990	3.4870220000000001
W	4.5251500000000000	33.2727059999999994	3.3626239999999998
W	27.7565249999999999	-1.2813760000000001	3.5469550000000001
W	29.2294429999999998	1.0319300000000000	3.6096910000000002
W	26.0299849999999999	1.0216920000000000	3.5454810000000001
W	24.5406189999999995	4.6939390000000003	3.3696500000000000
W	23.0748549999999994	7.1643179999999997	3.4453350000000000
W	21.1508530000000015	10.4741999999999997	3.4511250000000002
W	19.5981130000000014	13.1153809999999993	3.4823710000000001
W	18.0115380000000016	15.7820350000000005	3.3246929999999999
W	15.6518020000000000	19.0174750000000010	3.2620830000000001
W	13.9647070000000006	21.2097979999999993	3.3787660000000002
W	12.7412650000000003	24.8323059999999991	3.3249190000000000
W	10.5650689999999994	27.2434699999999985	3.4049820000000000
W	9.6364950000000000	30.3787519999999986	3.3808790000000002
W	7.1845400000000001	33.1902929999999969	3.4452919999999998
W	6.1381589999999999	36.0519419999999968	3.3616860000000002
W	30.9843809999999991	-1.2677410000000000	3.5654119999999998
W	27.7391560000000013	4.7013809999999996	3.3592580000000001
W	26.1593599999999995	6.9785089999999999	3.4722240000000002
W	24.2634919999999994	10.3008900000000008	3.4294840000000000
W	22.5469979999999985	13.0713190000000008	3.4721050000000000
W	21.0696310000000011	15.7174490000000002	3.4225870000000000
W	19.3822669999999988	18.9376040000000003	3.3922110000000001
W	17.8219139999999996	21.5381719999999994	3.4037590000000000
W	15.8927390000000006	24.7793370000000017	3.3696419999999998
W	14.3394659999999998	27.0749989999999983	3.4913319999999999
W	12.3632340000000003	30.5701280000000004	3.4721540000000002
W	9.1923490000000001	36.5439190000000025	3.5057079999999998
W	11.2355540000000005	33.0681810000000027	3.3805740000000002
W	7.7881210000000003	38.9017440000000008	3.5054660000000002
W	34.3767759999999996	-1.2737120000000000	3.7001260000000000

W	36.178159999999983	1.4170689999999999	3.7363189999999999
W	32.3375830000000022	1.0717200000000000	3.6422070000000000
W	30.9726409999999994	4.7237349999999996	3.4446970000000001
W	29.3617990000000013	6.9556889999999996	3.5464519999999999
W	27.2158820000000006	10.1832419999999999	3.4589059999999998
W	25.7375860000000003	12.6957760000000004	3.4707270000000001
W	23.8636130000000009	15.8394440000000003	3.4579490000000002
W	22.2129769999999986	18.5833620000000010	3.3344740000000002
W	20.5996670000000002	21.4119230000000016	3.3414860000000002
W	18.9533079999999998	24.1772740000000006	3.3467539999999998
W	17.4691180000000017	27.0095080000000003	3.5048789999999999
W	16.2101970000000009	30.6967299999999987	3.4566759999999999
W	13.9990729999999992	33.1824689999999975	3.5371579999999998
W	12.9978660000000001	35.8679599999999965	3.3637100000000002
W	10.6006029999999996	38.9428100000000015	3.6004320000000001
W	9.5075649999999996	41.6170090000000030	3.6611669999999998
W	37.4344809999999981	-1.2740270000000000	3.9150689999999999
W	34.1740989999999982	4.7194019999999997	3.6318429999999999
W	32.6462879999999984	6.9963949999999997	3.6989160000000001
W	31.2080410000000015	10.5826080000000005	3.6273200000000001
W	29.6617099999999994	13.3650640000000003	3.6192240000000000
W	27.9498139999999999	16.1471209999999985	3.5829249999999999
W	26.2852889999999988	19.0138980000000011	3.5815750000000000
W	24.6335790000000010	21.8305959999999999	3.5619350000000001
W	23.0027879999999989	24.6386429999999983	3.5775549999999998
W	21.3808450000000008	27.4221579999999996	3.5826220000000002
W	19.3472630000000017	30.6490569999999991	3.5379700000000001
W	15.8710459999999998	36.3649660000000026	3.6396009999999999
W	17.8454189999999997	32.9400899999999979	3.6224310000000002
W	14.6156059999999997	38.7411760000000029	3.5929790000000001
W	12.7029060000000005	42.1368129999999965	3.7716330000000000
W	11.2516999999999996	44.4123990000000006	3.9665629999999998
W	40.3937609999999978	-1.4515750000000001	3.8657770000000000

W	38.835630999999993	1.258370000000000	3.758054000000000
W	37.414354000000003	4.008487999999999	3.738379999999999
W	35.891818999999998	6.966340999999999	3.977392000000000
W	33.981696999999999	10.345257000000001	3.734726000000002
W	32.368898999999999	13.169173999999999	3.559451999999999
W	30.720382000000007	15.952759000000004	3.553065000000001
W	29.058215000000006	18.736131000000003	3.573064000000000
W	27.430707999999992	21.548489000000000	3.582672000000001
W	25.794940000000004	24.349394000000002	3.575655999999999
W	24.170798000000001	27.133572000000009	3.526694000000000
W	22.546720000000005	29.925961000000009	3.568700000000002
W	20.995065000000003	32.902580999999979	3.808055000000000
W	19.064057999999993	36.237369999999985	3.851707000000002
W	17.391709999999998	38.955810999999971	3.777740000000001
W	15.853752000000001	41.603422000000019	3.784717000000001
W	14.132676999999993	44.416724999999996	3.951992999999999
W	12.694610000000008	47.167547999999965	4.069613999999996
Se	18.085354999999998	41.162771999999968	4.730177000000003
Se	14.484811999999998	42.846764999999978	2.015880999999998
Se	12.695292000000002	45.675097999999984	2.155822000000001
Se	22.470779000000003	-2.882811999999999	4.348245000000004
Se	20.921426000000003	0.541001000000000	5.190455000000000
Se	19.092401999999999	3.343788000000000	5.290813000000000
Se	17.392153000000004	6.144245999999999	5.275807000000004
Se	15.679544999999992	8.896955999999994	5.229080999999999
Se	14.033346999999991	11.693778000000000	5.183968000000001
Se	12.382346000000001	14.549894000000001	5.100168000000000
Se	10.667723999999998	17.592817000000001	4.732699000000002
Se	9.015971000000004	20.567636000000003	5.056972000000000
Se	7.463842999999998	23.500509000000010	5.286918000000000
Se	5.863223999999998	26.427983000000011	5.361799999999997
Se	4.260340000000002	29.307075999999986	5.297348000000004
Se	25.908069999999998	-2.980944000000000	4.402506999999999

Se	24.343724999999992	0.391778000000000	5.352090999999997
Se	22.669872999999991	3.385743999999999	4.729535000000003
Se	20.975860999999983	6.208988999999999	4.822612999999996
Se	19.251936000000006	9.138464000000008	4.783471999999997
Se	17.561455999999997	11.941829999999995	4.763009000000003
Se	15.907412000000008	14.738993000000007	4.734151999999999
Se	14.049079000000008	17.565829000000008	4.653444000000004
Se	12.399544999999998	20.509090000000005	5.210893999999997
Se	10.860359000000008	23.504231000000008	4.680016000000002
Se	9.130950999999996	26.376422000000016	5.247789000000000
Se	7.611691000000004	29.403840999999999	4.785685000000000
Se	19.161135000000016	-0.856479000000000	2.427835000000000
Se	17.228155000000010	2.024458000000001	2.611314999999998
Se	15.564287000000002	4.923767999999999	2.442781999999998
Se	13.885009999999994	7.763242000000000	2.349546000000001
Se	12.181181000000005	10.622495999999999	2.291452000000000
Se	10.446491999999992	13.465524000000003	2.356171999999999
Se	9.013925000000004	16.629232999999993	2.138449000000000
Se	6.946442000000002	19.545714000000003	2.499026999999999
Se	5.394806000000000	22.471773999999999	2.570792000000000
Se	3.771649000000000	25.390812000000004	2.663338000000000
Se	2.175721999999999	28.400275000000006	2.587663000000000
Se	22.918202000000009	-0.686244000000000	1.546750000000001
Se	21.089165000000013	2.278655999999998	1.740701000000001
Se	19.224999000000004	5.240268000000004	1.505104000000000
Se	17.602206999999999	8.071039000000007	1.501201000000000
Se	15.868484999999997	10.864620000000004	1.434520000000000
Se	14.198458999999997	13.687245000000008	1.366114000000001
Se	12.566658000000003	16.710015999999995	1.525964000000001
Se	10.759116000000006	19.598867999999995	1.332764000000001
Se	9.219443999999993	22.608872999999991	1.737787000000000
Se	7.410779999999999	25.495730999999993	1.516556999999999
Se	5.936131999999997	28.534237000000010	1.825496000000000

Se	4.160442999999999	31.524705000000009	1.543990000000000
Se	2.118300000000001	32.413048000000004	4.366966999999998
Se	5.758744000000001	32.344292000000029	5.330772999999998
Se	3.817438999999998	35.479398000000033	4.234403999999996
Se	29.238362999999997	-2.923776999999998	4.593261000000000
Se	27.614878000000009	0.363064000000000	5.430017000000003
Se	26.031356999999999	3.323191000000000	4.896404999999997
Se	24.471816000000005	6.286064999999998	5.320001999999997
Se	22.570188999999992	9.112434000000004	5.062223999999996
Se	20.971146000000010	12.078502999999995	5.331940000000003
Se	19.303297000000006	14.898747000000002	5.245091000000004
Se	17.415957999999998	17.783445000000004	4.784962000000002
Se	15.803554000000001	20.638252000000014	5.077944999999997
Se	14.137812999999995	23.441185999999983	4.847889999999996
Se	12.508122000000002	26.470112000000003	5.152417999999999
Se	10.950167999999997	29.271088999999999	5.154377000000002
Se	32.598691999999998	-3.044797000000000	4.208739999999997
Se	30.856911000000002	0.302850000000000	5.501911999999999
Se	29.269671999999999	3.315901999999999	4.917322000000004
Se	27.726994999999987	6.334369999999998	5.338841999999996
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Se	24.214141999999989	12.036341000000002	5.278203999999997
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Se	14.318775000000005	29.383344999999985	4.813366000000003
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Se	8.996444000000003	43.946652999999977	4.758982999999997
Se	7.195365999999999	41.251395999999997	4.367377000000003

W₁₀₅Se₂₁₀; $E_{tot} = -61\,508\,146.791\,805\,60$ eV; $E_{rel} = 38.883\,347\,819\,0$ meV/f.u.

W	22.514139000000001	-4.429917999999998	3.115355999999998
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W	21.3062940000000012	-2.2227299999999999	3.0378560000000001
W	19.4774239999999992	1.0583530000000001	3.1848150000000000
W	17.9210570000000011	3.8644140000000000	3.3474260000000000
W	16.3448950000000011	6.6441150000000002	3.3560560000000002
W	14.7188479999999995	9.4458889999999993	3.3683109999999998
W	13.0832840000000008	12.2750769999999996	3.3374830000000002
W	11.4604479999999995	15.1244650000000007	3.2930500000000000
W	9.8440899999999996	17.9693970000000007	3.2671470000000000
W	8.2218879999999999	20.7857340000000015	3.2692350000000001
W	6.6140990000000004	23.5737850000000009	3.3142090000000000
W	5.0269399999999997	26.3988130000000005	3.2816649999999998
W	3.4204819999999998	29.3603670000000001	3.1384400000000001
W	1.7655270000000001	32.0181540000000027	3.1961539999999999
W	22.8181329999999996	0.3895180000000000	3.2364169999999999
W	24.1687130000000003	-1.9211190000000000	3.2935729999999999
W	20.6855919999999998	3.5456340000000002	3.2147690000000000
W	19.1205010000000009	6.3405360000000002	3.2871220000000001
W	17.5066470000000010	9.1928490000000007	3.3550040000000001
W	15.8480559999999997	12.0300659999999997	3.3649789999999999
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W	4.8442239999999996	31.9286679999999983	3.1723729999999999
W	25.7855230000000013	0.7116220000000000	3.2895520000000000
W	24.6985910000000004	3.8225730000000002	3.3373599999999999
W	23.2347169999999998	6.6067070000000001	3.4751859999999999
W	21.5879440000000002	9.4380880000000005	3.4585050000000002
W	19.8809100000000001	12.4606390000000005	3.5751759999999999
W	18.2119639999999983	15.2702050000000007	3.5631960000000000
W	16.6172870000000010	18.0944250000000011	3.5437449999999999

W	14.9845360000000003	21.0129869999999990	3.5185330000000001
W	13.3296690000000009	23.8880429999999997	3.4716700000000000
W	11.6808870000000002	26.7065100000000015	3.4216039999999999
W	10.0392039999999998	29.4436570000000017	3.3196140000000001
W	7.9168550000000000	31.9890940000000015	3.1975340000000001
W	27.5375210000000017	3.3995270000000000	3.0456799999999999
W	26.0405039999999985	6.1824070000000004	3.2927450000000000
W	24.3638170000000009	9.4634990000000005	3.4432269999999998
W	22.9982940000000013	11.8868849999999995	3.4671989999999999
W	20.9512350000000005	15.0543200000000006	3.4887210000000000
W	19.4161940000000008	17.7732729999999997	3.4582449999999998
W	17.7510690000000011	20.6522299999999994	3.3960659999999998
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W	29.5626199999999990	6.6907269999999999	3.2918020000000001
W	28.4252560000000010	9.2264490000000006	3.3709600000000002
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W	30.1237059999999985	11.9548190000000005	3.4321470000000001
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Se	28.015090000000007	22.761451999999985	4.859843999999998
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Se	24.703855999999983	28.700165999999994	4.895703000000001
Se	23.076491999999982	31.892286999999996	5.275655000000004
Se	34.944991000000017	16.729282000000013	5.299546000000003
Se	33.027436999999990	19.760452999999983	4.864265999999998
Se	31.424783000000015	22.765805000000003	4.987302999999998
Se	29.691537000000003	25.696187999999994	5.357503999999996
Se	28.008209000000008	28.664327000000001	4.877970999999996
Se	26.342030999999986	31.899570000000006	5.246531000000001
Se	36.514865000000004	19.668831000000008	5.187286000000003
Se	34.753537000000015	22.675929000000000	4.740073999999999
Se	33.007052000000016	25.710492999999996	5.310252000000002
Se	31.295542999999986	28.640451999999998	4.833688999999997
Se	29.598010999999996	31.858829000000001	5.220238000000002
Se	17.241250999999983	1.498102000000000	2.435584000000000
Se	15.720672999999997	4.427004000000002	2.281007999999999
Se	14.057855999999992	7.236888999999997	2.389018000000001
Se	12.427457999999997	10.066371000000002	2.381472000000000
Se	10.800836000000003	12.915552999999992	2.336091999999998
Se	9.179411000000000	15.752031000000006	2.307817000000000
Se	7.559364999999997	18.566534000000008	2.294900000000002
Se	5.941582999999996	21.405394000000011	2.268437000000000
Se	4.235419000000003	24.249318999999998	2.480551999999999
Se	2.712813999999998	27.203887000000017	2.252657000000001
Se	1.192984000000000	30.147176999999992	1.895005000000001
Se	-0.077843000000000	33.045189000000006	4.034004000000004
Se	21.114187000000011	1.666368000000001	1.516613999999999
Se	19.340551999999989	4.616456999999996	1.397219999999999

Se	17.798836999999989	7.492367999999999	1.482064000000000
Se	16.179518000000016	10.310771000000008	1.517406000000000
Se	14.553157000000006	13.144467999999998	1.497478000000001
Se	12.937279000000002	15.998428999999998	1.465795000000000
Se	11.320446999999997	18.835934000000017	1.432862000000001
Se	9.667832999999999	21.642099999999992	1.398894000000001
Se	7.981772000000003	24.419585999999989	1.367496000000000
Se	6.380555000000002	27.430396999999993	1.551091999999999
Se	4.714927999999996	30.359397999999988	1.268130000000000
Se	3.131219000000002	33.554668999999970	2.030669000000001
Se	24.371905999999992	1.733522999999999	1.647542000000001
Se	22.733526000000012	4.614967000000000	1.861175000000000
Se	21.158277999999993	7.410648000000001	1.951322000000000
Se	19.537555999999986	10.318175000000001	2.049348000000002
Se	17.873228999999985	13.140803999999993	2.069715000000000
Se	16.237352000000013	15.999143999999994	2.017014000000001
Se	14.620589000000007	18.875026999999993	2.027296999999999
Se	12.998032000000003	21.739623000000017	1.983965999999999
Se	11.332800000000007	24.562425000000011	1.938954000000001
Se	9.695686999999995	27.360358000000015	1.838823000000001
Se	8.055305000000006	30.214529999999999	1.631200000000000
Se	6.346734999999998	33.683900000000013	2.279836000000000
Se	28.181591999999984	1.191801000000001	2.389358000000001
Se	26.191573999999992	4.480756000000004	1.338802000000000
Se	24.633203999999992	7.497656000000001	1.638811000000000
Se	22.930568999999984	10.252506000000003	1.511670000000001
Se	21.389953999999995	13.171032000000003	1.771226000000000
Se	19.664207999999986	16.037144999999989	1.593283999999999
Se	18.048884999999985	18.903690999999985	1.608938999999999
Se	16.404157000000014	21.845859999999983	1.603024000000000
Se	14.744459000000009	24.755945000000005	1.520613999999999
Se	13.080605999999995	27.575572000000011	1.452981000000001
Se	11.372669999999994	30.415784999999996	1.343892000000001

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Se	27.9270490000000002	7.3582780000000003	1.6526160000000001
Se	26.3853839999999984	10.2884799999999998	2.0294430000000001
Se	24.5963780000000014	13.1459170000000007	1.7753080000000001
Se	22.9856470000000002	16.0581500000000013	2.1322549999999998
Se	21.2902030000000018	18.9736009999999986	1.8263620000000000
Se	19.7763169999999988	21.8240470000000002	2.0999170000000000
Se	18.0913280000000007	24.6502279999999985	1.7071689999999999
Se	16.4696649999999991	27.6260000000000012	2.0130550000000000
Se	14.7307419999999993	30.4460669999999993	1.6103390000000000
Se	12.9776229999999995	33.4975870000000029	2.1909019999999999
Se	31.7854780000000012	7.0583819999999999	2.5072749999999999
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Se	28.1027829999999987	13.0801029999999994	2.1465869999999998
Se	26.3890619999999991	16.0221419999999988	1.6752540000000000
Se	24.7272390000000009	18.7711439999999996	1.8751860000000000
Se	23.2076649999999987	21.8803219999999996	1.9040410000000001
Se	21.4423950000000012	24.7365630000000003	1.5791510000000000
Se	19.8179400000000001	27.7708429999999993	2.0367590000000000
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Se	16.3939009999999996	33.9638369999999981	2.5076410000000000
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Se	26.3141500000000015	21.8436629999999994	2.0901369999999999
Se	24.6887520000000009	24.7850800000000007	1.6236800000000000
Se	23.0733169999999994	27.7747829999999993	2.0496300000000001
Se	21.4393339999999988	30.6801880000000011	1.5386690000000001
Se	19.7194280000000006	33.9512519999999967	2.4013380000000000
Se	35.1618130000000022	12.8090499999999992	2.4508150000000000
Se	33.0954169999999976	15.8760499999999993	1.5696120000000000

Se	31.384637999999989	18.762212000000017	2.0584739999999999
Se	29.518411000000004	21.818092000000000	1.7988590000000000
Se	28.026524999999995	24.703924000000007	1.6862040000000000
Se	26.358558999999996	27.741517000000018	2.0947420000000001
Se	24.713733000000013	30.637523999999991	1.5456650000000001
Se	23.045500000000005	34.006093999999974	2.4306160000000001
Se	36.803316000000024	15.716585999999995	2.4141270000000001
Se	34.698680000000031	18.740023000000008	1.4881770000000001
Se	32.935163000000029	21.728373000000013	2.0409120000000001
Se	31.348503000000009	24.666727999999991	1.5537620000000001
Se	29.624447000000000	27.695954000000004	2.0527760000000002
Se	27.971869999999991	30.606850000000014	1.5198730000000000
Se	26.339590999999986	33.990293000000012	2.3913560000000000
Se	22.838515000000010	-3.165859000000002	5.1406120000000000
Se	19.190464999999997	-1.321471000000001	2.1393080000000002
Se	26.448285999999995	-1.522202000000001	2.4201560000000000
Se	22.768374999999989	-1.282459000000000	1.2994230000000000
Se	24.478528000000007	-4.179441999999999	1.8489819999999999
Se	20.332968999999985	-4.561600000000003	2.2561279999999999
Se	29.605810999999992	33.974750999999977	2.3628079999999998
Se	32.829928000000024	31.809909000000011	5.2163420000000000
Se	31.219045000000013	30.621400999999988	1.4683210000000000
Se	34.537677999999997	28.638995000000013	4.8021459999999996
Se	32.898164999999988	27.715621999999998	1.9744740000000001
Se	36.288355000000028	25.683883000000016	5.1993169999999997
Se	34.617137999999971	24.688866000000009	1.4587330000000001
Se	38.145037000000021	22.776154999999993	4.7038000000000002
Se	36.247467000000003	21.811146000000008	1.5909050000000000
Se	38.457794999999973	18.598248999999991	2.4356960000000001
Se	39.663426999999987	25.734667999999992	4.9526750000000002
Se	39.784070999999973	21.782063000000008	2.1356630000000001
Se	37.926482999999975	24.734905000000013	1.3135650000000001
Se	37.830218999999996	28.656328999999995	4.6158320000000002

Se	36.0878310000000013	31.7006550000000011	5.1976599999999999
Se	36.1389160000000018	27.7179159999999989	1.8495269999999999
Se	34.4664420000000007	30.6870219999999989	1.4134720000000001
Se	32.8869469999999993	33.9550369999999972	2.3398949999999998
Se	41.1971169999999987	28.5656019999999984	5.0600670000000001
Se	41.8000290000000021	24.5980680000000014	2.2865470000000001
Se	39.4196590000000029	31.6125630000000015	5.0500650000000000
Se	39.4381569999999968	27.6918889999999998	1.6209190000000000
Se	36.2179140000000004	33.9972810000000010	2.5515390000000000
Se	37.8784709999999976	30.5429150000000007	1.5776859999999999
Se	43.3038939999999997	27.4034650000000006	2.2455500000000002
Se	42.7513390000000015	31.4601770000000016	5.0327520000000003
Se	41.2546930000000032	30.4965849999999996	1.2801430000000000
Se	39.5395159999999990	33.8038560000000032	2.2872319999999999
Se	45.9998209999999972	33.2507739999999998	4.0592819999999996
Se	42.8527020000000007	33.6304409999999976	1.9270740000000000
Se	44.8193869999999990	30.2384979999999999	2.0332629999999998

$W_{105}Se_{210}$; $E_{tot} = -61\,508\,147.850\,709\,12$ eV; $E_{rel} = 28.798\,552\,390\,4$ meV/f.u.

W	21.3480239999999988	-1.1248970000000000	3.3461900000000000
W	19.4789360000000009	1.6886000000000001	3.4007160000000001
W	17.8143600000000006	4.4728149999999998	3.4206599999999998
W	16.1781889999999997	7.2449110000000001	3.3833839999999999
W	14.5102250000000002	10.0008199999999992	3.3751000000000002
W	12.8664769999999997	12.7627699999999997	3.3704879999999999
W	11.2130890000000001	15.5466479999999994	3.2461859999999998
W	9.2173169999999995	18.8526449999999990	2.9834230000000002
W	7.5336499999999997	21.9166600000000003	3.2107450000000002
W	6.0813709999999999	24.6389659999999999	3.2367539999999999
W	4.5562220000000000	27.3046979999999984	3.1199450000000000
W	2.7449530000000002	30.7243759999999995	3.0530789999999999
W	1.2769260000000000	33.3747690000000006	3.1328630000000000

W	-0.2681410000000000	36.1196970000000022	3.0628299999999999
W	-1.9398560000000000	38.7172330000000002	3.0099170000000002
W	24.5718710000000016	-1.2379869999999999	3.4307960000000000
W	22.8631540000000015	1.0645950000000000	3.4572720000000001
W	20.6132910000000003	4.1785909999999999	3.3164440000000002
W	18.9791659999999993	6.9658629999999997	3.3416210000000000
W	17.2764960000000016	9.7867700000000006	3.3272979999999999
W	15.6002539999999996	12.5643750000000001	3.3021699999999998
W	13.9839800000000007	15.3295949999999994	3.3061090000000002
W	12.4524369999999998	18.8877580000000016	3.2659410000000002
W	10.9410249999999998	21.1673669999999987	3.3814289999999998
W	8.9962879999999998	24.6685550000000013	3.3559899999999998
W	7.6670639999999999	27.0012860000000003	3.3921039999999998
W	6.0482329999999997	30.6227760000000018	3.2345950000000001
W	2.4546489999999999	36.2893869999999978	3.2001230000000001
W	4.5069600000000003	32.9157579999999967	3.3044889999999998
W	1.1865960000000000	38.6442920000000001	3.0481889999999998
W	27.7907340000000005	-1.2841739999999999	3.5439560000000001
W	29.2581349999999993	1.0308780000000000	3.6105220000000000
W	26.0612239999999993	1.0149630000000001	3.5352779999999999
W	24.5706460000000000	4.6841109999999997	3.3556900000000001
W	23.0947279999999999	7.1545449999999997	3.4514469999999999
W	21.2442740000000008	10.3730039999999999	3.4668649999999999
W	19.6560260000000007	13.1213180000000005	3.5360779999999998
W	17.9768630000000016	15.8030930000000005	3.4179750000000002
W	15.6482410000000005	18.9377339999999990	3.4014650000000000
W	14.1440819999999992	21.1751189999999987	3.5312640000000002
W	12.6820839999999997	24.7924250000000015	3.3850539999999998
W	10.9536320000000007	26.9761440000000015	3.5451760000000001
W	9.3192450000000004	30.6594939999999987	3.3161079999999998
W	7.6846509999999997	32.9045020000000008	3.4364390000000000
W	6.2331630000000002	36.5814200000000014	3.2520560000000001
W	4.5372219999999999	38.7835320000000010	3.2944049999999998

W	31.016300999999986	-1.2634810000000001	3.5639539999999998
W	27.768439999999982	4.6974739999999997	3.3628680000000002
W	26.1814210000000003	6.9610110000000001	3.4772729999999998
W	24.2208679999999994	10.2804529999999996	3.4388600000000000
W	22.6779879999999991	12.7848910000000000	3.4742959999999998
W	20.7921049999999994	15.9988550000000007	3.4611760000000000
W	19.4246890000000008	18.6556500000000014	3.4411440000000000
W	17.3694209999999991	21.1405010000000004	3.6059950000000001
W	15.8515020000000000	24.8332979999999992	3.4254190000000002
W	14.2252220000000005	27.0620300000000000	3.5627979999999999
W	12.5738939999999992	30.6850510000000014	3.3592800000000000
W	9.4191780000000005	36.6327399999999983	3.3044739999999999
W	10.9060570000000006	32.9254689999999997	3.4975520000000002
W	7.7557790000000004	38.8728740000000030	3.4100169999999999
W	34.4016360000000034	-1.2648070000000000	3.6991580000000002
W	36.2032340000000019	1.4274370000000001	3.7480210000000000
W	32.3664720000000017	1.0768240000000000	3.6487479999999999
W	30.9973530000000004	4.7316200000000004	3.4581130000000000
W	29.3811929999999997	6.9639949999999997	3.5559479999999999
W	27.2278780000000005	10.2136379999999996	3.4659149999999999
W	25.7431769999999993	12.7036180000000005	3.4510630000000000
W	23.8161169999999984	15.9085280000000004	3.4618679999999999
W	22.2517800000000001	18.5753960000000014	3.3952010000000001
W	20.6768520000000002	21.2260139999999993	3.4724100000000000
W	19.0491670000000006	24.8606200000000008	3.4885709999999999
W	17.4033599999999993	27.0987650000000002	3.6195230000000000
W	15.8561280000000000	30.7452480000000001	3.3635920000000001
W	14.1038460000000008	32.9435829999999967	3.5210919999999999
W	12.6619930000000007	36.6121509999999972	3.3513250000000001
W	10.9527920000000005	38.8997099999999989	3.4283489999999999
W	37.4602670000000018	-1.2648230000000000	3.9167860000000001
W	34.1974220000000031	4.7321910000000003	3.6510630000000002
W	32.6637219999999999	7.0081080000000000	3.7124039999999998

W	31.223240000000005	10.597435000000008	3.622099000000000
W	29.665731999999984	13.376751000000005	3.592200000000001
W	27.941310999999989	16.172903999999991	3.527038000000001
W	26.273918999999994	19.067668999999986	3.545612000000002
W	24.585483000000000	21.896792999999988	3.586929000000000
W	22.885687000000008	24.665282999999987	3.608334999999998
W	21.121316000000002	27.223690999999988	3.643202000000001
W	19.093233000000015	30.676321000000015	3.576085000000000
W	15.852664000000008	36.497945999999989	3.418660000000000
W	17.811744999999984	33.049033999999989	3.539861999999998
W	14.169449999999994	38.839238999999992	3.478180000000000
W	40.416905999999973	-1.445133000000000	3.860903000000000
W	38.860272000000019	1.268799000000000	3.768500000000000
W	37.436369999999966	4.017624999999998	3.761286000000001
W	35.909439999999965	6.983819000000004	4.004360000000001
W	33.991889000000005	10.363656000000006	3.735656000000001
W	32.372939999999998	13.183735000000004	3.526219000000002
W	30.717477999999998	15.957316999999998	3.477831999999998
W	29.064806999999983	18.742121000000009	3.472084000000002
W	27.430730000000005	21.550522000000008	3.495035000000001
W	25.769497999999987	24.337700999999991	3.561481000000001
W	24.086103000000014	27.092566000000015	3.630792000000000
W	22.513130000000003	29.987625999999988	3.772412000000001
W	20.664162999999985	33.390675000000017	3.763106000000001
W	19.162109000000009	35.872411999999971	3.602945000000001
W	17.420815000000010	38.658912000000008	3.523321000000001
Se	22.507421000000008	-2.897829000000002	4.332774999999998
Se	20.952968999999995	0.521438000000000	5.165046000000002
Se	19.116378999999985	3.311789000000001	5.265082999999997
Se	17.422554000000017	6.105413000000004	5.261096000000002
Se	15.735198000000005	8.862742000000008	5.242015000000003
Se	14.084500999999995	11.651794000000007	5.235402999999998
Se	12.399160999999994	14.489304000000006	5.192120000000001

Se	10.6527519999999996	17.5836019999999991	4.7610180000000000
Se	8.9366760000000003	20.5258339999999997	4.9055650000000002
Se	7.4465240000000001	23.5159519999999986	5.1039539999999999
Se	5.8119280000000000	26.4173819999999999	5.0894820000000003
Se	4.1482099999999997	29.3270610000000005	4.7042979999999996
Se	25.9447909999999986	-2.9836239999999998	4.4071680000000004
Se	24.3723630000000000	0.3816160000000000	5.3383159999999998
Se	22.7006119999999996	3.3665270000000000	4.7121380000000004
Se	21.0067890000000013	6.1751639999999997	4.8210569999999997
Se	19.3162850000000006	9.0870870000000004	4.7988400000000002
Se	17.6125200000000000	11.9071549999999995	4.8008600000000001
Se	15.9314269999999993	14.7017830000000007	4.8129130000000000
Se	14.0266420000000007	17.5176440000000007	4.8110700000000000
Se	12.4234589999999994	20.4819540000000018	5.2638379999999998
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Se	9.2303189999999997	26.3621489999999987	5.2715350000000001
Se	7.6087100000000003	29.2641649999999984	4.7699290000000003
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Se	6.9729880000000000	19.5179590000000012	2.3767589999999998
Se	5.3519899999999998	22.3847270000000016	2.2939530000000001
Se	3.7771629999999998	25.2000999999999991	2.2663050000000000
Se	2.4270170000000002	28.2956930000000000	2.2224119999999998
Se	0.5492060000000000	31.1300579999999982	2.1675249999999999
Se	22.9595209999999987	-0.7044780000000000	1.5272960000000000
Se	21.1279830000000004	2.2622779999999998	1.7178389999999999
Se	19.2563630000000003	5.2150660000000002	1.4851630000000000
Se	17.6523900000000005	8.0661939999999994	1.5033289999999999

Se	15.924175999999992	10.860561999999998	1.4736950000000000
Se	14.228426999999999	13.677255999999999	1.4429719999999999
Se	12.581265999999994	16.6760130000000011	1.6155759999999999
Se	10.8366900000000008	19.5870810000000013	1.3452160000000000
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Se	7.5164220000000004	25.4015410000000017	1.3983200000000000
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Se	2.6545359999999998	32.3395679999999999	4.9847400000000004
Se	1.0177259999999999	35.0945109999999971	4.9813599999999996
Se	-0.5714980000000000	38.0031600000000012	4.8828370000000003
Se	5.9968070000000004	32.2591449999999966	5.2034760000000002
Se	4.4209280000000000	35.2230500000000006	4.5926410000000004
Se	2.7628480000000000	38.1670700000000025	4.9843970000000004
Se	-1.0083970000000000	33.9142719999999969	2.2250060000000000
Se	-2.5084460000000002	36.7531829999999999	1.8322630000000000
Se	-3.8035109999999999	39.7677490000000020	3.7693989999999999
Se	2.8731460000000002	34.2227519999999998	1.5934919999999999
Se	1.0601860000000001	37.0180519999999973	1.1776190000000000
Se	-0.5812820000000000	40.1623090000000005	1.7495920000000000
Se	29.2742520000000006	-2.9264850000000000	4.5879729999999999
Se	27.6406190000000009	0.3587200000000000	5.4266800000000002
Se	26.0561480000000003	3.3124189999999998	4.8885350000000001
Se	24.5003039999999999	6.2628079999999997	5.3178630000000000
Se	22.6313379999999995	9.0709540000000004	5.1270259999999999
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Se	15.7283439999999999	20.5118630000000017	5.4051400000000003
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Se	10.9296260000000007	29.2880439999999993	4.8415249999999999
Se	32.6296749999999989	-3.0453410000000001	4.1944509999999999

Se	30.8834270000000011	0.3016500000000000	5.5047850000000000
Se	29.2946939999999998	3.3148700000000000	4.9247100000000001
Se	27.7480629999999984	6.3300510000000001	5.3460279999999996
Se	25.8896480000000011	9.1211050000000000	5.1334530000000003
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Se	14.2442270000000004	29.3461169999999996	4.8718290000000000
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Se	22.5852889999999995	5.2540600000000000	1.8556049999999999
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Se	9.3175299999999996	28.3538829999999997	1.9585750000000000
Se	7.7000500000000000	31.2730280000000000	1.4592680000000000
Se	29.4337389999999992	-0.7474499999999999	1.7011490000000000
Se	27.7389979999999987	2.3742209999999999	2.0421849999999999
Se	26.1126509999999996	5.2955220000000001	1.5139920000000000
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Se	10.9628499999999995	35.2326830000000015	4.8265589999999996
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Se	9.3640439999999998	34.3266729999999995	1.9650960000000000
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Se	14.232537000000007	31.333659000000008	1.543369000000000
Se	35.971769999999994	-0.470966000000000	1.968815000000000
Se	34.279567999999976	2.421717000000001	2.342036999999999
Se	32.727257999999991	5.363856000000002	1.734561000000000
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Se	14.202400000000008	35.207216000000025	4.918889000000001
Se	12.552027000000007	38.358871999999981	5.304787000000001
Se	19.343696999999988	32.361950999999977	5.516283999999997

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Se	11.0624810000000000	37.2859910000000028	1.5012509999999999
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Se	42.2062790000000021	-2.5927110000000000	3.0609459999999999
Se	41.0465850000000003	0.4950340000000000	5.0563180000000001
Se	39.5848080000000024	3.4524480000000000	4.8182590000000003
Se	38.1224350000000030	6.3790500000000003	4.6931209999999997
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Se	33.0224010000000021	15.3537189999999999	4.5172280000000002
Se	31.3348319999999987	18.1974869999999989	4.4573460000000003
Se	29.6799520000000001	21.0349739999999983	4.4444879999999998
Se	27.9942940000000000	23.8812959999999990	4.5154040000000002
Se	26.2876539999999999	26.6976340000000008	4.5985750000000003
Se	24.6769190000000016	29.5237279999999984	4.6010629999999999
Se	39.1534059999999968	-0.5703040000000000	1.9956790000000000
Se	37.7235909999999990	2.4413550000000002	1.8696870000000001
Se	36.1316849999999974	5.3590359999999997	2.0311669999999999
Se	34.5233569999999972	8.3050379999999997	2.2416309999999999
Se	32.8337730000000008	11.4059460000000001	1.7498250000000000
Se	31.1645779999999988	14.2864190000000004	1.6438260000000000
Se	29.4742880000000014	17.0928289999999983	1.6157830000000000
Se	27.8295570000000012	19.9202730000000017	1.6241600000000000
Se	26.1672989999999999	22.7383750000000013	1.6702429999999999
Se	24.4990209999999990	25.5331370000000000	1.7262169999999999
Se	22.6916319999999985	28.3548250000000017	1.8937690000000000
Se	21.1075699999999991	31.3703989999999990	2.1119690000000002
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Se	21.397988000000016	35.553376999999976	4.638029999999997
Se	19.588062000000008	38.380152000000025	4.478597999999999
Se	19.325659999999992	34.167521999999982	1.785595000000000
Se	17.768395000000017	36.990448000000007	1.733192000000001
Se	16.270741999999985	40.455407000000010	2.561968999999999

$W_{105}Se_{210}$; $E_{tot} = -61\,508\,148.504\,960\,48$ eV; $E_{rel} = 22.567\,587\,057\,1$ meV/f.u.

W	58.889468999999983	-66.583776000000003	3.473085000000002
W	57.051962000000032	-63.763440000000028	3.569354000000001
W	60.363013000000023	-64.388195999999935	3.531315000000002
W	55.389980999999988	-60.998970999999974	3.614690000000000
W	53.786020000000006	-58.235970999999993	3.593599000000002
W	52.210349000000008	-55.424667999999969	3.521242000000000
W	50.667634999999971	-52.413899000000007	3.402337999999999
W	62.141190000000017	-66.728977999999979	3.469551000000001
W	58.175663999999976	-61.271286000000035	3.463779999999999
W	56.516736999999991	-58.486305999999990	3.442596000000000
W	54.945788999999978	-55.673067000000032	3.437158999999999
W	53.316429999999969	-52.180382999999991	3.493548000000001
W	52.143894000000031	-49.537519000000032	3.355723999999999
W	65.417439000000017	-66.779599000000046	3.450098999999998
W	63.583289999999981	-64.469787999999941	3.518523000000001
W	62.093750999999975	-60.812998999999978	3.437959999999999
W	60.507396000000000	-58.046914000000010	3.543076000000001
W	58.927875999999977	-55.214637000000033	3.555060000000001
W	57.282635999999966	-52.466608000000008	3.386846999999999
W	54.816684000000022	-49.338057999999966	3.473348000000001
W	53.690353999999992	-46.729813999999975	3.332676999999999
W	68.695650999999980	-66.778861000000062	3.435410000000001
W	66.914186999999983	-64.509038000000039	3.491925000000002
W	65.326702999999949	-60.797727999999993	3.297867999999998
W	63.315899999999992	-58.405980999999970	3.381329000000000

W	61.8458970000000008	-55.6356499999999983	3.4186410000000000
W	59.9925849999999983	-52.2172509999999974	3.4764970000000002
W	58.8343220000000002	-49.6526470000000018	3.3227880000000001
W	56.4504710000000003	-46.4365900000000025	3.4604990000000000
W	55.3079979999999978	-43.9270670000000010	3.3426540000000000
W	71.9600449999999938	-66.7856179999999995	3.4399950000000001
W	70.2550880000000006	-64.5221329999999966	3.4888990000000000
W	68.5859760000000023	-60.8555130000000020	3.3410549999999999
W	67.1993750000000034	-58.4453590000000034	3.3795489999999999
W	65.0161659999999983	-55.0399919999999980	3.4506869999999998
W	63.9570289999999986	-52.4908980000000014	3.3386860000000000
W	61.5756569999999996	-49.3820630000000023	3.5038529999999999
W	60.4441410000000019	-46.8635980000000032	3.3293180000000002
W	58.1773779999999974	-43.5404339999999976	3.4862000000000002
W	56.9780810000000031	-41.1548530000000028	3.3861629999999998
W	75.2208250000000049	-66.7787720000000036	3.4854759999999998
W	73.5824829999999963	-64.5254529999999988	3.5177559999999999
W	71.9013900000000064	-60.8556549999999987	3.3441960000000002
W	70.1176509999999951	-58.5565929999999994	3.4339100000000000
W	68.9507260000000031	-55.6222070000000031	3.3230160000000000
W	66.7362420000000043	-52.3321940000000012	3.4555030000000002
W	65.4963240000000013	-49.8729730000000018	3.3608520000000000
W	63.2522149999999996	-46.5938620000000014	3.4753289999999999
W	62.0774850000000029	-44.1377960000000016	3.3967760000000000
W	59.8777400000000029	-40.8331549999999979	3.5180650000000000
W	58.7426600000000008	-38.4366709999999969	3.4435470000000001
W	78.4699679999999944	-66.7526969999999977	3.5450740000000001
W	76.8955629999999957	-64.5090339999999998	3.5934849999999998
W	75.3292110000000008	-60.8536420000000007	3.4414030000000002
W	73.7252009999999984	-58.6208179999999999	3.5555569999999999
W	71.7646799999999985	-55.1086790000000022	3.4070670000000001
W	70.0640750000000025	-52.8524310000000028	3.4138730000000002
W	68.2402579999999972	-49.6406399999999977	3.4323000000000001

W	67.1690080000000052	-46.4952669999999983	3.4518680000000002
W	65.2959160000000054	-44.1758370000000014	3.5824140000000000
W	63.7245479999999986	-40.4990039999999993	3.4656340000000001
W	62.1143929999999997	-38.2824010000000001	3.5725330000000000
W	81.6870530000000059	-66.7146620000000041	3.6187909999999999
W	80.1853919999999931	-64.4673949999999962	3.6589860000000001
W	78.5352189999999979	-60.8037100000000024	3.4919730000000002
W	76.9785609999999991	-58.5189200000000014	3.5848860000000000
W	75.4275080000000031	-54.9808870000000027	3.5043090000000001
W	73.8980980000000045	-52.3090460000000022	3.5085950000000001
W	72.2787450000000007	-49.4993559999999988	3.5019999999999998
W	70.3178079999999994	-46.3999949999999970	3.4581529999999998
W	68.5797500000000042	-44.1175110000000004	3.5772010000000001
W	66.9605930000000029	-40.4493399999999994	3.4653470000000000
W	65.3129150000000038	-38.2248700000000028	3.6270970000000000
W	84.8761269999999968	-66.7018549999999948	3.8800129999999999
W	83.4258130000000051	-64.3980530000000044	3.7545829999999998
W	81.7067329999999998	-60.7589240000000004	3.5514459999999999
W	80.0833259999999996	-58.4992900000000020	3.6062810000000001
W	78.1946999999999974	-55.3167150000000021	3.4610420000000000
W	76.6494270000000029	-52.5057130000000001	3.3975890000000000
W	75.0354650000000021	-49.7161040000000014	3.3706130000000001
W	73.3498270000000048	-46.9092709999999968	3.3459859999999999
W	71.7524719999999974	-44.1108819999999966	3.4956920000000000
W	70.3168830000000042	-40.4785230000000027	3.4454889999999998
W	68.4998489999999975	-38.1997349999999969	3.5836420000000002
W	88.7466830000000044	-66.8793610000000029	3.8112330000000001
W	86.6608980000000031	-63.8893879999999967	3.7409659999999998
W	90.3147419999999954	-64.3493770000000040	3.8600319999999999
W	85.4377379999999960	-61.0597449999999995	3.7219280000000001
W	83.8592170000000010	-58.4178739999999976	3.6342170000000000
W	82.1547269999999941	-54.9388299999999970	3.5844779999999998
W	80.6502859999999941	-52.1008950000000013	3.5435910000000002

W	79.0410590000000042	-49.2679830000000010	3.5281449999999999
W	77.3812139999999999	-46.4382540000000006	3.5015209999999999
W	75.6850309999999951	-43.6390469999999979	3.4923240000000000
W	73.5551719999999989	-40.5814620000000019	3.4183949999999999
W	71.7355089999999933	-38.2089879999999980	3.5102080000000000
W	88.1849119999999971	-61.0158470000000008	3.9325489999999999
W	86.5685270000000031	-58.3431879999999978	3.6939820000000001
W	84.9392529999999937	-55.2946579999999983	3.5245419999999998
W	83.3867709999999960	-52.4139849999999967	3.4542109999999999
W	81.8217219999999941	-49.5639099999999999	3.4651169999999998
W	80.1884249999999952	-46.7311649999999972	3.4540920000000002
W	78.5118570000000062	-43.9376370000000023	3.3858180000000000
W	76.8238079999999997	-41.1620849999999976	3.3841239999999999
W	74.9892080000000050	-38.3557449999999989	3.4468559999999999
Se	60.0627909999999972	-68.3607709999999997	4.4372550000000004
Se	58.5250630000000029	-64.9469490000000036	5.3103650000000000
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Se	53.4553009999999986	-56.4946339999999978	5.4044179999999997
Se	51.9125119999999995	-53.5263769999999965	5.2427320000000002
Se	49.7068370000000002	-50.4703659999999985	4.2983430000000000
Se	63.5435459999999992	-68.4642869999999988	4.3821360000000000
Se	61.9509880000000024	-65.0961460000000045	5.3602390000000000
Se	60.2581240000000022	-62.1077709999999996	4.8381740000000004
Se	58.5462010000000035	-59.1925900000000027	4.9355989999999998
Se	56.9130249999999975	-56.3520019999999988	4.9125610000000002
Se	55.2466549999999970	-53.4303400000000011	4.7918370000000001
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Se	51.3821870000000018	-47.4162340000000029	4.3330669999999998
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Se	63.6611469999999997	-62.1823679999999968	4.8814229999999998
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Se	75.2033200000000051	-65.1178900000000027	5.3776659999999996
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Se	71.8991000000000042	-59.2423399999999987	5.2335760000000002
Se	70.3744889999999970	-56.4826240000000013	5.1209239999999996
Se	68.4948870000000056	-53.6150080000000031	5.0862129999999999
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Se	77.174651999999947	-42.8174229999999980	1.5378250000000000
Se	75.3692920000000015	-39.9971200000000024	1.6196219999999999
Se	73.772499999999937	-36.5822629999999975	2.5141760000000000

W₁₀₅Se₂₁₀; $E_{tot} = -61\,508\,148.650\,619\,92$ eV; $E_{rel} = 21.180\,354\,295\,2$ meV/f.u.

W	21.0482750000000003	-0.7996410000000000	3.4312339999999999
W	19.2525440000000003	1.8973120000000001	3.3712640000000000
W	17.5476169999999989	4.6727340000000002	3.3055639999999999
W	15.909499999999995	7.5031309999999998	3.2760090000000002

W	14.2926380000000002	10.3258010000000002	3.2741400000000001
W	12.6819539999999993	13.1336929999999992	3.2829839999999999
W	11.0684050000000003	15.9318209999999993	3.2898209999999999
W	9.4517240000000005	18.7290080000000003	3.2869290000000002
W	7.8340600000000000	21.5293400000000013	3.2788670000000000
W	6.2178550000000001	24.3339819999999989	3.2755619999999999
W	4.6023430000000003	27.1411699999999989	3.2847070000000000
W	2.9828320000000001	29.9523870000000016	3.3036740000000000
W	1.3559600000000001	32.7713170000000034	3.3256480000000002
W	-0.2254140000000000	35.6185270000000003	3.3569870000000002
W	-1.6937480000000000	38.5158429999999967	3.3734820000000001
W	24.3751180000000005	-0.8866650000000000	3.5094129999999999
W	22.1392020000000009	1.6250610000000001	3.3544420000000001
W	20.4508180000000017	4.3060190000000000	3.2967689999999998
W	18.7922930000000008	7.1021939999999999	3.2794349999999999
W	17.1476110000000013	9.9383970000000001	3.2646530000000000
W	15.5109080000000006	12.7779150000000001	3.2609919999999999
W	13.8743289999999995	15.6148659999999992	3.2659690000000001
W	12.2375670000000003	18.4486020000000011	3.2696299999999998
W	10.6038730000000001	21.2790479999999995	3.2682340000000001
W	8.9737310000000008	24.1098159999999986	3.2640229999999999
W	7.3439969999999999	26.9433469999999993	3.2640359999999999
W	5.7099140000000004	29.7842689999999983	3.2733490000000001
W	2.4638309999999999	35.4880350000000035	3.3097880000000002
W	4.0741540000000001	32.6404489999999967	3.2914800000000000
W	0.9547450000000000	38.2699110000000005	3.3322940000000001
W	-0.1005090000000000	41.3843350000000001	3.5086179999999998
W	27.5408189999999991	-0.8832380000000000	3.5738259999999999
W	28.7834450000000004	1.6216219999999999	3.5337550000000002
W	26.0719759999999994	1.6625360000000000	3.5028060000000001
W	24.3414609999999989	4.9271250000000002	3.5122969999999998
W	22.7571310000000011	7.6532470000000004	3.5087570000000001
W	21.1416530000000016	10.4119030000000006	3.4802000000000000

W	19.518080000000012	13.216796000000004	3.4676390000000001
W	17.8867079999999987	16.0487390000000012	3.4678650000000002
W	16.2522200000000012	18.8875880000000009	3.4716119999999999
W	14.6226350000000007	21.7158240000000013	3.4743860000000000
W	12.9982070000000007	24.5340929999999986	3.4740799999999998
W	11.3714420000000000	27.3534679999999994	3.4729980000000000
W	9.7417040000000004	30.1765630000000016	3.4757330000000000
W	8.1162910000000004	33.0043039999999976	3.4866429999999999
W	6.5032189999999996	35.8326860000000025	3.5072820000000000
W	4.8950790000000000	38.6557919999999982	3.5216400000000001
W	3.1707999999999998	41.5292699999999968	3.5273639999999999
W	1.3343700000000001	43.9454459999999969	3.6653940000000000
W	30.6852739999999997	-0.9029550000000000	3.6888920000000001
W	27.1302349999999990	4.4825299999999997	3.3784100000000001
W	25.5413050000000013	7.3828750000000003	3.4004750000000001
W	23.9218750000000000	10.1640540000000001	3.4029720000000001
W	22.2946360000000006	12.9541699999999995	3.3858739999999998
W	20.6611830000000012	15.7740530000000003	3.3770859999999998
W	19.0264780000000009	18.6088309999999986	3.3795910000000000
W	17.3982680000000016	21.4382750000000009	3.3869060000000002
W	15.7753329999999998	24.2567559999999993	3.3912360000000001
W	14.1518979999999992	27.0721460000000000	3.3900899999999998
W	12.5246300000000002	29.8917819999999992	3.3881579999999998
W	9.2802450000000007	35.5361059999999966	3.3983629999999998
W	10.8992540000000009	32.7138840000000002	3.3910160000000000
W	7.6603070000000004	38.3609650000000002	3.3943159999999999
W	6.0362929999999997	41.1654880000000034	3.3921380000000001
W	4.4074910000000003	43.9428740000000033	3.5043820000000001
W	3.2031269999999998	47.2221440000000001	3.6784599999999998
W	33.9390569999999983	-0.8176030000000000	3.8801120000000000
W	35.3896099999999976	1.6951200000000000	3.9942910000000000
W	32.7033640000000005	1.5789310000000001	3.7406869999999999
W	31.0624150000000014	4.9812409999999998	3.6547109999999998

W	29.538709999999982	7.7920100000000003	3.6114160000000002
W	27.941639999999996	10.604212999999997	3.6108240000000000
W	26.311813999999983	13.413748999999993	3.6183580000000002
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W	23.044820999999989	19.023067000000011	3.6323590000000001
W	21.418255999999995	21.845355999999989	3.6370700000000000
W	19.794868999999985	24.675929000000000	3.6380580000000000
W	18.166129000000015	27.505482000000007	3.6368399999999999
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W	14.904806000000007	33.158175000000000	3.6388479999999999
W	13.281131999999995	35.980493000000027	3.6420100000000000
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W	17.698359000000000	32.870167999999996	3.6584690000000002
W	14.464456000000002	38.510382999999974	3.6725569999999998
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W	11.192021000000004	44.106309000000031	3.5741830000000001
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Se	14.1831259999999997	13.9088759999999994	1.4195629999999999
Se	12.5495599999999996	16.7415120000000002	1.4236020000000000
Se	10.9165960000000002	19.5701539999999987	1.4227719999999999
Se	9.2848459999999999	22.3988569999999996	1.4184140000000001
Se	7.6513460000000002	25.2300709999999988	1.4164159999999999
Se	6.0121890000000002	28.0645039999999995	1.4241230000000000
Se	4.3674340000000003	30.9042479999999991	1.4435610000000001
Se	2.5898450000000000	31.6185490000000016	5.1734669999999996
Se	0.9957410000000000	34.4560600000000008	5.1990939999999997
Se	-0.5809280000000000	37.3335170000000005	5.2323009999999996
Se	-2.5322779999999998	40.5648740000000032	4.2743050000000000
Se	6.0985889999999996	31.8462290000000010	4.7764579999999999
Se	4.4804709999999996	34.6773590000000027	4.8063209999999996
Se	2.8922330000000001	37.4944559999999996	4.8702160000000001
Se	1.3185990000000001	40.2976170000000025	5.0559149999999997
Se	-0.9252450000000000	43.4764290000000031	4.5248749999999998
Se	-1.0591500000000000	33.5675790000000021	2.4224450000000002
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Se	25.7198519999999995	3.6097570000000001	5.2226119999999998
Se	24.1199359999999992	6.5688209999999998	5.3782470000000000
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Se	20.8376769999999993	12.1171720000000001	5.3175179999999997
Se	19.2111820000000009	14.9267830000000004	5.3046829999999998
Se	17.5767400000000009	17.7556620000000009	5.3059510000000003
Se	15.9413820000000008	20.5867870000000011	5.3134870000000003
Se	14.3107179999999996	23.4122960000000013	5.3178999999999998
Se	12.6839270000000006	26.2346959999999996	5.3161250000000004
Se	11.0591849999999994	29.0568190000000008	5.3141010000000000
Se	32.3554180000000002	-2.5694300000000001	4.6331009999999999
Se	30.6533920000000002	0.8731400000000000	5.2800219999999998
Se	29.0924660000000017	3.7445240000000002	4.9888130000000004
Se	27.5459309999999995	6.5890890000000004	4.8817579999999996
Se	25.9374539999999989	9.4594039999999993	4.9299800000000003
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Se	15.8817959999999996	16.7872300000000010	1.9602980000000001
Se	14.2460719999999998	19.6140770000000018	1.9613240000000001
Se	12.6142360000000000	22.4358289999999982	1.9588250000000000
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Se	9.3595760000000006	28.0852040000000009	1.9564790000000001

Se	7.730439999999998	30.9161940000000008	1.9635080000000000
Se	29.2189380000000014	-0.2157480000000000	1.7805800000000001
Se	27.5148650000000004	2.7150099999999999	1.6398530000000000
Se	25.823499999999992	5.6368929999999997	1.5640710000000000
Se	24.220611999999991	8.4626330000000003	1.5543629999999999
Se	22.6076920000000001	11.2537660000000006	1.5450670000000000
Se	20.9786870000000008	14.0652779999999993	1.5397609999999999
Se	19.3424680000000002	16.8953050000000005	1.5405560000000000
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Se	16.083733999999998	22.5538600000000002	1.5447489999999999
Se	14.4609570000000005	25.3740629999999996	1.5454220000000001
Se	12.8348410000000008	28.1954080000000005	1.5454730000000001
Se	11.204076999999998	31.0198870000000007	1.5472390000000000
Se	9.4368800000000004	31.8779290000000017	5.3192009999999996
Se	7.821089999999999	34.7009820000000033	5.3343959999999999
Se	6.2141690000000001	37.5371099999999984	5.3505630000000002
Se	4.5878629999999996	40.4064460000000025	5.3258450000000002
Se	2.8310909999999998	43.2375060000000033	5.4350430000000003
Se	0.8569720000000000	46.3480539999999976	4.2699009999999999
Se	12.8916810000000002	31.9905539999999995	4.9183310000000002
Se	11.2707020000000000	34.8134190000000032	4.9235139999999999
Se	9.6515660000000008	37.6441919999999968	4.9233789999999997
Se	8.0243830000000003	40.4730709999999974	4.9253439999999999
Se	6.3492660000000001	43.2462340000000012	5.0006430000000002
Se	6.1049759999999997	33.7492250000000027	1.9805159999999999
Se	4.4982049999999996	36.5693669999999997	1.9961549999999999
Se	2.9160720000000002	39.4031680000000009	2.0152230000000002
Se	1.3898040000000000	42.3425340000000006	1.7591230000000000
Se	9.5741370000000003	33.8432749999999984	1.5543060000000000
Se	7.9483470000000001	36.6596079999999986	1.5620630000000000
Se	6.3125809999999998	39.4745810000000006	1.5578120000000000
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Se	35.581158999999995	-2.438982999999999	5.161798000000001
Se	33.984487999999989	0.750996000000000	5.798598000000001
Se	32.380313999999985	3.652416999999998	5.397164000000001
Se	30.859977000000007	6.666812000000002	5.497238000000003
Se	29.257242999999990	9.480135999999999	5.462862999999996
Se	27.635501000000014	12.292818999999997	5.468426000000000
Se	25.993769000000003	15.095045000000007	5.483625000000000
Se	24.351516000000002	17.897814000000003	5.492129000000003
Se	22.718572999999992	20.713847999999987	5.495312000000002
Se	21.093744000000009	23.541712000000004	5.494684000000003
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Se	17.837710999999988	29.200659999999992	5.491075000000004
Se	38.892730000000002	-2.050873999999999	3.320383000000001
Se	37.565004000000018	0.925711000000000	5.327417999999998
Se	36.099392000000017	3.847306000000001	4.834435000000000
Se	34.619473999999967	6.786003000000000	4.504477999999998
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Se	31.373326999999997	12.545016000000004	4.596955000000003
Se	29.736050999999998	15.383516999999994	4.620044000000000
Se	28.084440000000007	18.191686000000007	4.664206000000001
Se	26.457377000000010	21.003184000000010	4.662596999999999
Se	24.820806999999985	23.811260999999982	4.680842000000002
Se	23.206976000000009	26.640170000000012	4.651545999999997
Se	21.564682999999987	29.458085000000005	4.676788000000002
Se	32.423395999999968	-0.276004000000000	1.940762000000001
Se	30.835718000000000	2.745956000000001	2.295573999999998
Se	29.173372000000005	5.663115999999996	2.092117000000000
Se	27.570765999999990	8.504827999999998	2.090552999999999
Se	25.943863000000003	11.319608000000006	2.106580999999998
Se	24.318041000000009	14.127903999999991	2.104445000000001
Se	22.690273000000012	16.943784999999983	2.105979000000000
Se	21.061551000000015	19.767606000000007	2.112115000000002
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Se	16.178729000000006	28.243397000000016	2.120315999999999
Se	14.548700999999994	31.069150000000005	2.119561000000000
Se	35.767890000000013	-0.139954000000000	2.130093000000000
Se	34.223827999999975	2.802141000000002	2.017544000000000
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Se	27.919737999999988	14.339035000000009	1.761908000000000
Se	26.291062000000002	17.155394000000011	1.782194000000001
Se	24.659288000000001	19.971022000000014	1.791705000000001
Se	23.028280999999998	22.789573000000007	1.791504999999999
Se	21.396031000000007	25.609165999999983	1.784160000000000
Se	19.770043000000011	28.432082999999987	1.779660000000000
Se	18.143377999999985	31.253336000000009	1.779741000000000
Se	16.205269999999987	32.024800999999965	5.493903000000004
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Se	12.962348000000004	37.675618000000001	5.501900000000000
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Se	9.778570999999995	43.324375000000034	5.507593000000000
Se	19.950665999999982	32.291952999999995	4.651859000000000
Se	18.308033999999993	35.105687000000032	4.695433000000004
Se	16.710889000000017	37.943182000000002	4.657976999999998
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Se	13.431675000000003	43.620710000000025	4.601765999999996
Se	12.920721000000003	33.893391999999986	2.120448000000001
Se	11.297442999999995	36.715198999999984	2.119053000000001
Se	9.676838000000001	39.531055000000021	2.102549999999999
Se	8.053824000000005	42.320158999999968	2.077604000000000
Se	6.364372000000004	45.185308999999966	2.247657999999999
Se	16.525231999999990	34.075763000000020	1.788103000000000
Se	14.906757000000007	36.892960000000022	1.794567000000000
Se	13.295802000000001	39.700009999999989	1.787538000000001

Se	11.634162999999991	42.465755000000015	1.7463569999999999
Se	9.8768360000000008	45.2164789999999996	1.7199469999999999
Se	8.1127649999999996	48.0481229999999968	1.8275060000000001
Se	6.2651380000000003	50.813251000000011	1.8806799999999999
Se	4.6217519999999999	48.029119000000014	1.8132280000000001
Se	11.7498760000000004	46.4986760000000032	4.3752139999999997
Se	9.9026200000000006	49.2327439999999967	4.6574140000000002
Se	8.0453299999999999	52.0146080000000026	4.9878119999999999
Se	7.9088909999999997	46.1628270000000001	5.3173570000000003
Se	6.1625569999999996	49.0677779999999970	5.5921159999999999
Se	4.1016490000000001	51.9897589999999994	4.8685159999999996
Se	4.6117070000000000	46.0969139999999982	5.2185689999999996
Se	2.4038689999999998	49.2703080000000000	4.6756650000000004
Se	6.1124400000000003	54.5093510000000023	2.8339020000000001

$W_{105}Se_{210}$; $E_{tot} = -61\,508\,149.075\,138\,38$ eV; $E_{rel} = 17.137\,321\,342\,8$ meV/f.u.

W	20.8969769999999997	-0.8651890000000000	3.4378129999999998
W	19.1419819999999987	1.8501350000000001	3.4172050000000000
W	17.4571639999999988	4.6217280000000001	3.3862860000000001
W	15.8099100000000004	7.4411940000000003	3.3514759999999999
W	14.1780659999999994	10.2665179999999996	3.3185899999999999
W	12.5530050000000006	13.0924090000000000	3.2959309999999999
W	10.9290570000000002	15.9190939999999994	3.2961559999999999
W	9.3133499999999998	18.7497240000000005	3.3162850000000001
W	7.7271400000000003	21.5808339999999994	3.3499270000000001
W	6.1825299999999999	24.3995929999999994	3.3734139999999999
W	4.6480110000000003	27.2370030000000014	3.2617240000000001
W	3.0593819999999998	30.1740560000000002	2.9817399999999998
W	1.4042319999999999	32.8225860000000011	2.9414030000000002
W	24.2191669999999988	-1.0144869999999999	3.3729589999999998
W	22.0450510000000008	1.5316740000000000	3.3505889999999998
W	20.3510710000000010	4.2390900000000000	3.3243350000000000

W	18.6636990000000011	7.0616000000000003	3.3041190000000000
W	16.9996119999999991	9.9198660000000007	3.2820649999999998
W	15.3632390000000001	12.7723289999999992	3.2718820000000002
W	13.7397150000000003	15.6098239999999997	3.2748560000000002
W	12.1192510000000002	18.4377700000000004	3.2859769999999999
W	10.5067140000000006	21.2704759999999986	3.2994050000000001
W	8.9232399999999998	24.0964129999999983	3.3065199999999999
W	7.3994460000000002	26.9067299999999996	3.2768730000000001
W	5.7530340000000004	30.3017900000000004	3.2093959999999999
W	4.5025919999999999	32.6853210000000018	3.0818219999999998
W	27.3714340000000007	-1.0666359999999999	3.3652950000000001
W	28.9487319999999997	1.1718519999999999	3.5594359999999998
W	25.7949570000000001	1.1996590000000000	3.4821200000000001
W	24.2913929999999993	4.8435920000000001	3.4464670000000002
W	22.6408260000000006	7.5809680000000004	3.4800130000000000
W	20.9995650000000005	10.3629840000000009	3.4527120000000000
W	19.3730070000000012	13.1897380000000002	3.4490690000000002
W	17.7523650000000011	16.0344480000000011	3.4607600000000001
W	16.1345400000000012	18.8719360000000016	3.4680240000000002
W	14.5240790000000004	21.6816129999999987	3.4646400000000002
W	12.9234130000000000	24.4919620000000009	3.4706969999999999
W	11.3365760000000009	27.4211920000000013	3.4903080000000002
W	9.6863019999999995	30.2615809999999996	3.3557039999999998
W	7.7772699999999997	32.7796250000000029	3.2301579999999999
W	30.5226569999999988	-1.0914640000000000	3.6061369999999999
W	27.5226720000000000	4.8717370000000004	3.3656600000000001
W	25.4382120000000000	7.3374410000000001	3.3472040000000001
W	23.7747589999999995	10.0955490000000001	3.3216850000000000
W	22.1425759999999983	12.9054920000000006	3.3265330000000000
W	20.5232899999999994	15.7413779999999992	3.3406430000000000
W	18.9070169999999997	18.5851579999999998	3.3571819999999999
W	17.2957619999999999	21.4101089999999985	3.3611819999999999
W	15.6933279999999993	24.1988899999999987	3.3398379999999999

W	14.1202260000000006	26.971417999999999	3.322986999999999
W	12.4020700000000001	30.2092840000000002	3.320053999999999
W	10.9207529999999995	32.7609390000000005	3.2611640000000000
W	34.3767580000000024	-1.043021999999999	3.9274410000000000
W	35.4303129999999982	1.6284940000000001	3.619553999999999
W	32.7414240000000021	1.6291350000000000	3.6234050000000000
W	30.7161830000000009	4.8157110000000003	3.469666999999999
W	29.3676649999999988	7.3715650000000004	3.4488310000000002
W	27.7002540000000010	10.6524129999999992	3.508719999999999
W	26.1417280000000005	13.4007740000000002	3.5556190000000001
W	24.5418909999999997	16.1750849999999993	3.571518999999999
W	22.9281450000000007	18.9957460000000005	3.588341999999999
W	21.3051819999999985	21.8433969999999995	3.5966600000000000
W	19.6792419999999986	24.6885149999999989	3.5865980000000000
W	18.0583540000000013	27.5115850000000002	3.5455450000000002
W	16.4133420000000001	30.2776360000000011	3.4301010000000001
W	14.0533590000000004	32.8514479999999978	3.2103090000000001
W	37.5221540000000005	-0.8991770000000000	3.8341870000000000
W	33.7289349999999999	4.3284360000000000	3.4246590000000001
W	32.1123100000000008	7.2364119999999996	3.4210090000000002
W	30.4896749999999983	10.1698880000000003	3.3508100000000001
W	28.9295900000000010	13.0945879999999999	3.418232999999999
W	27.3284340000000014	15.8962289999999999	3.4623480000000000
W	25.7084879999999991	18.7018209999999989	3.473666999999999
W	24.0773790000000005	21.5409720000000000	3.474731999999999
W	22.4427629999999994	24.3946719999999999	3.465469999999999
W	20.8067150000000005	27.2444920000000010	3.4315730000000002
W	19.1618649999999988	30.0913930000000001	3.3523250000000000
W	17.5330189999999995	32.9211859999999987	3.008703999999999
W	40.5797919999999976	-0.8702550000000000	3.9023010000000000
W	42.0198600000000013	1.7079040000000001	3.897708999999999
W	39.3620170000000016	1.6023419999999999	3.7576540000000000
W	37.6473579999999970	4.9793930000000000	3.6935730000000002

W	36.0785880000000034	7.7178120000000003	3.6298740000000000
W	34.4985220000000012	10.5405350000000002	3.5774640000000000
W	32.9336830000000020	13.4165189999999992	3.5803950000000002
W	31.3433880000000009	16.2880409999999998	3.6254860000000000
W	29.7255429999999983	19.1340809999999983	3.6532070000000001
W	28.0904269999999983	21.9673589999999983	3.6617199999999999
W	26.4469579999999986	24.8082199999999986	3.6559110000000001
W	24.7955010000000016	27.6628569999999989	3.6414540000000000
W	23.1327959999999990	30.4941190000000013	3.6291430000000000
W	21.4742029999999993	33.2966049999999996	3.6293180000000000
W	43.6621900000000025	-0.9626240000000000	3.9164810000000001
W	40.4188380000000009	4.6591339999999999	3.6789410000000000
W	38.8402770000000004	7.4807670000000002	3.5835370000000002
W	37.2640110000000035	10.2641299999999998	3.5798429999999999
W	35.7057760000000002	13.0951290000000000	3.5681470000000002
W	34.1338810000000024	15.9500609999999998	3.5830460000000000
W	32.5375640000000033	18.8006589999999996	3.6120739999999998
W	30.9147019999999983	21.6338420000000013	3.6282169999999998
W	29.2842289999999998	24.4500500000000009	3.6229320000000000
W	27.6607079999999996	27.2618970000000012	3.6080410000000001
W	26.0409550000000003	30.0737729999999992	3.6123069999999999
W	22.8578270000000003	35.4416569999999993	3.7824110000000002
W	24.4125100000000010	32.8374760000000023	3.6787380000000001
Se	22.1953020000000016	-2.5908790000000002	4.3890900000000004
Se	20.4735469999999999	0.7219520000000000	5.2802730000000002
Se	18.7477379999999982	3.4934360000000000	5.2522250000000001
Se	17.0637079999999983	6.2846229999999998	5.2183260000000002
Se	15.4120690000000007	9.0991450000000000	5.1899879999999996
Se	13.7717840000000002	11.9140119999999996	5.1668940000000001
Se	12.1436220000000006	14.7284229999999994	5.1587280000000000
Se	10.5277860000000008	17.5477190000000007	5.1700130000000000
Se	8.9316089999999999	20.3743720000000010	5.1981000000000002
Se	7.3655239999999997	23.2196899999999999	5.2281420000000001

Se	5.8293179999999998	26.1258219999999994	5.1859370000000000
Se	4.2518279999999997	29.0855539999999984	4.9518380000000004
Se	25.6270179999999996	-2.7829310000000000	4.2344340000000003
Se	23.9260300000000008	0.6567000000000000	5.1086210000000003
Se	22.3651780000000002	3.6024690000000001	4.8476939999999997
Se	20.6676110000000008	6.3894520000000004	4.7997019999999999
Se	19.0065929999999987	9.2109419999999993	4.7663900000000003
Se	17.3677799999999998	12.0442300000000007	4.7604899999999999
Se	15.7419250000000002	14.8795889999999993	4.7660840000000002
Se	14.1231240000000007	17.7118959999999994	4.7752150000000002
Se	12.5124490000000002	20.5421440000000004	4.7829040000000003
Se	10.9060380000000006	23.3802389999999995	4.8037549999999998
Se	9.3158550000000009	26.2351260000000011	4.8099629999999998
Se	7.6483179999999997	29.1432679999999991	4.6291560000000000
Se	18.7573079999999983	-0.7722850000000000	2.5006510000000000
Se	16.9355399999999996	2.1605010000000000	2.4831140000000000
Se	15.2464200000000005	5.0429909999999998	2.4322100000000000
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Se	10.3177590000000006	13.6281130000000008	2.3199120000000000
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Se	7.0613109999999999	19.3388309999999990	2.3559980000000000
Se	5.4683729999999997	22.2245770000000000	2.3524750000000001
Se	3.8327990000000001	25.0977280000000000	2.4709870000000000
Se	2.3376999999999999	28.0200159999999983	2.1649530000000001
Se	0.8716090000000000	30.9280019999999993	1.6567130000000001
Se	22.4893250000000009	-0.3562840000000000	1.5982810000000001
Se	20.6309959999999997	2.4899589999999998	1.5041180000000001
Se	18.9453700000000005	5.3186879999999999	1.4906820000000001
Se	17.2974539999999983	8.1762859999999993	1.4678880000000001
Se	15.6550609999999999	11.0405270000000009	1.4416650000000000
Se	14.0269790000000008	13.8956990000000005	1.4291650000000000
Se	12.4013659999999994	16.7350080000000005	1.4335310000000001

Se	10.7815770000000004	19.5675939999999997	1.4493720000000001
Se	9.1771809999999991	22.3990690000000008	1.4592950000000000
Se	7.5813959999999998	25.2177119999999988	1.4344410000000001
Se	6.0565189999999998	28.2264699999999991	1.5491820000000001
Se	4.4462479999999998	31.1158269999999995	1.1628400000000001
Se	2.6850939999999999	32.0184259999999981	4.8419390000000000
Se	6.0523709999999999	32.1620530000000002	5.0009860000000002
Se	-0.4598650000000000	33.9111350000000016	3.6447210000000001
Se	2.8437420000000002	34.2959290000000010	1.7961100000000001
Se	29.0081190000000007	-2.8180380000000000	4.3490479999999998
Se	27.3309770000000007	0.4723320000000000	5.3772080000000004
Se	25.8002590000000005	3.4648829999999999	4.8929229999999997
Se	24.0369929999999989	6.4740789999999997	5.3157969999999999
Se	22.3482109999999992	9.2822350000000000	5.2988910000000002
Se	20.7066589999999984	12.0810720000000007	5.2813319999999999
Se	19.0808800000000005	14.9063459999999992	5.2850510000000002
Se	17.4567720000000008	17.7446349999999988	5.2989240000000004
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Se	12.6696059999999999	26.2667690000000000	5.2905709999999999
Se	11.0021249999999995	29.1963310000000007	5.2337559999999996
Se	32.4564049999999966	-2.4518080000000002	4.6847580000000004
Se	30.7603000000000009	0.6173600000000000	5.2890009999999998
Se	29.0007179999999991	3.4644889999999999	4.9147580000000000
Se	27.4049210000000016	6.5906690000000001	5.0654519999999996
Se	25.7776950000000014	9.4307119999999998	4.8697369999999998
Se	24.1561020000000006	12.2137619999999991	4.8452240000000000
Se	22.5329690000000014	15.0157249999999998	4.8519699999999997
Se	20.9115169999999999	17.8414290000000015	4.8678549999999996
Se	19.2910550000000001	20.6839830000000013	4.8830429999999998
Se	17.6656939999999985	23.5256040000000013	4.8804350000000003
Se	16.0523400000000009	26.3451640000000005	4.8652519999999999
Se	14.3760739999999991	29.2122610000000016	4.7187409999999996

Se	25.802265999999995	-0.471216000000000	1.504087000000000
Se	24.094004999999992	2.599480999999999	2.048751999999999
Se	22.312039999999997	5.415068999999999	1.965541000000000
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Se	10.9059320000000000	25.293490999999995	2.009770000000001
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Se	7.782309999999998	30.999210999999990	1.642304999999999
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Se	20.812139999999994	14.035157999999991	1.501323000000000
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Se	17.577688999999995	19.701406999999997	1.522747000000001
Se	15.9621110000000002	22.502577999999997	1.506412000000001
Se	14.325613999999998	25.303343999999992	1.480172000000000
Se	12.7298010000000001	28.270610000000013	1.608717000000000
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Se	12.604684999999999	32.138930999999995	5.094107000000002
Se	6.066043999999998	34.452700000000001	2.341133999999998
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Se	35.8942890000000006	-2.706383000000002	4.740622000000001
Se	34.0960880000000017	0.680111000000000	5.613340000000000
Se	32.250835999999996	3.545058000000000	5.238192999999999
Se	30.7270140000000005	6.446951000000003	5.391949000000003
Se	29.0841010000000004	9.314120000000008	5.197570999999999

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Se	25.880413000000008	15.080064999999994	5.414909999999999
Se	24.260601000000012	17.883665000000006	5.418523999999997
Se	22.637862999999994	20.719529999999989	5.422037999999997
Se	21.006926000000000	23.574262000000009	5.420100999999998
Se	19.373785000000016	26.436111000000004	5.395834999999999
Se	17.710073000000013	29.318564999999995	5.315058999999998
Se	39.064242999999976	-2.594557000000000	4.809051000000002
Se	37.367615999999982	0.906102000000000	5.365429999999999
Se	35.702236999999967	3.765782999999999	5.056966000000001
Se	34.101681999999967	6.520069999999996	4.936817999999997
Se	32.502648000000006	9.383065000000002	4.891129000000003
Se	30.944552999999991	12.252090000000008	4.879184000000004
Se	29.349046000000013	15.153876999999996	4.963696999999998
Se	27.727827999999988	17.992640000000015	4.985221000000001
Se	26.093416999999988	20.817513000000017	4.984109000000001
Se	24.452064000000000	23.658122999999998	4.977723000000001
Se	22.799717000000011	26.519261000000002	4.959484999999999
Se	21.104773999999990	29.390955000000017	4.921636000000003
Se	32.535355000000027	-0.510473000000000	2.102725000000000
Se	30.741378000000010	2.499763000000002	2.179594999999999
Se	29.130402000000001	5.561473000000003	1.601420000000001
Se	27.441062999999998	8.471356000000001	2.067994000000001
Se	25.761981999999997	11.300141000000000	1.985567000000001
Se	24.153994000000009	14.084645999999993	2.030396999999998
Se	22.537675000000001	16.907130999999997	2.055130999999998
Se	20.922481000000012	19.743528999999988	2.075940000000001
Se	19.301300000000012	22.577424000000006	2.077411999999998
Se	17.678428000000003	25.405322000000017	2.048639999999998
Se	16.056205999999995	28.208247000000001	1.963924000000000
Se	14.368216000000003	31.051358000000005	1.711900000000000
Se	35.857607999999990	-0.331917000000000	1.994571000000001
Se	34.106768999999999	2.545436000000000	1.689109999999999

Se	32.407868999999980	5.453674999999996	1.6227210000000001
Se	30.809167999999997	8.419470999999997	1.5818129999999999
Se	29.1741670000000006	11.3625030000000002	1.5588460000000000
Se	27.5923330000000000	14.2057640000000003	1.5962499999999999
Se	25.9938910000000014	17.0086690000000011	1.6251720000000001
Se	24.372911999999995	19.829799999999988	1.6430800000000001
Se	22.742709999999989	22.6694640000000014	1.6453480000000000
Se	21.1119740000000000	25.5109190000000012	1.6248940000000001
Se	19.4828860000000006	28.3534620000000004	1.5708789999999999
Se	17.759306999999997	31.1127770000000012	1.4097590000000000
Se	15.9346270000000008	32.3395330000000030	4.9280819999999999
Se	19.3116790000000016	32.3302270000000007	4.8120320000000003
Se	12.5558460000000007	34.5074350000000010	2.3257040000000000
Se	15.846126999999992	34.5426300000000026	2.3974289999999998
Se	42.277008999999996	-2.4788540000000001	5.0860029999999998
Se	40.698774999999977	0.7412540000000000	5.7683590000000002
Se	39.0349640000000022	3.6680779999999999	5.4076789999999999
Se	37.455368999999975	6.6649060000000002	5.5295220000000000
Se	35.8030380000000008	9.4326889999999999	5.4529249999999996
Se	34.2347850000000022	12.2579130000000003	5.4225209999999997
Se	32.664439999999990	15.1182090000000002	5.4438129999999996
Se	31.0658870000000000	17.9916720000000012	5.4804890000000004
Se	29.435023999999985	20.8444439999999993	5.4996179999999999
Se	27.7930540000000015	23.689493999999998	5.4972870000000000
Se	26.1505070000000011	26.540853999999995	5.4822210000000000
Se	24.4964280000000016	29.3920400000000015	5.4778140000000004
Se	45.5181100000000001	-2.0007830000000002	3.1234810000000000
Se	44.2192080000000018	0.9287339999999999	5.1959869999999997
Se	42.7159350000000018	3.8769220000000000	4.7576700000000001
Se	41.2082860000000011	6.8177789999999998	4.4530919999999998
Se	39.520426999999980	9.6515310000000003	4.6195519999999997
Se	37.950552999999993	12.4926060000000003	4.5628880000000001
Se	36.3904550000000029	15.3471109999999999	4.5290059999999999

Se	34.7881130000000027	18.2131550000000004	4.5633590000000002
Se	33.1617409999999992	21.0843260000000008	4.5871919999999999
Se	31.5161489999999986	23.9390420000000006	4.6004019999999999
Se	29.8836060000000003	26.7897740000000013	4.5719050000000001
Se	28.2738289999999992	29.6408389999999997	4.5126470000000003
Se	39.0702649999999991	-0.2210480000000000	1.9699030000000000
Se	37.4534859999999981	2.7307760000000001	2.3357060000000001
Se	35.7435389999999984	5.5624880000000001	2.1270080000000000
Se	34.1207539999999980	8.4002479999999995	2.0999070000000000
Se	32.5293559999999999	11.3163769999999992	2.0802030000000000
Se	30.9414620000000014	14.2040989999999994	2.1029450000000001
Se	29.3343039999999995	17.0404699999999991	2.1505470000000000
Se	27.7146569999999990	19.8631819999999983	2.1678470000000001
Se	26.0844689999999986	22.6928629999999991	2.1691470000000002
Se	24.4520860000000013	25.5380770000000012	2.1579860000000002
Se	22.8197270000000003	28.3981749999999984	2.1208770000000001
Se	21.1956980000000001	31.3008610000000012	2.0578919999999998
Se	42.3514529999999993	-0.1126560000000000	2.0647120000000001
Se	40.8145659999999992	2.8431129999999998	1.9732120000000000
Se	39.2041550000000001	5.7566910000000000	1.7702110000000000
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Se	32.9332530000000006	17.1712279999999993	1.7362759999999999
Se	31.3202449999999999	20.0004950000000008	1.7605290000000000
Se	29.6906660000000002	22.8123010000000015	1.7656099999999999
Se	28.0514149999999987	25.6196120000000001	1.7559810000000000
Se	26.4154869999999988	28.4347220000000007	1.7485360000000001
Se	24.8020040000000002	31.2567909999999998	1.7599290000000001
Se	22.7419699999999985	32.2142860000000013	5.4867610000000004
Se	26.6215420000000016	32.4642550000000014	4.5663879999999999
Se	24.6699920000000006	35.0520339999999990	5.2025259999999998
Se	19.3993029999999997	34.2334049999999976	2.1956340000000001

Se	23.262513999999995	34.150613999999974	1.7632310000000000
Se	20.801867999999989	35.6340160000000026	4.8547110000000000

$W_{105}Se_{210}$; $E_{tot} = -61\,508\,149.347\,597\,52$ eV; $E_{rel} = 14.542\,472\,390\,4$ meV/f.u.

W	20.699018999999998	-0.8685420000000000	3.2590990000000000
W	19.034735999999988	1.8955569999999999	3.4338030000000002
W	17.347480999999984	4.6572449999999996	3.4175730000000000
W	15.683192999999993	7.4798450000000001	3.3767429999999998
W	14.0605750000000000	10.3444699999999994	3.3451480000000000
W	12.4639860000000002	13.2137949999999993	3.3306399999999998
W	10.906515999999999	16.0859150000000000	3.3309359999999999
W	9.402836999999999	18.939654999999984	3.3228730000000000
W	7.863051999999997	21.7829610000000002	3.2119719999999998
W	6.2542220000000004	24.716855999999999	2.9700920000000002
W	4.5986510000000003	27.372831999999989	2.9236320000000000
W	24.2055240000000005	-1.3810810000000000	3.2370109999999999
W	21.8374600000000001	1.6738270000000000	3.3167830000000000
W	20.142914999999986	4.3998290000000004	3.3617349999999999
W	18.482231999999998	7.193724999999997	3.3630439999999999
W	16.8485890000000005	10.0382140000000000	3.3500420000000002
W	15.2542380000000009	12.8935040000000001	3.3373940000000002
W	13.6839110000000002	15.7442430000000009	3.2995619999999999
W	12.1330550000000006	18.618497999999989	3.2458550000000002
W	10.6210710000000006	21.460409999999995	3.2083800000000000
W	8.9380860000000002	24.823458999999997	3.1148080000000000
W	7.728165999999999	27.2298860000000005	2.9486770000000000
W	27.015720999999992	-0.9327720000000000	3.4345889999999999
W	28.6839930000000010	1.9042669999999999	3.4208210000000001
W	25.9012810000000009	1.9111350000000000	3.3765399999999999
W	24.2073110000000007	4.8487629999999999	3.5363039999999999
W	22.4915750000000010	7.6477610000000000	3.5327809999999999
W	20.8457340000000002	10.4495410000000000	3.5168499999999998

W	19.246760999999993	13.2772810000000003	3.5315370000000001
W	17.700296999999991	16.1635570000000008	3.5403950000000002
W	16.0994160000000015	19.000599999999986	3.4002370000000002
W	14.565580999999999	21.475851999999997	3.2872640000000000
W	12.724983999999992	25.0066330000000008	3.2024249999999999
W	11.0945870000000006	27.260775999999999	3.1914549999999999
W	31.128493999999999	-1.2310120000000000	3.2580179999999999
W	27.304525999999992	4.3196380000000003	3.4148250000000000
W	25.2608940000000004	7.455982999999998	3.4135080000000002
W	23.6105310000000017	10.1802720000000004	3.4013439999999999
W	22.033294999999990	12.954511999999994	3.4117389999999999
W	20.510034999999985	15.729680000000001	3.4485649999999999
W	18.9128070000000008	19.073679999999995	3.4727830000000002
W	17.601303999999990	21.4502920000000010	3.4518909999999998
W	15.9499800000000008	25.1134860000000018	3.2636599999999998
W	14.328865999999997	27.3192100000000018	3.3234290000000000
W	33.9156550000000010	-0.9517660000000000	3.3412120000000001
W	35.5458830000000034	1.8300790000000000	3.4101309999999998
W	32.7543160000000029	1.5865910000000001	3.3426369999999999
W	30.4156820000000003	4.8922200000000000	3.5439099999999999
W	29.350384999999993	7.4674240000000003	3.4589370000000002
W	27.590987999999994	10.6844380000000001	3.5721569999999998
W	25.9725430000000017	13.425217999999992	3.6360920000000001
W	24.4364880000000007	16.265043999999996	3.6628069999999999
W	22.705097999999996	19.1692590000000003	3.5270269999999999
W	20.912580999999994	21.465623999999983	3.5799919999999998
W	19.223017999999997	25.1590750000000014	3.3463090000000002
W	17.551248999999985	27.398945999999987	3.3706480000000001
W	34.4384060000000005	4.409577999999998	3.3953530000000001
W	32.0993700000000004	7.665918999999997	3.5747650000000002
W	30.8240470000000002	10.1230790000000006	3.4957989999999999
W	28.718030999999999	13.1977460000000004	3.4937830000000001
W	27.215158999999999	15.847094999999995	3.5330189999999999

W	25.6260440000000003	19.2052769999999988	3.5586250000000001
W	24.1798509999999993	21.5515059999999998	3.6013440000000001
W	22.5202939999999998	25.1987670000000001	3.3964330000000000
W	20.7934079999999994	27.4465199999999996	3.4056259999999998
W	37.1865710000000007	4.6273020000000002	3.4566780000000001
W	36.1169000000000011	7.2780240000000003	3.4138549999999999
W	33.7071090000000027	10.4992450000000002	3.6124809999999998
W	32.6876809999999978	13.5057620000000007	3.6095709999999999
W	31.1310299999999991	16.3368129999999994	3.6654730000000000
W	29.4952949999999987	19.1241650000000014	3.6356139999999999
W	27.4532309999999988	21.5360370000000003	3.6473870000000002
W	25.8591209999999982	25.2200600000000001	3.4113620000000000
W	24.0560539999999996	27.4734410000000011	3.4290729999999998
W	38.8410190000000028	7.4348330000000002	3.4780080000000000
W	37.7773180000000011	10.1576850000000007	3.4107599999999998
W	35.3983029999999985	13.2855609999999995	3.5058769999999999
W	33.8567099999999996	16.0528100000000009	3.4398059999999999
W	32.2717140000000029	18.8312239999999989	3.4420030000000001
W	30.6649799999999999	21.5758979999999987	3.5153189999999999
W	29.1841819999999998	25.2124859999999984	3.3945870000000000
W	27.3376599999999996	27.5070459999999990	3.4351189999999998
W	40.4614690000000010	10.2546710000000001	3.4805450000000002
W	39.3494990000000016	12.9670579999999998	3.4103119999999998
W	37.8247959999999992	16.4355629999999984	3.4875710000000000
W	36.2753159999999966	19.2755499999999991	3.5029640000000000
W	34.6205539999999985	22.0497990000000001	3.4795150000000001
W	32.3865669999999994	25.1484370000000013	3.3855879999999998
W	30.6136750000000006	27.4808090000000007	3.4290289999999999
W	42.0006160000000008	13.1163340000000002	3.4683660000000001
W	40.5393740000000022	16.1511719999999990	3.3700980000000000
W	39.0035370000000015	18.9900510000000011	3.3135500000000002
W	37.4148550000000029	21.7742059999999995	3.3036150000000002
W	35.7389730000000014	24.5403950000000002	3.3437090000000000

W	33.8642210000000006	27.3518089999999994	3.4248750000000001
Se	22.2373389999999986	-2.2993999999999999	4.7605969999999997
Se	20.3941310000000016	0.6806650000000000	5.2199470000000003
Se	18.6008309999999994	3.5077060000000002	5.2880060000000002
Se	16.8962770000000013	6.3122509999999998	5.2575870000000000
Se	15.2478309999999997	9.1422220000000003	5.2223090000000001
Se	13.6403820000000007	11.9970040000000004	5.2013619999999996
Se	12.0852190000000004	14.8712529999999994	5.1933860000000003
Se	10.5975210000000004	17.7683280000000003	5.1810039999999997
Se	9.0621050000000007	20.6803719999999984	5.1264500000000002
Se	7.4838480000000001	23.6259289999999993	4.9095060000000004
Se	5.9367400000000004	26.6022460000000009	4.7937830000000003
Se	25.6569700000000012	-2.1268090000000002	5.1873259999999997
Se	23.8907820000000015	0.7512350000000000	4.6902410000000003
Se	22.1863859999999988	3.6539210000000000	4.8661040000000000
Se	20.5066060000000014	6.4686839999999997	4.8638529999999998
Se	18.8532399999999996	9.2975110000000001	4.8429390000000003
Se	17.2359809999999989	12.1394199999999994	4.8440300000000001
Se	15.6577620000000000	15.0002220000000008	4.8088470000000001
Se	14.1025379999999991	17.8643740000000015	4.7475470000000000
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Se	10.8534740000000003	23.7161320000000018	4.5243460000000004
Se	9.2883169999999993	26.6971960000000017	4.8838640000000000
Se	18.4687710000000003	-0.5077420000000000	2.4932189999999999
Se	16.8048649999999995	2.3542909999999999	2.4153660000000001
Se	15.0836150000000000	5.1967059999999998	2.4343430000000001
Se	13.4228790000000000	8.0715970000000006	2.4068600000000000
Se	11.8137310000000006	10.9611169999999998	2.3589709999999999
Se	10.2016240000000007	13.8378110000000003	2.3881000000000001
Se	8.6633399999999998	16.7547479999999993	2.3285410000000000
Se	7.0595489999999996	19.6322310000000009	2.4184009999999998
Se	5.5394319999999997	22.5439650000000000	2.1598549999999999
Se	4.0254490000000001	25.4416720000000005	1.7098780000000000

Se	2.745070000000001	28.455863999999983	3.662370000000001
Se	22.317689999999989	-0.202038000000000	1.601839000000000
Se	20.447338999999995	2.669235000000000	1.488715000000000
Se	18.786611000000006	5.473497000000001	1.522143999999999
Se	17.150327999999982	8.308659999999997	1.517029000000000
Se	15.541888999999994	11.168981999999997	1.496678000000000
Se	13.948404999999993	14.016391999999997	1.470288000000000
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Se	5.993831000000001	28.808522000000000	1.690411000000001
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Se	27.288730000000010	0.786323000000000	5.242638000000004
Se	25.614209999999999	3.641115000000001	5.237142000000004
Se	23.883659999999990	6.546829999999999	5.363747000000000
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Se	20.569396999999986	12.150185999999997	5.364722000000004
Se	19.007688000000017	15.010184999999999	5.372906000000004
Se	17.466751999999996	17.947029000000006	5.292306000000000
Se	15.885476999999998	20.800111999999986	5.255499000000004
Se	14.272221000000000	23.708804000000007	4.749635999999997
Se	12.630146999999991	26.750833000000001	5.115274999999996
Se	32.674492999999982	-2.128026999999999	5.185933000000003
Se	30.702456000000015	0.801984999999999	4.782948000000002
Se	28.994780999999997	3.669220999999998	5.245400000000001
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Se	23.993144999999984	12.246173999999999	4.959379000000002
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Se	19.200468999999982	20.849840000000004	5.321072000000000
Se	17.557565000000003	23.761146000000001	4.786899000000000

Se	15.9081480000000006	26.8629290000000012	5.2045329999999996
Se	25.6209859999999985	-0.0571760000000000	1.5888270000000000
Se	23.8759709999999998	2.7275730000000000	1.9628460000000001
Se	22.1672909999999987	5.5025729999999999	2.0578520000000000
Se	20.4700869999999995	8.3235550000000007	2.0211320000000002
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Se	17.2453630000000011	14.0515810000000005	2.0329890000000002
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Se	20.6752250000000011	14.0846789999999995	1.5657200000000000
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Se	15.9927720000000004	22.8311080000000004	1.8390409999999999
Se	14.3098379999999992	25.6985390000000002	1.3827460000000000
Se	12.5623509999999996	29.0225310000000007	2.4213600000000000
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Se	25.8039829999999988	17.1417420000000007	1.8255880000000000
Se	24.1522539999999992	19.9503179999999993	1.6150450000000001
Se	22.5137539999999987	22.8835020000000000	2.0854180000000002
Se	20.8886889999999994	25.7689500000000002	1.5373500000000000
Se	19.1904240000000001	29.0881749999999997	2.3871869999999999
Se	37.5934859999999986	6.2846440000000001	5.3201479999999997
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Se	32.4966599999999985	15.2057830000000003	5.4541009999999996
Se	30.8704689999999999	18.0823630000000009	5.4663190000000004
Se	29.1682279999999992	20.9200869999999988	5.4326520000000000
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Se	32.2987630000000010	11.4624740000000003	1.8545840000000000
Se	30.6786230000000018	14.2536869999999993	2.1091210000000000
Se	29.1060729999999985	17.0119439999999997	2.1309450000000001
Se	27.5343310000000017	19.8216070000000002	1.9044239999999999
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Se	34.1527370000000019	23.9691749999999999	5.0913839999999997
Se	32.2909879999999987	26.9495310000000003	5.2862140000000002
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Se	41.3883369999999999	18.2514329999999987	4.1685270000000001
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Se	36.0433000000000021	27.1089020000000005	4.3091239999999997
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Se	32.5150580000000033	22.8554199999999987	2.1117689999999998
Se	30.8125050000000016	25.8402120000000011	1.5465130000000000
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Se	36.0564499999999981	22.8939030000000017	1.4856900000000000
Se	34.2329349999999977	25.6972479999999983	1.6061289999999999
Se	32.6762200000000007	29.1130719999999990	2.4498310000000001
W	30.6924010000000003	-6.5247880000000000	3.2031239999999999
W	32.3217130000000026	-3.7303419999999998	3.3095420000000000
W	29.5585470000000008	-3.9870310000000000	3.1854030000000000
W	27.4703780000000002	-12.1718670000000007	2.9919060000000002
W	28.9391269999999992	-9.4036000000000008	2.9937520000000002
W	27.5038820000000008	-7.1548550000000004	3.1410730000000000
W	25.5500079999999983	-3.7389519999999998	3.2714010000000000
W	26.0062910000000009	-9.4561360000000008	3.0193889999999999

W	24.408000999999987	-6.8127230000000001	3.0846469999999999
W	22.7157680000000006	-4.1806320000000001	2.9731139999999998
Se	34.54736900000000033	-3.1969430000000001	2.2964289999999998
Se	32.9521519999999981	-6.1125520000000000	2.4378370000000000
Se	30.9238350000000004	-2.9525450000000002	1.3589460000000000
Se	31.1614140000000006	-8.9144620000000003	2.1330950000000000
Se	29.12920700000000010	-5.8460109999999998	1.4748220000000001
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Se	29.3779350000000008	-11.6998979999999992	1.7043349999999999
Se	27.43348200000000015	-8.7454450000000001	1.1319079999999999
Se	25.8914329999999993	-5.7870929999999996	1.5411090000000001
Se	24.0500779999999992	-3.0683850000000001	1.2775190000000001
Se	27.49889500000000010	-14.3012840000000008	3.7781440000000002
Se	25.4618639999999985	-11.7324929999999998	1.8289489999999999
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Se	22.03422700000000013	-6.3402289999999999	2.1855000000000002
Se	20.5285699999999984	-3.2501970000000000	2.2071779999999999
Se	29.3153919999999992	-7.7831910000000004	4.9122659999999998
Se	27.5165340000000000	-4.9327980000000000	4.5523959999999999
Se	27.5465400000000002	-10.6098750000000006	4.8448520000000004
Se	25.7835169999999998	-7.8185399999999996	4.9405250000000001
Se	24.0748029999999993	-5.0851340000000000	4.9128829999999999

W₁₀₅Se₂₁₀; $E_{tot} = -61\,508\,149.350\,902\,72$ eV; $E_{rel} = 14.510\,994\,295\,2$ meV/f.u.

W	19.4136479999999985	1.3328660000000001	3.2947229999999998
W	17.7857449999999986	4.1688000000000001	3.2792560000000002
W	16.1546050000000001	6.9987009999999996	3.2920110000000000
W	14.5007280000000005	9.8221319999999999	3.3221750000000001
W	12.8665269999999996	12.6493420000000008	3.3583840000000000
W	11.2909509999999997	15.4743239999999993	3.3728419999999999
W	9.6996219999999997	18.2936900000000016	3.2135159999999998

W	7.823576000000001	21.704522000000008	3.074368999999999
W	6.335791000000004	24.442980999999996	3.250563000000001
W	4.825693000000002	27.145921000000013	3.237473000000000
W	3.171981999999999	29.749756000000014	3.258357999999999
W	6.300925999999996	29.673100000000016	3.196095999999998
W	22.202660999999991	1.067698000000000	3.304289999999999
W	20.581904999999990	3.894150999999999	3.301372999999999
W	18.959004000000002	6.717220000000002	3.303973000000000
W	17.304427000000004	9.549787999999995	3.334801000000001
W	15.636920999999992	12.385723000000005	3.342709000000002
W	14.012802999999999	15.204893999999995	3.322401000000002
W	12.472789000000006	18.032261999999993	3.281031000000000
W	11.100623000000006	21.634667000000003	3.242483000000000
W	9.601551999999999	23.924934000000004	3.354004000000002
W	7.559764000000004	27.310628999999987	3.304327999999999
W	28.963228999999983	1.296407000000001	3.384109000000000
W	26.218914000000016	1.507644000000000	3.490533999999998
W	24.606448000000003	4.286074000000002	3.500595999999998
W	22.994137999999995	7.147545000000000	3.532121000000001
W	21.353737999999999	9.923818000000007	3.531226000000002
W	19.657737000000009	12.839762999999996	3.572514000000000
W	18.004127000000004	15.657959000000000	3.543626000000002
W	16.454615000000004	18.382058000000007	3.420535000000001
W	14.358757999999999	21.666211000000006	3.327367999999999
W	12.792429000000003	23.906037000000013	3.446759000000001
W	11.333621000000008	27.573233999999994	3.284211000000000
W	9.670346000000003	29.793399000000009	3.346855000000001
W	27.388223000000000	3.989517999999999	3.340485000000001
W	25.793869999999983	6.767236999999997	3.389536000000001
W	24.143647000000014	9.797988999999994	3.485001000000000
W	22.645144999999994	12.367174999999996	3.496722999999998
W	20.733467000000010	15.586691000000001	3.494415000000000
W	19.321891999999983	18.149291999999991	3.482988000000002

W	17.6291040000000017	21.6449630000000006	3.3889360000000002
W	16.0492260000000009	23.9227200000000018	3.4940210000000000
W	14.5186060000000001	27.6126490000000011	3.3045339999999999
W	12.9022830000000006	29.8602319999999999	3.3969250000000000
W	32.8519170000000003	0.8361070000000000	3.3968029999999998
W	31.2915090000000014	4.5475370000000002	3.3869319999999998
W	29.8479010000000002	7.1836070000000003	3.5871800000000000
W	28.2548980000000007	9.8286239999999996	3.5233590000000001
W	25.6284990000000015	12.6675559999999994	3.5645539999999998
W	24.7001379999999990	15.7594989999999999	3.5251160000000001
W	22.4309890000000003	18.0890750000000011	3.5231520000000001
W	21.1136960000000009	21.7474799999999995	3.4119180000000000
W	19.3722589999999997	23.9507289999999990	3.5544500000000001
W	17.7713539999999988	27.6261410000000005	3.3376690000000000
W	16.1075039999999987	29.8882919999999999	3.3683450000000001
W	34.5545400000000029	4.4354760000000004	3.2528329999999999
W	32.9712120000000013	6.7076300000000000	3.4542790000000001
W	30.9846590000000006	10.0576690000000006	3.5843769999999999
W	29.7250869999999985	12.6363249999999994	3.5051960000000002
W	27.8152879999999989	15.9160799999999991	3.5532960000000000
W	26.3150620000000011	18.4363540000000015	3.5310750000000000
W	24.3312449999999991	21.7003360000000001	3.4553400000000001
W	22.6627830000000010	23.9925919999999984	3.5681609999999999
W	21.0793630000000007	27.6473680000000002	3.3652519999999999
W	19.3383670000000016	29.9054159999999989	3.3762680000000000
W	36.1319919999999968	7.3615719999999998	3.4255480000000000
W	35.0064550000000025	9.9196369999999998	3.3960669999999999
W	32.4380930000000021	12.8256759999999996	3.5434230000000002
W	30.7213080000000005	15.5798220000000001	3.4237730000000002
W	29.0935780000000008	18.3919579999999989	3.4437310000000001
W	27.4155559999999987	21.1697430000000004	3.4053770000000001
W	25.8521450000000002	23.9539459999999984	3.5164860000000000
W	24.3943140000000014	27.6335279999999983	3.3724249999999998

W	22.589645999999983	29.922951999999987	3.4021940000000002
W	37.6742180000000033	10.1094290000000004	3.5174840000000001
W	36.4570870000000014	12.7044090000000001	3.4116710000000001
W	34.7336179999999999	16.0817760000000014	3.5517650000000001
W	33.1045530000000028	18.8769430000000007	3.5840869999999998
W	31.4414760000000015	21.6774410000000017	3.5804100000000001
W	29.7628570000000003	24.4623320000000000	3.5544220000000002
W	27.6161239999999992	27.5309670000000004	3.4097759999999999
W	25.8416609999999984	29.8884369999999997	3.4264839999999999
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W	35.8487330000000028	18.6672499999999992	3.4726469999999998
W	34.2204490000000021	21.4318489999999997	3.5178929999999999
W	32.5726429999999993	24.1895330000000008	3.4757319999999998
W	30.9005660000000013	26.9464280000000009	3.4588510000000001
W	29.0805030000000002	29.7472490000000001	3.4629189999999999
Se	20.6037469999999985	0.1657380000000000	5.1847110000000001
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Se	10.8853740000000005	17.2370459999999994	5.1720069999999998
Se	9.2580139999999993	20.3411870000000015	4.7474420000000004
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Se	6.1708509999999999	26.1226050000000001	5.1235530000000002
Se	4.6024940000000001	29.0305870000000006	5.0784750000000001
Se	24.2162199999999999	0.3440270000000000	4.8186380000000000
Se	22.5834079999999986	3.1526960000000002	4.8079559999999999
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Se	13.889461000000007	7.594566000000004	2.306191999999998
Se	12.224994000000006	10.431233999999999	2.351046000000002
Se	10.603002999999993	13.324237999999994	2.324971000000001
Se	8.913023000000008	16.174979000000004	2.454299999999999
Se	7.578719000000004	19.355640999999985	2.190087999999998
Se	5.578223999999996	22.154976999999988	2.357019999999999
Se	4.063709000000002	24.957930999999985	2.362525000000002
Se	2.550808000000000	27.794817999999994	2.088916999999999
Se	20.888870000000007	2.185998999999998	1.450244000000001
Se	19.270015000000008	5.020384000000000	1.444901000000000
Se	17.643045000000008	7.866437000000003	1.466733000000001
Se	15.986110999999993	10.688022999999994	1.490707999999999
Se	14.310403000000009	13.498559000000002	1.484045000000001
Se	12.680113999999997	16.344744999999996	1.446268000000001
Se	11.108919999999995	19.398873999999993	1.590587999999999
Se	9.434272000000000	22.299277000000000	1.364481000000001
Se	7.925621999999997	25.247672999999989	1.682323000000000
Se	6.108062000000003	28.054221999999993	1.326816999999999
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Se	27.581288000000007	0.410027000000000	5.344885999999998
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Se	24.332515999999983	6.003918999999998	5.340963000000003
Se	22.681276000000004	8.816337000000008	5.375460000000003
Se	21.002791999999995	11.679731999999996	5.348920999999998
Se	19.333776000000003	14.541639999999992	5.386122000000003
Se	17.690708999999982	17.432297999999994	5.354015000000004

Se	15.9837760000000006	20.3678130000000017	4.9525550000000003
Se	14.3964110000000005	23.3021050000000010	5.2997670000000001
Se	12.8448200000000003	26.2164329999999985	4.8119490000000003
Se	11.2596900000000009	29.2808640000000011	5.2266849999999998
Se	30.9253490000000006	0.3227660000000000	4.9030790000000000
Se	29.4502479999999984	3.3134070000000002	4.8816629999999996
Se	27.8137289999999986	6.0517040000000000	4.8680050000000001
Se	26.1879510000000018	8.8783689999999993	4.8901399999999997
Se	24.2849089999999990	11.6551919999999996	5.3612520000000004
Se	22.7268989999999995	14.5941949999999991	4.8258669999999997
Se	20.9443869999999990	17.3715750000000000	5.3668790000000000
Se	19.3734339999999996	20.3761779999999995	4.8434119999999998
Se	17.7056089999999990	23.3103839999999991	5.3240850000000002
Se	16.0958140000000007	26.2361350000000009	4.8180209999999999
Se	14.5087419999999998	29.3798470000000016	5.2411050000000001
Se	24.2025630000000014	2.1975600000000002	1.9709280000000000
Se	22.5763120000000015	5.0544900000000004	2.0013130000000001
Se	20.9590360000000011	7.8673289999999998	1.9854730000000000
Se	19.3180909999999990	10.7194830000000003	2.0569340000000000
Se	17.6469960000000015	13.5510719999999996	2.0436429999999999
Se	15.9957320000000003	16.3664379999999987	1.9890150000000000
Se	14.4290649999999996	19.3211280000000016	2.0062609999999999
Se	12.7517750000000003	22.2689319999999995	1.4649040000000000
Se	11.2170310000000004	25.2935620000000014	1.8809199999999999
Se	9.4710789999999996	28.1106690000000015	1.6102909999999999
Se	7.7999879999999999	31.3796689999999998	2.3241070000000001
Se	27.6677779999999984	2.2707869999999999	1.4930040000000000
Se	26.0166560000000011	5.0880150000000004	1.5250459999999999
Se	24.4370569999999994	7.9993960000000000	1.6573410000000000
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Se	21.1166860000000014	13.6517339999999994	1.7873810000000001
Se	19.3675759999999997	16.4905760000000008	1.5569530000000000
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Se	26.126055999999984	14.641638000000004	5.185645000000001
Se	24.382374999999997	17.581315000000000	5.156919000000003
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Se	21.028988999999993	23.377127000000015	5.387649999999998
Se	19.387427999999999	26.270060999999983	4.839896999999997
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Se	16.146177000000016	28.226151000000015	1.477942000000001

Se	14.4698410000000006	31.5427129999999991	2.3649580000000001
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Se	26.1278080000000017	16.6129590000000000	1.6946749999999999
Se	24.3178930000000015	19.3947700000000012	2.1755949999999999
Se	22.7340990000000005	22.3711790000000015	1.5923060000000000
Se	21.0625549999999997	25.3408179999999987	2.0502270000000000
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Se	17.7842370000000010	31.5597190000000012	2.3624040000000002
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Se	32.8091799999999978	14.8872789999999995	4.9702180000000000
Se	31.1318519999999985	17.6630660000000006	4.9246610000000004
Se	29.4299420000000005	20.5358039999999988	4.9212090000000002
Se	27.8029319999999984	23.3315909999999995	4.9728029999999999
Se	25.9585940000000015	26.2410180000000004	4.9141199999999996
Se	24.2269359999999985	29.4223940000000006	5.2715329999999998
Se	37.9598399999999998	11.8306670000000000	5.3597370000000000
Se	36.1838720000000009	14.7582649999999997	5.1749960000000002
Se	34.5083389999999994	17.7702419999999996	5.4104799999999997
Se	32.7934119999999965	20.5866229999999995	5.4210589999999996
Se	31.1380380000000017	23.4388089999999991	5.4046709999999996
Se	29.2893979999999985	26.3574979999999996	5.1820399999999998
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Se	36.6237270000000024	5.1453660000000001	2.1582520000000001
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Se	24.3539610000000017	25.3498160000000006	2.0302530000000001
Se	22.731208999999998	28.252448999999986	1.5396220000000000
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Se	36.3650960000000012	10.989300999999993	1.5513090000000000
Se	34.4595130000000012	13.8792290000000005	2.1521629999999998
Se	32.742744999999993	16.7480340000000005	2.0962459999999998
Se	31.081161999999991	19.563864999999998	2.1036410000000001
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Se	39.916823999999983	14.9547260000000009	4.4322809999999997
Se	38.263835999999977	17.9784770000000016	4.3172180000000004
Se	36.5030670000000015	20.8361310000000017	4.5197180000000001
Se	34.786270999999993	23.713924999999997	4.5321680000000004
Se	33.1251790000000028	26.6364120000000000	4.3070740000000001
Se	31.2212420000000002	29.522297999999993	4.4293370000000003
Se	40.0579430000000016	11.0196710000000007	2.5510730000000001
Se	37.8277190000000019	14.080026999999994	1.6661120000000000
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Se	32.977088999999994	22.5543480000000010	1.6436010000000001
Se	31.262346999999983	25.302690999999994	1.6125560000000001
Se	29.475322999999995	28.0895490000000017	1.6572279999999999
Se	27.9159310000000005	31.517911999999990	2.4753300000000000
W	26.1382750000000001	-9.852358999999999	2.9249260000000001
W	22.7132930000000002	-4.2411040000000000	3.3689629999999999
W	24.402138999999982	-6.994697999999996	3.2439460000000002
W	27.591370999999988	-7.6029890000000000	3.1637279999999999
W	25.496342999999995	-4.4447380000000001	3.2748260000000000
W	29.5616780000000006	-4.205970999999999	3.3613729999999999

W	21.054445999999987	-1.478453999999999	3.3377970000000001
W	23.8340560000000004	-1.7232970000000001	3.3136890000000001
W	27.8989620000000009	-1.2790750000000000	3.5077080000000000
W	31.0457169999999998	-1.8184670000000001	3.3742540000000001
Se	25.6841720000000002	-12.1056500000000007	1.5699770000000000
Se	23.914864999999989	-9.3631150000000005	2.1046550000000002
Se	27.6417369999999991	-9.115892999999998	1.0981620000000001
Se	22.1307690000000008	-6.6207250000000002	2.4784649999999999
Se	25.9612200000000009	-6.260304999999998	1.5313829999999999
Se	29.2302460000000011	-6.204057999999999	1.6079520000000000
Se	20.474450999999984	-3.7613010000000000	2.3490929999999999
Se	24.126319999999998	-3.4409660000000000	1.4335990000000001
Se	27.5736400000000010	-3.3850760000000002	1.9240459999999999
Se	31.032703999999990	-3.525660999999999	1.4381860000000000
Se	25.7875170000000011	-8.295042999999997	4.9113150000000001
Se	24.037355999999991	-5.418447999999997	5.1746930000000004
Se	27.548535999999986	-5.3998840000000001	4.6042180000000004
Se	22.505759999999987	-0.6423170000000000	1.4586410000000001
Se	25.8779240000000001	-0.6281530000000000	2.0224940000000000
Se	29.4405690000000000	-0.551320999999999	1.7018960000000001
Se	32.713191999999994	-0.8453730000000000	1.5586949999999999
Se	22.2779880000000006	-2.625519999999999	5.2223819999999996
Se	25.8681480000000015	-2.4668570000000001	4.8293499999999998
Se	29.300028999999985	-2.531006999999998	5.1952439999999998
Se	18.795073999999996	-0.9243350000000000	2.3346490000000002
W	29.0472010000000012	-9.885597999999999	2.9867319999999999
W	27.5981150000000000	-12.6173120000000001	2.8335659999999998
W	30.748221999999984	-7.151737999999999	3.1791179999999999
Se	27.596979999999985	-14.778988999999993	3.5275850000000002
Se	27.548024999999991	-11.128909999999994	4.7499650000000004
Se	29.593278999999990	-12.1138790000000007	1.6826000000000001
Se	29.337258999999995	-8.3217470000000002	4.9424330000000003
Se	31.348380999999998	-9.4227570000000007	2.2132820000000000

Se	30.8945490000000014	-5.5412819999999998	5.0945939999999998
W	32.3433980000000005	-4.4961330000000004	3.2940239999999998
Se	33.0503440000000026	-6.6771969999999996	2.3552089999999999
Se	32.6086820000000017	-2.8168030000000002	5.2171859999999999
W	33.9810950000000034	-1.7847729999999999	3.4464039999999998
Se	34.7857819999999975	-3.9047850000000000	2.5710850000000001
Se	34.2661050000000031	-0.1112680000000000	5.3748509999999996
W	35.5657580000000024	0.9958030000000000	3.6060949999999998
Se	36.5009560000000022	-0.9823600000000000	2.7514590000000001
Se	36.6167119999999997	2.8733309999999999	4.5528769999999996
Se	1.3466710000000000	30.8074860000000008	4.0967240000000000

W₁₀₅Se₂₁₀; $E_{tot} = -61\,508\,150.632\,896\,76$ eV; $E_{rel} = 2.301\,527\,247\,6$ meV/f.u.

W	21.0579760000000000	-1.0589720000000000	3.3988980000000000
W	19.2547430000000013	1.7945670000000000	3.4503200000000001
W	17.5962530000000008	4.5793850000000003	3.4437120000000001
W	15.9731299999999994	7.3852349999999998	3.3885070000000002
W	14.3452710000000003	10.2089689999999997	3.3716029999999999
W	12.7385380000000001	13.0318050000000003	3.3813190000000000
W	11.1690570000000005	15.8427760000000006	3.3610790000000001
W	9.5711750000000002	18.6476049999999987	3.1684999999999999
W	7.6588099999999999	22.0375370000000004	2.9850020000000002
W	6.1488540000000000	24.7495040000000017	3.1193399999999998
W	4.6142390000000004	27.4592339999999986	3.0571009999999998
W	2.9440450000000000	30.0541230000000006	3.0114770000000002
W	24.2936259999999997	-1.2381340000000001	3.4020480000000002
W	22.5746080000000013	1.1183170000000000	3.4746720000000000
W	20.4075829999999989	4.2835510000000001	3.3652340000000001
W	18.7815970000000014	7.0524269999999998	3.3547400000000001
W	17.1528889999999983	9.8928340000000006	3.3643790000000000
W	15.5071209999999997	12.7462140000000002	3.3552900000000001
W	13.8873449999999998	15.5744600000000002	3.3163600000000000

W	12.352560000000004	18.397183999999993	3.2580930000000001
W	10.942828000000004	21.9898130000000016	3.1857210000000000
W	9.4196100000000005	24.265886999999993	3.2818450000000001
W	7.344358999999999	27.6359020000000015	3.1817020000000000
W	6.071793999999997	29.986537999999995	3.0356990000000001
W	27.525331999999988	-1.3174370000000000	3.3996640000000000
W	29.106076999999991	0.9264990000000000	3.5021830000000000
W	25.7824670000000005	0.9860200000000000	3.4957560000000001
W	24.354583999999991	4.6819160000000002	3.3914080000000002
W	22.823740999999983	7.459160999999999	3.5334819999999998
W	21.176709999999999	10.274205999999995	3.5164149999999998
W	19.5419230000000006	13.179840999999997	3.5641470000000002
W	17.893616999999990	16.009046999999989	3.5315880000000002
W	16.3405290000000001	18.7393220000000014	3.4045550000000002
W	14.216801999999995	22.030387999999985	3.2901639999999999
W	12.614402999999994	24.2612160000000010	3.4086660000000002
W	11.1150110000000009	27.918959999999984	3.2292109999999998
W	9.4290430000000001	30.128859999999995	3.2621799999999999
W	27.556301999999987	4.6180430000000001	3.3701099999999999
W	25.9466740000000016	6.9063400000000001	3.5273650000000001
W	23.982922999999995	10.258701999999995	3.4976600000000002
W	22.583190999999993	12.6795760000000008	3.5256479999999999
W	20.635989999999996	15.964904999999999	3.5013869999999998
W	19.2040730000000011	18.498111999999990	3.4718849999999999
W	17.5222160000000002	22.025300999999989	3.3675329999999999
W	15.8878710000000005	24.292066999999994	3.4736910000000001
W	14.293744999999995	27.978419999999998	3.2864830000000000
W	12.6555710000000001	30.2175970000000014	3.3643120000000000
W	35.5761540000000025	1.0299240000000001	3.5494080000000001
W	32.383611999999994	0.9388649999999999	3.5271910000000002
W	30.8010410000000014	4.6157029999999999	3.4036190000000000
W	29.1887960000000000	6.8556910000000002	3.5786509999999998
W	27.6976270000000007	10.5069409999999994	3.4762140000000001

W	25.929998999999987	12.680260000000005	3.6566109999999998
W	24.396913999999989	16.309077999999995	3.4898189999999998
W	22.550429999999986	18.480429999999984	3.6254119999999999
W	20.911763000000005	22.140782000000015	3.4070930000000001
W	19.186467000000004	24.356629000000016	3.5245099999999998
W	17.534341000000013	28.027422999999989	3.3358960000000000
W	15.851653999999999	30.274725000000001	3.3739270000000001
W	34.054223000000004	4.649754999999999	3.4445760000000001
W	32.471403999999997	6.879208000000002	3.5937999999999999
W	30.816217999999992	10.548256999999996	3.4290790000000002
W	29.178872999999994	12.795602000000006	3.6133620000000000
W	27.591674000000011	16.426158999999984	3.4450740000000000
W	25.861035000000011	18.627358000000010	3.6018789999999998
W	24.133504999999995	22.215969999999987	3.4080910000000002
W	22.435483999999989	24.443773000000002	3.5452370000000002
W	20.827642000000009	28.093498000000003	3.3636230000000000
W	19.071414999999982	30.331230999999989	3.4028800000000001
W	42.497298000000007	1.8512150000000001	3.6482250000000001
W	39.458759000000006	1.588446999999999	3.6918039999999999
W	37.321981000000010	4.711062000000001	3.5853860000000002
W	35.712572000000015	6.941033000000000	3.6230419999999999
W	33.979422999999970	10.608401000000006	3.4439829999999998
W	32.334848000000009	12.835796999999995	3.5767300000000000
W	30.837194000000002	16.490707000000004	3.4260419999999998
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W	25.622999000000001	24.503609000000009	3.5324089999999999
W	24.125109999999994	28.130167000000001	3.3615370000000002
W	22.318000000000014	30.392610000000012	3.4286580000000000
W	40.893866000000027	4.0316729999999996	3.6391049999999998
W	38.821795000000016	7.361056999999997	3.6428639999999999
W	37.733888999999978	10.327427000000001	3.5870600000000001
W	36.127302000000002	12.977672000000001	3.4877080000000000

W	34.0386510000000015	16.4732430000000001	3.4686319999999999
W	32.4482739999999978	18.7626519999999992	3.5946129999999998
W	30.7559600000000017	22.3747650000000000	3.4484119999999998
W	29.3024619999999985	24.6578300000000006	3.4872570000000001
W	27.3298479999999984	28.0691339999999983	3.3778310000000000
W	25.5756030000000010	30.3901949999999985	3.4477199999999999
W	45.6182319999999990	1.8855200000000001	3.6033680000000001
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W	42.3506599999999978	6.9007310000000004	3.8254640000000002
W	40.4589580000000026	10.2796040000000009	3.6985950000000001
W	38.8560209999999984	13.0045289999999998	3.4376959999999999
W	37.2687299999999979	16.0359529999999992	3.4975480000000001
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W	33.9004249999999985	22.0839260000000017	3.6681100000000000
W	32.2778660000000031	24.7200130000000016	3.5408140000000001
W	30.6905740000000016	27.3979040000000005	3.4984920000000002
W	28.8321049999999985	30.2496189999999991	3.4545759999999999
Se	22.2283049999999989	-2.8507910000000001	4.3541040000000004
Se	20.6931459999999987	0.5971860000000000	5.2163100000000000
Se	18.8981780000000015	3.4332419999999999	5.3026520000000001
Se	17.1978140000000010	6.2278900000000004	5.2711779999999999
Se	15.5451599999999992	9.0187390000000001	5.2426539999999999
Se	13.9287949999999991	11.8403039999999997	5.2429680000000003
Se	12.3392420000000005	14.6945700000000006	5.2385970000000004
Se	10.7513100000000001	17.6178239999999988	5.1437590000000002
Se	9.0977420000000002	20.6981399999999987	4.6811080000000000
Se	7.5389790000000003	23.6514850000000010	4.9385100000000000
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Se	4.3285429999999998	29.3549219999999984	4.8782680000000003
Se	25.7089140000000000	-2.9673959999999999	4.3741450000000004
Se	24.1166039999999988	0.3732490000000000	5.3158019999999997
Se	22.4715190000000007	3.4169269999999998	4.7608730000000001
Se	20.7979109999999991	6.3029039999999998	4.8607500000000003

Se	19.171096999999996	9.1402750000000008	4.8483060000000000
Se	17.5098360000000000	12.0024409999999992	4.8359430000000003
Se	15.8657979999999998	14.8667829999999999	4.8412309999999996
Se	14.2404279999999996	17.7215519999999991	4.8086099999999998
Se	12.5035360000000004	20.6250099999999996	4.6978770000000001
Se	10.9162710000000001	23.6139809999999990	5.1691690000000001
Se	9.3085249999999995	26.5702779999999983	4.5778299999999996
Se	7.6607630000000002	29.5176249999999989	4.9611570000000000
Se	18.9088120000000011	-0.7849590000000000	2.4692259999999999
Se	17.0377760000000009	2.1085340000000001	2.6208179999999999
Se	15.3881470000000000	5.0355939999999997	2.4341070000000000
Se	13.7458580000000001	7.9194040000000001	2.3827769999999999
Se	12.1063880000000008	10.7914720000000006	2.3654869999999999
Se	10.4777269999999998	13.6764820000000000	2.3426779999999998
Se	8.8014130000000002	16.5253410000000009	2.4063829999999999
Se	7.4415699999999996	19.6799019999999985	2.1268470000000002
Se	5.4154660000000003	22.4580090000000006	2.2379449999999999
Se	3.8891260000000001	25.2575199999999995	2.1851460000000000
Se	2.3674309999999998	28.0855589999999999	1.8432180000000000
Se	1.0878350000000001	31.1112059999999992	3.7817409999999998
Se	22.6368280000000013	-0.6480640000000000	1.5469560000000000
Se	20.8836009999999987	2.3634879999999998	1.7428239999999999
Se	19.0427579999999992	5.2914339999999997	1.5076290000000001
Se	17.4617669999999983	8.1763549999999992	1.5166900000000001
Se	15.8356960000000004	11.0262580000000003	1.5209090000000001
Se	14.1838599999999992	13.8534279999999992	1.4927760000000001
Se	12.5579870000000007	16.7023569999999992	1.4308149999999999
Se	10.9883690000000005	19.7488320000000002	1.5501220000000000
Se	9.2880939999999992	22.6357140000000001	1.2927299999999999
Se	7.7583750000000000	25.5666860000000007	1.5789089999999999
Se	5.9355409999999997	28.3580159999999992	1.1679459999999999
Se	4.2918050000000001	31.4937439999999995	1.7355000000000000
Se	29.1330820000000017	-0.8122170000000000	1.5480959999999999

Se	27.437570999999984	0.308620000000000	5.306880999999997
Se	25.831578000000004	3.252139000000001	4.878903000000002
Se	24.225314000000009	6.297813999999998	5.314128000000002
Se	22.559618000000004	9.158502999999996	5.345813999999998
Se	20.893910000000018	12.041776999999997	5.349314999999998
Se	19.227353999999983	14.897064999999996	5.368743000000003
Se	17.570757000000004	17.789242000000016	5.341872000000004
Se	15.850927999999997	20.735531999999992	4.910349000000001
Se	14.214648999999996	23.665279999999992	5.263485000000002
Se	12.619294000000000	26.571766000000002	4.775583000000001
Se	10.991049999999995	29.628233999999991	5.169356999999998
Se	30.745967000000003	0.274598000000000	5.330528000000002
Se	29.128547000000011	3.207692000000002	4.873681999999996
Se	27.520119999999986	6.225236999999999	5.368668999999997
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Se	24.218578999999983	12.029042999999997	5.372957999999997
Se	22.605147999999998	14.938928999999999	4.863743999999996
Se	20.853563000000012	17.785409000000014	5.334582000000002
Se	19.240985999999995	20.736247999999998	4.848799999999998
Se	17.531953000000015	23.694935000000010	5.306315999999998
Se	15.877656999999992	26.608726999999982	4.802361999999996
Se	14.241229000000006	29.741593000000017	5.228830000000003
Se	25.895692000000004	-0.764643000000000	1.552761000000001
Se	24.217697999999986	2.421774000000001	1.976361000000000
Se	22.398897999999991	5.363679000000003	1.949503999999999
Se	20.814457000000009	8.166126000000002	2.024346000000000
Se	19.156618999999992	11.054140999999996	2.054488000000001
Se	17.523544999999986	13.903098000000000	2.039485000000000
Se	15.875192999999994	16.729597999999993	1.980283999999999
Se	14.308025000000007	19.689361999999991	1.977992000000000
Se	12.614164000000006	22.633396999999987	1.423307000000001
Se	11.043404999999999	25.642385000000009	1.828319000000000
Se	9.279666999999999	28.444095999999983	1.522513999999999

Se	7.575440999999996	31.708670000000015	2.199930999999999
Se	27.498024999999984	2.339236999999998	2.027857000000000
Se	25.898662000000016	5.289444999999997	1.532443999999999
Se	24.347773000000001	8.266894000000006	1.818729000000000
Se	22.540908999999992	11.078898000000006	1.556477000000001
Se	21.034182000000013	14.001780000000001	1.812340000000001
Se	19.257352000000009	16.843392000000015	1.553698999999999
Se	17.732504999999997	19.811441999999996	1.734054000000000
Se	15.902668999999995	22.643328000000003	1.516108000000000
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Se	12.675003999999995	28.629488999999995	1.401281999999999
Se	10.884672000000001	31.916858000000013	2.498016999999999
Se	34.045020999999984	0.251020000000000	5.360625999999999
Se	32.435174000000035	3.217238000000000	4.905901000000001
Se	30.816811999999988	6.234118999999997	5.395233000000002
Se	29.228670999999985	9.136958999999992	4.986705999999999
Se	27.592248000000014	12.095874000000002	5.465212000000002
Se	25.957556000000003	15.001315000000000	4.993630999999997
Se	24.236653000000004	17.945931999999991	5.435891999999999
Se	22.535748000000017	20.802450000000003	4.923949999999996
Se	20.819337000000009	23.786799999999995	5.372786999999998
Se	19.161708999999983	26.672900999999995	4.829863999999997
Se	17.464244000000008	29.811761000000006	5.251542999999999
Se	37.542810000000029	0.399247000000000	5.182466999999999
Se	35.712684000000030	3.260123999999998	4.982713999999996
Se	34.091687000000003	6.273156000000002	5.431217000000002
Se	32.473297000000023	9.187697999999993	4.933397000000003
Se	30.833061000000007	12.149259999999999	5.448578999999996
Se	29.204173999999983	15.082160999999993	4.951854000000000
Se	27.537406000000007	18.067185999999995	5.418554000000003
Se	25.852503999999997	20.928000999999983	4.892051000000004
Se	24.092741000000002	23.836016000000008	5.395702000000000
Se	22.443094999999996	26.744129999999984	4.861883999999999

Se	20.707527999999999	29.871746999999992	5.2728330000000003
Se	30.790327000000013	2.3347549999999999	2.0459010000000002
Se	29.184768999999993	5.2518430000000000	1.5673990000000000
Se	27.604411999999999	8.2835560000000008	2.0534189999999999
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Se	24.283170999999994	14.0522460000000002	2.0952280000000001
Se	22.533339999999990	16.844917999999998	1.7961140000000000
Se	20.931754999999990	19.859180999999995	2.0518950000000000
Se	19.211348999999985	22.7326310000000014	1.5954109999999999
Se	17.5565660000000001	25.717090999999999	2.0056500000000002
Se	15.9185610000000004	28.6291590000000014	1.4708950000000001
Se	14.213060999999997	31.9197050000000004	2.3565190000000000
Se	34.066704999999989	2.3830540000000000	2.0467360000000001
Se	32.459145999999969	5.2604970000000000	1.6032869999999999
Se	30.827014999999994	8.2836890000000007	2.0927280000000001
Se	29.186053999999986	11.2121770000000005	1.5920190000000001
Se	27.517130999999991	14.1363930000000000	2.1316940000000000
Se	25.898517999999993	17.009745999999998	1.6166959999999999
Se	24.155910999999997	19.927707999999991	2.1093160000000002
Se	22.4876770000000015	22.8160710000000009	1.5687869999999999
Se	20.8279730000000001	25.7922830000000012	2.0275420000000000
Se	19.175999999999984	28.671355999999994	1.5204439999999999
Se	17.505867999999995	31.984311999999992	2.4040330000000001
Se	41.0760080000000016	0.2294780000000000	4.9589460000000001
Se	39.0645730000000029	3.3948670000000001	5.2959079999999998
Se	37.347988999999983	6.4090470000000002	5.4743110000000001
Se	35.7481140000000011	9.2653250000000007	4.9059980000000003
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Se	32.4481990000000025	15.1104160000000007	4.9657400000000003
Se	30.828786999999984	18.118808999999988	5.4027469999999997
Se	29.125621999999999	21.0145020000000002	4.9271300000000000
Se	27.4787800000000004	23.9764330000000001	5.2337410000000002
Se	25.692054999999999	26.774848999999997	4.9137829999999996

Se	23.9642039999999987	29.8914399999999993	5.2884760000000002
Se	44.3376179999999991	0.3448940000000000	4.8452289999999998
Se	42.4970250000000007	3.4794760000000000	5.5538900000000000
Se	40.6590819999999979	6.1663379999999997	5.3048770000000003
Se	39.1037490000000005	9.2018450000000005	5.4301360000000001
Se	37.5781050000000008	12.1573869999999999	5.3913539999999998
Se	35.7561430000000016	15.1144379999999998	5.0750240000000000
Se	34.1703949999999992	18.1458380000000012	5.4271390000000004
Se	32.3724070000000026	21.0328559999999989	5.1559920000000004
Se	30.8570899999999995	24.0187379999999990	5.4167009999999998
Se	29.0239930000000008	26.7789649999999995	5.0698650000000001
Se	27.2558669999999985	29.8474730000000008	5.3092639999999998
Se	37.4806639999999973	2.3393830000000002	2.2335759999999998
Se	35.7926059999999993	5.2432740000000004	1.6893730000000000
Se	34.0816560000000024	8.3011049999999997	2.0937030000000001
Se	32.4328259999999986	11.2425719999999991	1.5804990000000001
Se	30.7961419999999997	14.1974370000000008	2.0527000000000002
Se	29.1884520000000016	17.0750300000000017	1.6067149999999999
Se	27.4785770000000014	20.0288730000000008	2.0876540000000001
Se	25.7560690000000001	22.8751779999999982	1.5689869999999999
Se	24.0858899999999991	25.8388320000000000	2.0035750000000001
Se	22.4588010000000011	28.7523589999999984	1.5393289999999999
Se	20.8022850000000012	32.0594180000000009	2.4651369999999999
Se	40.8941590000000019	2.2378700000000000	1.7652639999999999
Se	39.2072580000000031	5.3298290000000001	2.0808890000000000
Se	37.3482270000000014	8.2806630000000006	1.9498990000000000
Se	35.8869139999999973	11.1559310000000007	1.8236939999999999
Se	34.1445819999999998	14.1530109999999993	2.1959569999999999
Se	32.4895100000000028	17.1294849999999990	1.6201070000000000
Se	30.8331899999999983	20.0940960000000004	2.1004849999999999
Se	29.1373399999999982	22.9207749999999990	1.5900140000000000
Se	27.4087460000000007	25.8024610000000010	2.0953080000000002
Se	25.7745530000000009	28.7850290000000015	1.5355129999999999

Se	24.1562570000000001	32.1024639999999977	2.4992549999999998
Se	46.1431490000000011	3.8078660000000002	4.9074460000000002
Se	44.5772929999999974	6.5715570000000003	4.6759399999999998
Se	42.6200440000000000	9.2166599999999992	4.6782349999999999
Se	41.2107120000000009	12.3775739999999992	4.5040769999999997
Se	39.6040050000000008	15.2948540000000008	4.1533470000000001
Se	38.0393889999999999	18.2257530000000010	4.4526329999999996
Se	36.0167379999999966	21.0883150000000015	4.5702319999999999
Se	34.6042259999999970	24.2443680000000015	4.4908659999999996
Se	32.9121430000000004	27.0826999999999991	4.3626170000000002
Se	31.0648139999999984	29.9562729999999995	4.2638660000000002
Se	44.1648110000000003	2.5582140000000000	1.7961220000000000
Se	42.4658829999999980	5.2941820000000002	1.8999550000000001
Se	40.8855130000000031	8.2591750000000008	2.1527340000000001
Se	39.2808050000000009	11.2498050000000003	1.6806270000000001
Se	37.5295139999999989	14.2307120000000005	1.6939000000000000
Se	35.8291400000000024	17.0281379999999984	1.7112069999999999
Se	34.3254120000000000	20.0591909999999984	2.0797279999999998
Se	32.5823570000000018	22.9222450000000002	1.7180690000000001
Se	30.8462059999999987	25.7339389999999995	1.6716190000000000
Se	29.2393859999999997	28.5693139999999985	1.6800459999999999
Se	27.6496470000000016	31.9965510000000002	2.4517000000000002
W	30.7535479999999986	-1.3313330000000001	3.3910019999999998
Se	29.0858740000000004	-3.0082320000000000	4.3668269999999998
Se	32.3462209999999999	-0.7575200000000000	1.5285810000000000
W	33.9386480000000006	-1.2702540000000000	3.3554499999999998
Se	32.4671870000000027	-2.9933320000000001	4.3661110000000001
Se	35.5800539999999970	-0.5861450000000000	1.5126350000000000
W	37.1586339999999993	-1.1389069999999999	3.3201950000000000
Se	35.9456879999999970	-2.9748969999999999	4.1469170000000002
Se	39.2939069999999973	-0.9915920000000000	2.3546939999999998
Se	47.4983689999999967	0.9581870000000000	2.7327919999999999

$W_{105}Se_{210}$; $E_{tot} = -61\,508\,150.655\,888\,57\text{ eV}$; $E_{rel} = 2.082\,557\,628\,5\text{ meV/f.u.}$

W	20.8434050000000006	-0.9987120000000000	3.4964750000000002
W	19.0548940000000009	1.7080740000000001	3.4829970000000001
W	17.3520789999999998	4.4824409999999997	3.4690289999999999
W	15.7094679999999993	7.3107930000000003	3.4634480000000001
W	14.1241679999999992	10.1505399999999995	3.4790399999999999
W	12.6054840000000006	12.9899450000000005	3.4595710000000000
W	11.0746909999999996	15.8229209999999991	3.2597999999999998
W	9.2196219999999993	19.2318719999999992	3.0069370000000002
W	7.7435179999999999	22.0550619999999995	3.1251500000000001
W	6.2745319999999998	24.7175680000000000	3.0429349999999999
W	4.6666650000000001	27.3324999999999996	3.0122949999999999
W	24.1961739999999992	-1.1349270000000000	3.3849030000000000
W	21.9675629999999984	1.4054990000000001	3.3775450000000000
W	20.2395159999999983	4.1026749999999996	3.3618709999999998
W	18.5454340000000002	6.9275479999999998	3.3705059999999998
W	16.8984689999999986	9.8015299999999996	3.3768199999999999
W	15.3170649999999995	12.6615090000000006	3.3693830000000000
W	13.8363169999999993	15.5187770000000000	3.3209550000000001
W	12.4839929999999999	19.1447029999999998	3.2270249999999998
W	11.0199920000000002	21.4616119999999988	3.2924110000000000
W	9.0314540000000001	24.8760300000000001	3.1685740000000000
W	7.8031249999999996	27.2365040000000000	3.0247440000000001
W	27.3930369999999996	-1.1550100000000001	3.3243369999999999
W	29.0010639999999995	1.0897330000000001	3.4850180000000002
W	25.7744140000000002	1.1074340000000000	3.4477000000000002
W	24.1658709999999992	4.7222119999999999	3.4305560000000002
W	22.5210110000000014	7.4406100000000004	3.4832000000000001
W	20.8948229999999988	10.2218339999999994	3.4833229999999999
W	19.3363160000000001	13.0261940000000003	3.5068009999999998
W	17.8141439999999989	15.8072800000000004	3.4294850000000001
W	15.7629719999999995	19.1261930000000007	3.3212079999999999

W	14.217838999999997	21.388362999999982	3.431528999999998
W	12.821262000000008	25.070751000000013	3.206124000000000
W	11.176002000000004	27.315927999999995	3.233175999999998
W	30.545864000000017	-1.126984999999999	3.332824000000000
W	27.416567000000006	4.812249999999997	3.301416999999998
W	25.377275000000009	7.151283000000003	3.365228999999998
W	23.704402000000017	9.913748999999993	3.332476999999999
W	22.089213999999984	12.713037999999992	3.357638000000001
W	20.585172000000000	15.509696999999992	3.381987000000001
W	19.088225999999988	19.060553999999998	3.375537000000000
W	17.513550999999996	21.344386000000001	3.503088000000000
W	15.992915999999992	25.054076999999995	3.266133000000000
W	14.422420000000007	27.340816000000002	3.312978000000002
W	33.783912999999983	-1.015962999999999	3.350525999999999
W	36.218231000000030	1.691850000000001	3.762776999999998
W	32.195869000000018	1.150485999999999	3.510959999999999
W	30.662188000000004	4.771011999999998	3.370845999999998
W	29.179480999999991	7.083065000000004	3.452672999999999
W	27.587111000000002	10.491595999999995	3.474482000000001
W	26.064143000000014	13.181919000000006	3.538097000000000
W	24.533666000000002	15.940020999999998	3.523982999999999
W	22.471682000000013	19.123156000000016	3.410651000000001
W	20.824929999999984	21.341888999999983	3.540954999999999
W	19.217888999999996	25.029174999999986	3.318264000000001
W	17.642858000000004	27.325928999999986	3.303180999999999
W	33.849946000000028	4.769339000000004	3.531696000000002
W	32.235357999999980	7.039453000000000	3.499750000000001
W	30.373360000000017	10.112595999999999	3.380882999999999
W	28.845942999999983	12.917602000000005	3.378124000000001
W	27.301432999999994	15.619903000000008	3.425406999999999
W	25.628028000000005	19.021399999999999	3.461514999999999
W	24.115386999999984	21.357966000000011	3.566039000000000
W	22.490556000000015	25.027122999999996	3.365613999999999

W	20.888127999999983	27.3099330000000009	3.3367810000000002
W	42.422269999999975	1.9213860000000000	3.7838630000000002
W	39.302011999999977	1.9035210000000000	3.7901150000000001
W	37.7571110000000019	4.3668740000000001	3.6230449999999998
W	35.9530320000000003	7.6814260000000001	3.5941860000000001
W	34.4063710000000000	10.5022190000000002	3.5828929999999999
W	32.829287999999982	13.3511450000000007	3.5743980000000000
W	31.1628340000000001	16.2014190000000013	3.5798540000000001
W	29.461342999999994	18.9746330000000007	3.5350700000000002
W	27.405909999999987	21.315843999999985	3.5960969999999999
W	25.768637999999993	25.028918999999984	3.3929079999999998
W	24.136874999999999	27.2972360000000016	3.4034740000000001
W	40.4691600000000022	4.4329049999999999	3.6287630000000002
W	38.753974999999970	7.2865560000000000	3.4514440000000000
W	37.177110999999965	10.179672999999993	3.4420080000000000
W	35.593125999999980	13.0279650000000000	3.4356870000000002
W	33.968066999999978	15.882754999999995	3.4240529999999998
W	32.3022050000000007	18.693771999999992	3.4063949999999998
W	30.639707999999988	21.4177810000000015	3.4548269999999999
W	29.034037999999989	25.009077999999988	3.4143859999999999
W	27.364889999999990	27.2778060000000018	3.4888070000000000
W	48.7895060000000029	1.9648289999999999	3.9949300000000001
W	45.6917720000000003	2.0636800000000002	3.8896329999999999
W	44.4042400000000015	4.4307040000000004	3.7490910000000000
W	42.709086999999967	7.8217220000000003	3.6498409999999999
W	41.1702200000000005	10.6319250000000007	3.6009050000000000
W	39.5761600000000016	13.469545999999994	3.5760079999999999
W	37.9488360000000000	16.338301999999988	3.5625100000000001
W	36.2785000000000011	19.209289999999993	3.5509490000000001
W	34.5629220000000004	22.043351999999987	3.5388060000000001
W	32.816690999999987	24.743794999999987	3.5075400000000001
W	30.5964330000000011	27.254584999999987	3.4804119999999998
W	47.097954999999989	4.5942959999999999	3.9531480000000001

W	45.4651840000000007	7.5124110000000002	3.6607150000000002
W	43.9098380000000006	10.3363110000000002	3.5280990000000001
W	42.3546049999999994	13.1494289999999996	3.5197360000000000
W	40.76364800000000034	15.9819499999999994	3.5101950000000000
W	39.1345049999999972	18.8200399999999988	3.4891980000000000
W	37.4731400000000008	21.6523579999999995	3.4646029999999999
W	35.7539310000000015	24.4375259999999983	3.4381590000000002
W	33.9498269999999991	27.1384380000000007	3.4056600000000001
Se	22.1776920000000004	-2.7061060000000001	4.4347159999999999
Se	20.4250760000000007	0.5967150000000000	5.3328020000000000
Se	18.6670179999999988	3.3546830000000001	5.3157199999999998
Se	16.9762570000000004	6.1400189999999997	5.3089089999999999
Se	15.3560909999999993	8.9636800000000001	5.3205020000000003
Se	13.7864780000000007	11.8329170000000001	5.3254440000000001
Se	12.2443410000000004	14.7818249999999995	5.2344970000000002
Se	10.6261910000000004	17.9028759999999991	4.7412729999999996
Se	9.1065819999999995	20.8774639999999998	4.9362529999999998
Se	7.6013460000000004	23.7392910000000015	4.9771619999999999
Se	6.0647320000000002	26.6395489999999988	4.8677469999999996
Se	25.6297089999999983	-2.8781520000000000	4.2218999999999998
Se	23.9133770000000005	0.5604900000000000	5.0945600000000004
Se	22.2804539999999989	3.4728409999999998	4.8726750000000001
Se	20.5790199999999999	6.2513930000000002	4.8385090000000002
Se	18.9329140000000002	9.0755330000000001	4.8292080000000004
Se	17.3169040000000010	11.9281229999999994	4.8521080000000003
Se	15.7300710000000006	14.8060930000000006	4.8605689999999999
Se	14.0305000000000000	17.7569949999999999	4.7364340000000000
Se	12.4944559999999996	20.7861609999999999	5.1904300000000001
Se	10.9727720000000009	23.7768000000000015	4.5675460000000001
Se	9.4045570000000005	26.7624090000000017	4.9401900000000003
Se	18.6866039999999991	-0.9168750000000000	2.5929359999999999
Se	16.8413809999999984	2.0315129999999999	2.5539679999999998
Se	15.1215150000000005	4.9422699999999997	2.5377239999999999

Se	13.4741160000000004	7.8689470000000004	2.5007210000000000
Se	11.8713739999999994	10.8109979999999997	2.4690219999999998
Se	10.2502410000000008	13.7131039999999995	2.5166740000000001
Se	8.9658650000000009	16.8876029999999986	2.1799650000000002
Se	6.9799020000000001	19.7167780000000015	2.3102770000000001
Se	5.5210290000000004	22.5356710000000007	2.1457790000000001
Se	4.0366150000000003	25.3717630000000014	1.8516180000000000
Se	2.8350450000000000	28.4172280000000015	3.8016740000000002
Se	22.4205590000000008	-0.4996240000000000	1.6412240000000000
Se	20.5220419999999990	2.3433269999999999	1.5489590000000000
Se	18.8123560000000012	5.1827740000000002	1.5517740000000000
Se	17.1692590000000003	8.0558589999999999	1.5590520000000001
Se	15.5409290000000002	10.9200199999999992	1.5488880000000000
Se	13.9840110000000006	13.8071889999999993	1.5007839999999999
Se	12.4881700000000002	16.8892559999999996	1.6137390000000000
Se	10.8539169999999991	19.8182790000000004	1.3164620000000000
Se	9.3820099999999993	22.7870470000000012	1.5744769999999999
Se	7.6078409999999996	25.6008670000000009	1.1636169999999999
Se	6.0280050000000003	28.7508939999999988	1.7241990000000000
Se	29.0255669999999988	-2.8046150000000001	4.3878389999999996
Se	27.3513190000000002	0.4190400000000000	5.2990870000000001
Se	25.7320959999999985	3.3768389999999999	4.8640429999999997
Se	23.9347710000000014	6.3343629999999997	5.3176769999999998
Se	22.2707709999999999	9.1345720000000004	5.3144039999999997
Se	20.6634829999999994	11.9293549999999993	5.3364240000000001
Se	19.0981759999999987	14.7985310000000005	5.3317059999999996
Se	17.3882359999999991	17.8101999999999983	4.9286320000000003
Se	15.8070819999999994	20.7699509999999989	5.2874400000000001
Se	14.2784969999999998	23.7125729999999990	4.7755820000000000
Se	12.7473410000000005	26.7997200000000007	5.1303369999999999
Se	32.5278190000000009	-2.8155380000000001	4.2043309999999998
Se	30.6472520000000017	0.4098260000000000	5.3281000000000001
Se	28.9697530000000008	3.4066399999999999	4.8383070000000004

Se	27.293632999999998	6.477792000000000	5.105350999999998
Se	25.699210000000000	9.286350999999998	4.871576000000000
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Se	20.787352999999995	17.726050999999982	4.819649000000000
Se	19.150432999999996	20.722170999999995	5.324753000000003
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Se	16.012443000000011	26.863607999999993	5.172312999999999
Se	25.744485999999984	-0.604129999999999	1.495323000000000
Se	23.999964999999995	2.461257999999999	2.054148999999998
Se	22.190712999999988	5.269487999999999	1.972559000000000
Se	20.519058999999986	8.076133000000005	1.989363000000000
Se	18.879925000000001	10.939282999999996	1.998119999999999
Se	17.301937999999998	13.793158000000000	2.010225000000002
Se	15.798548999999995	16.782160999999986	2.016214999999999
Se	14.164706999999999	19.746251000000009	1.458746000000000
Se	12.677462999999995	22.781773000000012	1.827700000000001
Se	10.978865000000008	25.621815999999990	1.506490000000001
Se	9.347219000000008	28.907655999999994	2.146859000000001
Se	28.982433000000003	-0.590121000000000	1.480666000000000
Se	27.385459000000009	2.475007999999999	1.974498000000001
Se	25.685469000000012	5.375550999999997	1.531590999999999
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Se	22.333081000000000	11.016738999999994	1.512176000000000
Se	20.746714000000008	13.856839000000008	1.514941000000001
Se	19.198437999999994	16.844546000000011	1.696027000000000
Se	17.457788999999982	19.702617000000000	1.545500000000001
Se	15.920690999999997	22.751364999999998	1.967827999999999
Se	14.387231999999991	25.730660000000003	1.369780999999999
Se	12.666579000000005	29.070820000000012	2.463328000000002
Se	35.949612999999994	-0.913447000000000	2.446801999999999
Se	34.149445999999975	0.578313000000000	5.168008000000004
Se	32.283690000000000	3.380153000000000	4.937891999999997

Se	30.6808210000000017	6.3874740000000001	5.3700859999999997
Se	29.0138220000000011	9.1968010000000007	5.1873079999999998
Se	27.4541329999999988	12.1111780000000007	5.3806669999999999
Se	25.8460239999999999	14.9074840000000002	5.4001320000000002
Se	24.0794660000000000	17.8406909999999996	5.1221389999999998
Se	22.4586359999999985	20.7658629999999995	5.3810599999999997
Se	20.8270209999999985	23.6682440000000014	4.8409909999999998
Se	19.2428029999999985	26.8769670000000005	5.1890260000000001
Se	37.6939479999999989	0.3172830000000000	5.0564410000000004
Se	35.7455259999999981	3.6135440000000001	5.1719379999999999
Se	34.0269899999999978	6.5398310000000004	5.2333639999999999
Se	32.3875710000000012	9.3264390000000006	4.8746910000000003
Se	30.8392969999999984	12.1843789999999998	4.8819809999999997
Se	29.2336020000000012	14.9857289999999992	4.9742509999999998
Se	27.5025469999999999	17.8223589999999987	4.8357500000000000
Se	25.7834479999999999	20.7025870000000012	5.3848599999999998
Se	24.1339520000000007	23.6673319999999983	4.8817539999999999
Se	22.4805390000000003	26.8677069999999993	5.2392880000000002
Se	32.2278809999999964	-0.4989040000000000	1.5078149999999999
Se	30.6862400000000015	2.4926550000000001	1.9824390000000001
Se	29.0586459999999995	5.4065040000000000	1.5178190000000000
Se	27.3451799999999992	8.2970559999999995	2.0584570000000002
Se	25.6535210000000014	11.1279310000000002	1.9368060000000000
Se	24.0570440000000012	13.9113939999999996	2.0352549999999998
Se	22.5030679999999990	16.8069179999999996	2.0763760000000002
Se	20.7978379999999987	19.7062169999999988	1.6033390000000001
Se	19.1972799999999992	22.7180749999999989	2.0132710000000000
Se	17.6266740000000013	25.6433299999999988	1.4353579999999999
Se	15.9934329999999996	28.9967089999999992	2.2858890000000001
Se	34.1770899999999997	2.3869829999999999	2.2448700000000001
Se	32.4002580000000009	5.3355740000000003	1.5912880000000000
Se	30.7299609999999994	8.2504439999999999	1.7193380000000000
Se	29.0674250000000001	11.1978840000000002	1.5176620000000001

Se	27.457035999999987	13.991690000000002	1.5320440000000000
Se	25.857019999999986	16.910560000000003	1.7223459999999999
Se	24.105408000000006	19.733049999999986	1.5794539999999999
Se	22.498134000000003	22.730951999999985	2.0508530000000000
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Se	19.278318999999998	28.977221000000001	2.3111869999999999
Se	40.913339999999980	0.2010920000000000	4.6919019999999998
Se	39.139600999999990	3.555724999999998	5.6126540000000000
Se	37.360044999999995	6.369741000000003	5.2846050000000000
Se	35.778897999999981	9.375750000000000	5.4229930000000000
Se	34.164048000000011	12.220646999999996	5.408508999999996
Se	32.543275000000013	15.084600000000000	5.390100999999996
Se	30.868976000000000	17.941539999999998	5.379464999999997
Se	29.151993000000009	20.745878999999986	5.364339000000002
Se	27.427375999999989	23.656998999999990	4.893469999999998
Se	25.724737999999986	26.815443999999994	5.306803999999996
Se	44.164332999999992	0.269056000000000	4.643994000000002
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Se	39.190198999999998	9.414225000000001	4.914456999999996
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Se	35.973534999999983	15.181397999999997	4.915110999999996
Se	34.307355999999986	18.047038000000006	4.908921000000003
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Se	37.647581999999999	2.413107000000001	1.881200000000000
Se	35.844214999999984	5.410425000000000	2.140870000000001
Se	34.046398000000035	8.356047999999995	2.066174999999999
Se	32.422901000000031	11.223193000000002	2.078097999999998
Se	30.819689000000003	14.057708999999991	2.065129000000002
Se	29.176850000000017	16.835094000000016	2.029757000000000
Se	27.522473000000015	19.643764000000009	1.805676000000001

Se	25.832898000000001	22.7020349999999986	2.0811549999999999
Se	24.1575799999999994	25.6092189999999995	1.5363970000000000
Se	22.5561010000000017	28.9673529999999992	2.3726240000000001
Se	40.9169190000000000	2.5704400000000001	1.9076489999999999
Se	39.1534570000000031	5.4745130000000000	1.7431360000000000
Se	37.4179760000000030	8.4136849999999992	1.6369800000000001
Se	35.8423330000000036	11.2961290000000005	1.6112420000000001
Se	34.2463679999999968	14.1535519999999995	1.6068009999999999
Se	32.5948599999999971	16.9785830000000004	1.5963590000000001
Se	30.8988970000000016	19.7932899999999989	1.5748380000000000
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Se	27.4472980000000000	25.6539159999999988	1.5653120000000000
Se	25.8559869999999989	28.9537200000000006	2.4393560000000001
Se	47.3823330000000027	0.4820080000000000	5.1680330000000003
Se	45.7385220000000032	3.6534209999999998	5.7927239999999998
Se	44.0714479999999966	6.5259080000000003	5.3855659999999999
Se	42.5197170000000000	9.5294270000000001	5.4775140000000002
Se	40.9071789999999993	12.3563740000000006	5.4243160000000001
Se	39.2932169999999985	15.2100170000000006	5.3956730000000004
Se	37.6528619999999989	18.0834319999999984	5.3765109999999998
Se	35.9906879999999987	20.9588199999999993	5.3605859999999996
Se	34.2666719999999998	23.8018749999999990	5.3477639999999997
Se	32.3524799999999999	26.6452899999999993	5.2473900000000002
Se	50.6561319999999995	0.8921510000000000	3.2731460000000001
Se	49.3121920000000031	3.8764379999999998	5.2574639999999997
Se	47.7918590000000023	6.7629080000000004	4.7539939999999996
Se	46.2646769999999989	9.6639990000000004	4.4347760000000003
Se	44.6092560000000020	12.5317880000000006	4.5290480000000004
Se	42.9965690000000009	15.4284339999999993	4.4936999999999996
Se	41.3607680000000002	18.3279850000000017	4.4458120000000001
Se	39.6860380000000035	21.2267270000000003	4.4078689999999998
Se	37.9670399999999972	24.1356670000000015	4.3505609999999999
Se	36.0912539999999993	27.0715730000000008	4.3415629999999998

Se	44.120069999999983	2.548350999999998	1.983115000000000
Se	42.492007000000010	5.561734999999997	2.333564000000000
Se	40.778758000000034	8.472592999999998	2.120987000000000
Se	39.180225000000001	11.328784999999999	2.104683000000001
Se	37.566384999999968	14.190823999999992	2.099288000000000
Se	35.932811000000009	17.046209999999985	2.090634000000001
Se	34.265140999999998	19.877144999999987	2.067880000000002
Se	32.539628000000004	22.656010999999995	2.021157999999998
Se	30.901198000000008	25.557569999999983	1.769562000000001
Se	29.190139999999995	29.006533000000010	2.647209000000001
Se	47.478025999999998	2.738947000000000	2.103510000000000
Se	45.877181000000002	5.652304000000000	1.985872000000001
Se	44.269097999999996	8.594120000000002	1.731490000000000
Se	42.713417999999972	11.487228000000000	1.663955000000001
Se	41.140754000000012	14.330954000000002	1.658279000000001
Se	39.525615999999994	17.161027000000007	1.648255000000000
Se	37.868372000000008	19.986067999999995	1.633096000000001
Se	36.161036000000028	22.783487999999984	1.609502000000000
Se	34.394410999999981	25.541264000000017	1.575599999999999
Se	32.627425000000023	28.840382999999992	2.444551000000001

$W_{105}Se_{210}$; $E_{tot} = -61\,508\,150.874\,557\,12\text{ eV}$; $E_{rel} = 0\text{ meV/f.u.}$

W	20.942357999999987	-1.046237000000001	3.403166999999998
W	19.261175000000015	1.687748999999999	3.384113999999998
W	17.568525000000011	4.470296000000003	3.336682999999998
W	15.895521000000005	7.286619000000000	3.291150000000000
W	14.239354999999998	10.119032000000007	3.275919000000000
W	12.593885999999995	12.953654000000002	3.300733000000001
W	10.979165000000001	15.789106999999996	3.363236000000001
W	9.426970000000007	18.620338000000003	3.402022000000001
W	7.862912999999998	21.444849000000014	3.239825000000002
W	5.998935999999996	24.859394000000018	3.015368000000000

W	4.530777999999998	27.613825999999995	3.129407000000000
W	3.045077000000000	30.331237999999990	3.049334000000000
W	1.418215000000000	32.9435920000000024	2.997046000000000
W	23.717669999999983	-1.263695999999999	3.305193000000000
W	22.055241999999998	1.478798000000000	3.351195000000000
W	20.356092000000003	4.250785999999997	3.349783000000000
W	18.675927999999990	7.059727999999998	3.304711000000000
W	17.0246740000000010	9.874907999999996	3.281470000000000
W	15.387202000000003	12.691174000000002	3.286220000000000
W	13.749738000000007	15.511798999999999	3.307272000000000
W	12.147909999999995	18.329156999999986	3.325591000000000
W	10.632410999999994	21.1586220000000012	3.308301999999999
W	9.275472999999999	24.770309999999985	3.227582000000000
W	7.810000999999997	27.072994999999988	3.305765000000000
W	5.784342999999998	30.4724700000000013	3.176721000000000
W	4.544241999999997	32.834977999999996	3.018898000000000
W	27.7817730000000012	-0.954489000000000	3.414041999999998
W	28.932244000000007	1.830155999999999	3.412449000000000
W	26.137041000000000	1.844314999999999	3.487744000000000
W	24.398223999999990	4.737593999999996	3.565110999999999
W	22.654242000000000	7.543400000000000	3.514130000000000
W	21.0332700000000017	10.332307000000000	3.490257000000000
W	19.411901000000003	13.139523999999998	3.493717000000000
W	17.777674999999986	15.946325999999991	3.496188000000000
W	16.167000999999991	18.728206000000000	3.514746000000000
W	14.607286000000002	21.507747999999994	3.469703000000000
W	12.539920000000004	24.764496999999986	3.335280000000000
W	11.008530999999996	27.0227150000000016	3.441279000000000
W	9.555281000000008	30.6974270000000011	3.231383000000000
W	7.910929999999996	32.9360100000000031	3.239433000000000
W	30.797357999999991	-1.546448000000000	3.339761999999999
W	27.391590000000008	4.286768000000004	3.435927000000000
W	25.381468999999992	7.387436000000000	3.404853999999998

W	23.784749999999989	10.111148999999993	3.383248000000000
W	22.179857999999994	12.890957999999995	3.394314000000000
W	20.551819999999993	15.694556999999996	3.398054000000000
W	18.936685000000007	18.468928999999993	3.391395000000000
W	17.367903999999993	21.199849000000004	3.399586999999999
W	15.716468000000008	24.629345000000007	3.436808999999998
W	14.264438999999994	26.986529000000009	3.525299000000000
W	12.730442000000000	30.696283000000011	3.303710000000000
W	11.148021000000000	32.970649000000016	3.352548999999998
W	34.092742999999987	-0.912836000000000	3.508899000000000
W	35.697026000000010	1.807482000000000	3.624937000000000
W	32.967333000000036	1.568813999999999	3.418022999999998
W	30.469792000000018	4.643614999999996	3.527420999999999
W	29.391904000000003	7.673853000000003	3.546091000000000
W	27.844601000000008	10.486625999999993	3.594927999999999
W	26.225753000000010	13.308681999999992	3.618856000000000
W	24.577173999999994	16.147881999999992	3.633436000000000
W	22.921793999999984	18.987704000000008	3.631686000000000
W	21.254417000000001	21.806588000000014	3.611721000000000
W	19.575585000000002	24.556934999999993	3.551476000000000
W	17.525200000000017	26.933569999999996	3.584295000000000
W	15.949998000000008	30.667822000000010	3.371931000000000
W	14.352643000000005	32.955213000000005	3.391109000000000
W	34.525199999999981	4.315062000000002	3.457695999999999
W	32.127217000000017	7.443731999999998	3.459077000000000
W	30.591605000000013	10.219117000000007	3.421955000000000
W	29.003837999999982	13.019337999999994	3.463607000000000
W	27.363174999999982	15.849776000000003	3.486670000000000
W	25.704004999999987	18.700202000000009	3.491499000000000
W	24.042238000000011	21.539207999999986	3.474953999999999
W	22.386146000000001	24.317643000000003	3.436481999999998
W	20.739502000000017	27.023717000000013	3.471670000000000
W	19.194523000000002	30.627190999999998	3.422877000000000

W	17.553243999999994	32.9141090000000034	3.4833550000000000
W	37.2351299999999981	4.5646829999999996	3.5667789999999999
W	36.1250840000000011	7.7139930000000003	3.5521750000000001
W	34.6246679999999998	10.5386810000000004	3.5690469999999999
W	33.0196929999999966	13.4181450000000009	3.5871719999999998
W	31.3713930000000012	16.2863119999999988	3.6125660000000002
W	29.7124769999999998	19.1365170000000013	3.6245470000000002
W	28.0498699999999985	21.9862900000000003	3.6167250000000002
W	26.3700450000000011	24.8377760000000016	3.5927970000000000
W	24.6557700000000004	27.6630679999999991	3.5699939999999999
W	22.9235720000000001	30.3609599999999986	3.5317750000000001
W	20.7604949999999988	32.8713010000000025	3.5008330000000001
W	38.7722329999999999	7.5140750000000001	3.4721500000000001
W	37.3005270000000024	10.3966139999999996	3.4794200000000002
W	35.7359440000000035	13.2397100000000005	3.4986609999999998
W	34.1179910000000035	16.0632510000000011	3.5232600000000001
W	32.4874719999999968	18.8744410000000009	3.5411790000000001
W	30.8517599999999987	21.6790640000000003	3.5417090000000000
W	29.2117429999999985	24.4832140000000003	3.5220880000000001
W	27.5598719999999986	27.2844709999999999	3.4919699999999998
W	25.8661029999999990	30.0520239999999994	3.4693179999999999
W	24.0854800000000004	32.7519149999999968	3.4474459999999998
Se	22.2550649999999983	-2.2275130000000001	5.2147059999999996
Se	20.5063579999999988	0.5612360000000000	5.2623689999999996
Se	18.7768839999999990	3.3296779999999999	5.2297950000000002
Se	17.0948120000000010	6.1246590000000003	5.1770410000000000
Se	15.4427950000000003	8.9349450000000008	5.1462560000000002
Se	13.8019400000000001	11.7479320000000005	5.1513330000000002
Se	12.1886039999999998	14.5727659999999997	5.1958450000000003
Se	10.6033430000000006	17.4317449999999994	5.2484469999999996
Se	9.0393240000000006	20.3833130000000011	5.2042679999999999
Se	7.4146340000000004	23.5154660000000000	4.7322430000000004
Se	5.9060969999999999	26.4934900000000013	4.9539150000000003

Se	4.342360000000002	29.3196459999999988	4.9768889999999999
Se	25.7866019999999985	-2.2100979999999999	4.6268589999999996
Se	24.1137879999999996	0.7221520000000000	4.8462550000000002
Se	22.3844290000000008	3.5497359999999998	4.8511629999999997
Se	20.6796509999999998	6.3626319999999996	4.8315400000000004
Se	19.0283170000000013	9.1663420000000002	4.7930279999999996
Se	17.3937190000000008	11.9699240000000007	4.7859369999999997
Se	15.7608160000000002	14.7838619999999992	4.7933709999999996
Se	14.1307639999999992	17.6057459999999999	4.8254089999999996
Se	12.5273800000000008	20.4526479999999999	4.8458889999999997
Se	10.8153760000000005	23.3806680000000000	4.7457469999999997
Se	9.2898569999999996	26.4086150000000011	5.1995310000000003
Se	7.7280389999999999	29.3875689999999992	4.5869580000000001
Se	18.7100639999999991	-0.5790860000000000	2.3585799999999999
Se	16.9768070000000009	2.2034240000000000	2.4007410000000000
Se	15.3023539999999993	5.0390410000000001	2.3242069999999999
Se	13.6258820000000007	7.8822190000000001	2.2993910000000000
Se	11.9721989999999998	10.7353539999999992	2.2905289999999998
Se	10.3116780000000006	13.5870210000000000	2.3518159999999999
Se	8.6997839999999993	16.4782359999999990	2.3721420000000002
Se	7.0511540000000004	19.3387810000000009	2.4826830000000002
Se	5.7446760000000001	22.5059889999999996	2.1829350000000001
Se	3.7624990000000000	25.3163950000000000	2.2769940000000002
Se	2.2886419999999998	28.1370399999999989	2.1806980000000000
Se	0.8061990000000000	30.9793699999999994	1.8365570000000000
Se	22.3578590000000013	-0.2321000000000000	1.4729570000000001
Se	20.7015780000000014	2.5442469999999999	1.5069859999999999
Se	19.0282589999999985	5.3362840000000000	1.4831540000000001
Se	17.3532429999999991	8.1571789999999993	1.4429430000000001
Se	15.6986580000000000	10.9892199999999995	1.4299360000000001
Se	14.0510760000000001	13.8164160000000003	1.4475110000000000
Se	12.4022659999999991	16.6348360000000000	1.4709110000000001
Se	10.8058969999999999	19.4797420000000017	1.4638070000000001

Se	9.2776890000000005	22.5275950000000016	1.6052029999999999
Se	7.6368830000000001	25.4337720000000012	1.3262810000000000
Se	6.1606199999999998	28.3855719999999998	1.5887830000000001
Se	4.3819660000000002	31.1983260000000016	1.1587140000000000
Se	2.7963580000000001	32.2408250000000010	4.8644049999999996
Se	6.1336810000000002	32.3632440000000017	4.9423139999999997
Se	-0.4197160000000000	34.0315510000000003	3.7693930000000000
Se	2.7846310000000001	34.3590119999999999	1.7118190000000000
Se	29.1312730000000002	-2.3201060000000000	5.0830640000000002
Se	27.5449400000000004	0.6788220000000000	5.2721510000000000
Se	25.7770550000000007	3.5772439999999999	5.3155760000000001
Se	24.0439089999999993	6.4655310000000004	5.3648680000000004
Se	22.3690449999999998	9.2482980000000001	5.3448430000000000
Se	20.7335269999999987	12.0323860000000007	5.3341969999999996
Se	19.0981899999999989	14.8369230000000005	5.3354439999999999
Se	17.4858399999999996	17.6423850000000009	5.3504529999999999
Se	15.8913449999999994	20.4800819999999995	5.3576180000000004
Se	14.1287000000000003	23.4440349999999995	5.0396919999999996
Se	12.5766989999999996	26.4016349999999989	5.3110020000000002
Se	11.0341769999999997	29.3406869999999991	4.7950070000000000
Se	32.5646089999999973	-2.1253180000000000	5.1811400000000001
Se	30.8859250000000003	0.6845300000000000	4.7317419999999997
Se	29.0699240000000003	3.5871580000000001	5.2865159999999998
Se	27.4100239999999999	6.5053060000000000	4.8201450000000001
Se	25.8079609999999988	9.3756909999999998	4.9370039999999999
Se	24.2003939999999993	12.1603320000000004	4.9194469999999999
Se	22.5667599999999986	14.9774010000000004	4.9248719999999997
Se	20.9264420000000015	17.7929349999999999	4.9326160000000003
Se	19.2943190000000016	20.5778959999999991	4.9603299999999999
Se	17.5773709999999994	23.4103999999999992	4.8149660000000001
Se	15.8891340000000003	26.3046180000000014	5.3608950000000002
Se	14.2909710000000008	29.3087079999999993	4.8441150000000004
Se	25.7691909999999993	-0.2191630000000000	1.9413840000000000

Se	24.0855630000000005	2.5973850000000001	2.0386009999999999
Se	22.3647649999999985	5.3861070000000000	2.0505779999999998
Se	20.6554549999999999	8.2232009999999995	1.9759070000000001
Se	19.0114160000000005	11.0412970000000001	1.9679080000000000
Se	17.3774659999999983	13.8484259999999999	1.9750010000000000
Se	15.7435820000000000	16.6634700000000002	1.9816920000000000
Se	14.1320470000000000	19.4891739999999984	2.0046659999999998
Se	12.5887680000000000	22.4301509999999986	2.0268299999999999
Se	10.9529899999999998	25.3828269999999989	1.4649859999999999
Se	9.4478200000000001	28.4127580000000002	1.8462069999999999
Se	7.7325629999999999	31.2387510000000006	1.5150159999999999
Se	29.3098390000000002	-0.1337870000000000	1.6806760000000001
Se	27.5134410000000003	2.6452030000000000	1.4950490000000001
Se	25.8393130000000006	5.5197630000000002	1.7102029999999999
Se	24.0546159999999993	8.3707259999999994	1.5298750000000001
Se	22.4595580000000012	11.1921079999999993	1.5401300000000000
Se	20.8515559999999986	13.9933720000000008	1.5554010000000000
Se	19.2206870000000016	16.7786200000000001	1.5468430000000000
Se	17.5766509999999982	19.5556899999999985	1.5290180000000000
Se	15.9561430000000009	22.5051909999999999	1.6980599999999999
Se	14.2266860000000008	25.3606699999999989	1.5410150000000000
Se	12.6984899999999996	28.4005870000000016	1.9813300000000000
Se	11.1373010000000008	31.3627940000000009	1.4047110000000000
Se	9.4626210000000004	32.4248460000000023	5.1533650000000000
Se	12.7094830000000005	32.4791269999999983	5.2325100000000004
Se	6.0804109999999998	34.5248009999999965	2.1615829999999998
Se	9.4075959999999998	34.6869990000000001	2.4626990000000002
Se	34.3456479999999971	0.6840110000000000	5.4190019999999999
Se	32.5127549999999985	3.5978850000000002	4.9346209999999999
Se	30.7581769999999999	6.4676559999999998	5.3209910000000002
Se	29.1984460000000006	9.3598009999999991	5.4017929999999996
Se	27.5813449999999989	12.1997090000000004	5.4345420000000004
Se	25.9361110000000004	15.0317580000000000	5.4489140000000003

Se	24.2834420000000009	17.8779539999999990	5.4543509999999999
Se	22.6258620000000015	20.7206940000000017	5.4429809999999996
Se	20.9487330000000007	23.5451300000000003	5.4133630000000004
Se	19.2401510000000009	26.3319989999999997	5.3694170000000003
Se	17.5626110000000004	29.2755529999999986	4.8870690000000003
Se	35.9672109999999989	3.5040950000000000	5.4493060000000000
Se	34.1672319999999985	6.4978389999999999	4.8638620000000001
Se	32.6295629999999974	9.4367509999999992	4.9425450000000000
Se	31.0344240000000013	12.2749869999999994	4.9525110000000003
Se	29.3876460000000002	15.1299869999999999	4.9672289999999997
Se	27.7244530000000005	17.9779739999999997	4.9740849999999996
Se	26.0635970000000015	20.8322229999999990	4.9706219999999997
Se	24.3953699999999998	23.6797669999999982	4.9604369999999998
Se	22.7256819999999991	26.4740409999999997	4.9553269999999996
Se	20.9211390000000002	29.2630090000000003	4.8624770000000002
Se	32.5700369999999992	-0.2902760000000000	1.7190820000000000
Se	30.9783140000000010	2.6604380000000001	2.0022009999999999
Se	29.0489139999999999	5.6056150000000002	1.8209750000000000
Se	27.3984039999999993	8.4366059999999994	2.0341060000000000
Se	25.8070500000000003	11.2307659999999991	2.0910190000000002
Se	24.1995849999999990	14.0463600000000000	2.1192940000000000
Se	22.5675190000000008	16.8640940000000015	2.1275840000000001
Se	20.9211980000000004	19.6636489999999995	2.1104400000000001
Se	19.2722039999999986	22.4361479999999993	2.0413800000000002
Se	17.6331300000000013	25.2559600000000017	1.8066720000000001
Se	15.9882419999999996	28.3417110000000001	2.0532130000000000
Se	14.3821770000000004	31.3004290000000012	1.4898640000000001
Se	36.3680250000000029	-0.5274150000000000	2.7426740000000001
Se	34.4013670000000005	2.5883240000000001	1.5920770000000000
Se	32.5717179999999971	5.4365309999999996	2.0222739999999999
Se	30.8379200000000004	8.4577109999999998	1.5799049999999999
Se	29.2448820000000005	11.3154009999999996	1.6090739999999999
Se	27.6334860000000013	14.1334610000000005	1.6520140000000001

Se	25.989197999999982	16.964625000000016	1.6726030000000001
Se	24.336048000000017	19.797294999999983	1.6660029999999999
Se	22.6778230000000001	22.601455000000014	1.6277919999999999
Se	20.9930190000000003	25.404208000000006	1.5916630000000000
Se	19.2074660000000002	28.360758000000006	2.0117520000000000
Se	17.635290999999987	31.294021000000008	1.5582450000000001
Se	15.9176850000000005	32.446919000000012	5.3001209999999999
Se	19.1686130000000006	32.353932000000004	5.3580280000000000
Se	12.7558430000000005	34.624358000000009	2.3392659999999998
Se	16.0719400000000014	34.605921999999996	2.4252680000000000
Se	37.5360540000000000	6.4073580000000003	5.3213759999999999
Se	36.000785999999980	9.430913999999996	5.390545999999996
Se	34.392811999999993	12.302025000000004	5.396888999999998
Se	32.7401040000000023	15.157667999999993	5.4202820000000003
Se	31.079595999999987	18.018291999999989	5.4424910000000004
Se	29.4144930000000002	20.875796000000011	5.4441860000000002
Se	27.7473630000000000	23.735627000000009	5.4239069999999998
Se	26.0820900000000009	26.593032999999984	5.3960400000000002
Se	24.3759070000000015	29.424189999999994	5.375944999999998
Se	39.7596750000000014	9.417045999999991	4.4050520000000004
Se	38.126488999999994	12.467627000000002	4.409347999999996
Se	36.4645300000000034	15.375899999999997	4.4558980000000004
Se	34.796332999999971	18.254948999999999	4.489372999999996
Se	33.121426999999971	21.121493000000010	4.5119420000000003
Se	31.453576999999992	23.991119999999987	4.489499999999996
Se	29.7780500000000004	26.865107999999993	4.4458880000000001
Se	28.081611999999998	29.754418000000011	4.3759839999999999
Se	38.0524180000000030	2.441167999999998	2.7381350000000002
Se	35.936444999999991	5.6414780000000002	1.8172459999999999
Se	34.1688509999999965	8.476276999999996	2.0525220000000002
Se	32.600006999999980	11.3358740000000004	2.0971320000000002
Se	30.979749999999992	14.177374999999996	2.1343410000000000
Se	29.3356250000000003	17.0144640000000003	2.1512080000000000

Se	27.6807720000000010	19.8531650000000006	2.1544129999999999
Se	26.0217290000000006	22.6857690000000005	2.1425640000000001
Se	24.3526859999999985	25.5008760000000017	2.1063339999999999
Se	22.6384979999999985	28.2720589999999987	2.0493500000000000
Se	21.0483440000000002	31.1870849999999997	1.7729649999999999
Se	39.6154799999999980	5.5120690000000003	2.5455459999999999
Se	37.6134490000000028	8.6682509999999997	1.6232599999999999
Se	36.0709459999999993	11.5487660000000005	1.6396930000000001
Se	34.4891099999999966	14.3977090000000008	1.6622539999999999
Se	32.8707139999999995	17.2199549999999988	1.6825939999999999
Se	31.2406129999999997	20.0266440000000010	1.6923070000000000
Se	29.6005830000000003	22.8262670000000014	1.6830870000000000
Se	27.9438719999999989	25.6235199999999992	1.6605090000000000
Se	26.2470950000000016	28.4030319999999996	1.6345780000000001
Se	24.5115820000000006	31.1600889999999993	1.6100540000000001
Se	22.4889370000000000	32.2558790000000002	5.2854799999999997
Se	26.2243269999999988	32.6737030000000033	4.3892870000000004
Se	19.3842700000000008	34.6460900000000009	2.6730049999999999
Se	22.7992530000000002	34.4673950000000033	2.4757780000000000
W	22.6082099999999997	-3.8030140000000001	3.2853930000000000
Se	22.0212259999999986	-6.1683399999999997	2.2204220000000001
Se	20.3384880000000017	-3.4155910000000000	2.5082570000000000
Se	24.1482980000000005	-3.0705010000000001	1.5550240000000000
Se	24.0256509999999999	-5.0859800000000002	4.9437870000000004
W	24.2782380000000018	-6.6412370000000003	2.9458090000000001
W	25.8061690000000006	-4.3950180000000003	3.1712349999999998
Se	23.7112349999999985	-8.8631510000000002	1.5868130000000000
Se	25.7248759999999983	-5.8961880000000004	1.0861860000000001
Se	25.6937910000000009	-7.9400310000000003	4.7384550000000001
Se	27.4480860000000000	-2.9709400000000001	1.6484920000000001
Se	27.6139170000000007	-5.2043609999999996	4.8582760000000000
W	25.6132500000000007	-9.4447510000000001	2.8380060000000000
W	27.1771470000000015	-6.7144930000000000	2.9017510000000000

W	29.064993999999987	-3.9523030000000001	3.1523010000000000
Se	25.506592999999987	-11.596869999999991	3.5514139999999998
Se	27.6033180000000016	-9.0370320000000000	1.6573070000000001
Se	29.2846200000000003	-6.2355049999999999	1.8041820000000000
Se	30.844149999999991	-3.2786520000000001	1.4174590000000000
W	32.358576999999968	-3.7220949999999999	3.3018610000000002
Se	31.248837999999992	-5.5341810000000002	4.2344549999999996
Se	34.5645340000000019	-3.4282560000000002	2.5133269999999999

W₁Se₂; $E_{tot} = -585\,786.557\,184\,49$ eV; $E_{rel} = 0$ meV/f.u.

W	-0.7471090000000000	2.9001999999999999	0.0991500000000000
Se	1.4886640000000000	2.7177539999999998	0.3196100000000000
Se	-1.6878730000000000	1.2033140000000000	-1.0477430000000001

W₂Se₄; $E_{tot} = -1\,171\,577.976\,800\,61$ eV; $E_{rel} = 56.080\,620\,500\,0$ meV/f.u.

W	0.6508389999999999	-0.2001480000000000	0.9445760000000000
Se	-0.7716499999999999	1.7252890000000001	1.6468719999999999
Se	-0.4337510000000000	-2.3270160000000000	0.2172230000000000
W	-0.2519010000000000	0.9276070000000000	-0.6588400000000000
Se	2.2424279999999999	0.9516340000000000	-0.5922150000000000
Se	-1.4359649999999999	-1.0773690000000000	-1.5576170000000000

W₂Se₄; $E_{tot} = -1\,171\,578.088\,961\,85$ eV; $E_{rel} = 0$ meV/f.u.

W	1.1288590000000001	0.2172830000000000	-0.6348310000000000
Se	1.1734819999999999	2.4281320000000002	-0.0971550000000000
Se	-0.6534600000000000	-0.4598890000000000	-2.1521020000000002
W	-0.7826320000000000	-1.0329530000000000	0.2131920000000000
Se	1.4116979999999999	-1.3214980000000001	1.2336890000000000
Se	-2.2779490000000000	0.1689240000000000	1.4372039999999999

W₃Se₆; $E_{tot}=-1\ 757\ 370.726\ 832\ 83\ \text{eV}$; $E_{rel}=138.034\ 723\ 666\ 6\ \text{meV/f.u.}$

W	-1.0722449999999999	0.8156330000000001	0.8688030000000000
Se	-2.2098369999999998	1.6938420000000001	-1.1620180000000000
Se	-2.1078929999999998	-0.8178430000000000	2.0665170000000002
W	1.2907660000000001	0.0673610000000000	0.2932570000000000
Se	0.9348940000000000	1.9130929999999999	1.8547220000000000
Se	1.6537580000000001	-2.3193350000000001	0.6790030000000000
W	-0.3970540000000000	0.0393300000000000	-1.4427829999999999
Se	1.8065519999999999	0.9788230000000000	-1.9301029999999999
Se	0.1010580000000000	-2.3709060000000002	-1.2273980000000000

W₃Se₆; $E_{tot}=-1\ 757\ 371.139\ 938\ 14\ \text{eV}$; $E_{rel}=0.332\ 953\ 666\ 6\ \text{meV/f.u.}$

W	1.4299630000000001	-0.1534170000000000	-0.3212400000000000
Se	3.2709850000000000	-1.4574790000000000	-0.7119510000000000
Se	0.0726680000000000	0.4906070000000000	-2.2581080000000000
W	-0.0523820000000000	0.6424609999999999	1.7265889999999999
Se	-1.9477400000000000	1.8805920000000000	0.8902160000000000
Se	-0.0373260000000000	-1.6966129999999999	1.0018819999999999
W	-1.4068760000000000	-0.1431650000000000	-0.4117440000000000
Se	1.8998500000000000	1.8686100000000001	1.0092030000000001
Se	-3.2291439999999998	-1.4315940000000000	-0.9248470000000000

W₄Se₈; $E_{tot}=-2\ 343\ 163.292\ 045\ 39\ \text{eV}$; $E_{rel}=26.548\ 352\ 750\ 0\ \text{meV/f.u.}$

W	-2.2172660000000000	1.3274900000000001	0.2271660000000000
Se	-1.4719110000000000	1.8087860000000000	-2.0412800000000000
Se	-3.7861370000000001	2.7797390000000002	1.0352380000000001
W	-0.4582380000000000	-0.8866120000000000	0.7030350000000000
Se	-2.9247049999999999	-1.0029800000000000	0.1909640000000000
Se	1.4720759999999999	-1.8088940000000000	2.0411280000000001
W	2.2173189999999998	-1.3273720000000000	-0.2268020000000000
Se	-0.2411930000000000	1.4395780000000000	1.6565900000000000

Se	3.7856160000000001	-2.7796699999999999	-1.0358010000000000
W	0.4585380000000000	0.8865610000000000	-0.7028460000000000
Se	2.9248509999999999	1.0028600000000001	-0.1909540000000000
Se	0.2410460000000000	-1.4394860000000000	-1.6564369999999999

W₄Se₈; $E_{tot} = -2\,343\,163.398\,238\,80$ eV; $E_{rel} = 0$ meV/f.u.

W	1.2622439999999999	-1.6482740000000000	-0.0381780000000000
Se	1.4567200000000000	-3.9033460000000000	-0.3574890000000000
Se	2.5707339999999999	-0.4919040000000000	-1.7360810000000000
W	-1.9499759999999999	0.6722310000000000	-0.2346870000000000
Se	-4.1190559999999996	0.1191730000000000	-0.6984030000000000
Se	-1.8225220000000000	1.5635159999999999	2.0279560000000001
W	0.3969030000000000	0.6714020000000001	1.4194880000000001
Se	-1.1276260000000000	2.1786539999999999	-1.9630300000000001
Se	1.8814270000000000	-1.1148769999999999	2.2560090000000002
W	0.8113690000000000	1.0445560000000000	-0.9424650000000000
Se	1.7916859999999999	2.5425339999999998	0.7126220000000000
Se	-1.1519050000000000	-1.6336660000000001	-0.4457410000000000

W₅Se₁₀; $E_{tot} = -2\,928\,954.275\,590\,47$ eV; $E_{rel} = 202.432\,842\,200\,0$ meV/f.u.

W	-0.4953670000000000	1.8638260000000000	-1.9647159999999999
Se	1.0217449999999999	3.2198410000000002	-0.7275940000000000
Se	0.4495300000000000	0.8384850000000000	-3.7693340000000002
W	-2.2219139999999999	0.7606050000000000	0.3468420000000000
Se	-2.9209390000000002	1.7050850000000000	-1.8078620000000001
Se	-3.4201410000000001	2.0893009999999999	1.7544709999999999
W	-0.4604010000000000	-1.4374180000000001	1.2461760000000000
Se	-2.8914260000000001	-1.5291580000000000	0.8000370000000000
Se	1.2675230000000000	-2.4282439999999998	2.6809150000000002
W	2.2149359999999998	-1.8163380000000000	0.5136920000000000
Se	-0.2683830000000000	0.9055320000000000	2.0296400000000001
Se	3.4888740000000000	-3.4852599999999998	-0.3773230000000000

W	0.7329390000000000	0.6329210000000000	-0.1773870000000000
Se	3.1920910000000000	0.3687480000000000	0.5159530000000000
Se	0.3109320000000000	-1.6879270000000000	-1.0635090000000000

W₅Se₁₀; $E_{tot} = -2\,928\,955.287\,754\,68$ eV; $E_{rel} = 0$ meV/f.u.

W	-2.1593249999999999	2.2980019999999999	0.5488600000000000
Se	0.1055820000000000	3.0327220000000001	0.6384240000000000
Se	-3.7740900000000002	3.8264670000000001	0.0379380000000000
W	-1.7932370000000000	-0.3913890000000000	0.9251170000000000
Se	-2.0596869999999998	0.7282040000000000	-1.3320060000000000
Se	-2.8054589999999999	1.1101770000000000	2.5964489999999998
W	0.4544860000000000	-1.9960230000000001	0.1958460000000000
Se	-1.9418160000000000	-2.6904400000000002	-0.0684150000000000
Se	2.6960780000000000	-2.8137770000000000	0.8114360000000000
W	2.7671709999999998	-1.2174320000000001	-1.0504500000000001
Se	0.4125240000000000	-0.3580360000000000	2.0570379999999999
Se	4.2959470000000000	-1.9359890000000000	-2.5837759999999999
W	0.2907250000000000	0.5471570000000000	-0.3081250000000000
Se	2.9119860000000002	1.0305780000000000	-0.2733920000000000
Se	0.5991160000000000	-1.1702210000000000	-2.1949420000000002

W₆Se₁₂; $E_{tot} = -3\,514\,746.992\,343\,94$ eV; $E_{rel} = 36.238\,360\,166\,6$ meV/f.u.

W	-1.4922740000000001	-2.6091120000000001	1.7015199999999999
Se	0.7287030000000000	-3.0015320000000001	2.3978609999999998
Se	-3.3901550000000000	-1.4554980000000000	2.5364369999999998
W	-1.7563489999999999	2.6817940000000000	-0.0206420000000000
Se	0.4720320000000000	3.4469850000000002	0.1477040000000000
Se	-3.0692970000000002	4.3193320000000002	-0.8743620000000000
W	-1.7266290000000000	-0.2804820000000000	0.8726030000000000
Se	-1.7834420000000000	0.8045909999999999	-1.5582250000000000
Se	-2.7173479999999999	1.8061460000000000	1.9874529999999999
W	0.7056730000000000	-1.6365149999999999	0.0985650000000000

Se	-1.6168469999999999	-2.5121349999999998	-0.6906040000000000
Se	3.1907230000000002	-2.0931419999999998	0.2860620000000000
W	2.9669569999999998	-0.5499230000000001	-1.5326820000000001
Se	0.5649030000000000	0.2964260000000000	1.6731000000000000
Se	4.4611499999999999	-0.9193010000000000	-3.2086380000000001
W	0.6358100000000000	0.9752800000000000	-0.7025410000000000
Se	3.0747770000000001	1.6887989999999999	-0.7128100000000001
Se	0.7516090000000000	-0.9617130000000000	-2.4008010000000000

W₆Se₁₂; $E_{tot} = -3\,514\,747.209\,774\,10$ eV; $E_{rel} = 0$ meV/f.u.

W	-3.7392050000000001	1.5155170000000000	0.6522740000000000
Se	-5.5663309999999999	2.2193619999999998	1.8182250000000000
Se	-3.8346380000000000	-0.7250360000000000	-0.1600260000000000
W	-1.1123010000000000	2.1466870000000000	-0.1487110000000000
Se	1.1105200000000000	2.8044039999999999	0.5602250000000000
Se	-3.1743749999999999	3.1263489999999998	-1.1021069999999999
W	-1.3076319999999999	-0.3533010000000000	0.3988610000000000
Se	-0.7144660000000000	0.5230910000000000	-1.9320459999999999
Se	-1.8493930000000001	1.4524010000000001	2.1764329999999998
W	1.1101610000000000	-2.1469870000000002	0.1434250000000000
Se	-1.1119049999999999	-2.8034599999999998	-0.5674709999999999
Se	3.1692290000000001	-3.1286820000000000	1.1010150000000001
W	3.7400229999999999	-1.5153479999999999	-0.6489590000000000
Se	0.7128090000000000	-0.5250870000000000	1.9285220000000001
Se	5.5739419999999997	-2.2170440000000000	-1.8053800000000000
W	1.3063780000000000	0.3532140000000000	-0.4017780000000000
Se	3.8324210000000001	0.7236740000000000	0.1667250000000000
Se	1.8547650000000000	-1.4497519999999999	-2.1792289999999999

W₇Se₁₄; $E_{tot} = -4\,100\,538.049\,657\,65$ eV; $E_{rel} = 96.713\,464\,428\,5$ meV/f.u.

W	-1.3851659999999999	-2.9522910000000002	1.8153340000000000
Se	0.9832910000000000	-3.0669759999999999	2.3694670000000002

Se	-1.8652340000000001	-0.9926070000000000	3.4258690000000001
W	-1.8441529999999999	2.6760510000000002	-0.0786590000000000
Se	0.3831960000000000	3.4661290000000000	0.0219840000000000
Se	-3.1545399999999999	4.2822319999999996	-0.9892190000000000
W	-1.7181999999999999	-0.4112630000000000	0.9001660000000000
Se	-1.8115300000000001	0.7101380000000000	-1.5092209999999999
Se	-2.7096510000000000	1.9031070000000001	1.9579990000000000
W	0.7347440000000000	-1.6368060000000000	0.2214160000000000
Se	-1.4780709999999999	-2.5721579999999999	-0.5848420000000000
Se	3.3449499999999999	-1.8636040000000000	0.4221020000000000
W	3.0343510000000000	-0.4593930000000000	-1.4592860000000001
Se	0.5776559999999999	0.3602430000000000	1.7093700000000001
Se	4.5573949999999996	-0.7906320000000000	-3.1162779999999999
W	0.6214870000000000	0.9693220000000000	-0.6626470000000000
Se	2.9953539999999998	1.8311530000000000	-0.7787120000000000
Se	0.8518559999999999	-1.0530210000000000	-2.2980630000000000
W	-3.6673190000000000	-2.2248779999999999	2.3964500000000002
Se	-3.1147320000000001	-4.5454150000000002	2.8141360000000000
Se	-4.3664670000000001	-1.0005510000000000	0.5207170000000000

W₇Se₁₄; $E_{tot} = -4\ 100\ 538.726\ 651\ 90\ \text{eV}$; $E_{rel} = 0\ \text{meV/f.u.}$

W	-3.4673910000000001	3.1717260000000000	1.0467830000000000
Se	-4.8980949999999996	4.8901909999999997	0.6070200000000000
Se	-1.2813720000000000	3.7363590000000002	1.7432350000000001
W	-3.1699720000000000	0.4074880000000000	0.8654690000000000
Se	-4.5975590000000004	1.5452560000000000	2.5011739999999998
Se	-3.2529830000000000	-1.5849040000000001	-0.4992160000000000
W	-0.8565510000000000	1.4921100000000000	0.2866210000000000
Se	1.5375900000000000	1.9963370000000000	0.9136160000000000
Se	-2.9809610000000002	2.0552940000000000	-1.0676270000000001
W	-0.7293040000000000	-1.2259659999999999	0.1734170000000000
Se	-0.3546300000000000	0.2893800000000000	-1.8504280000000000

Se	-1.2587860000000000	0.0250110000000000	2.3306650000000002
W	1.7719400000000001	-2.7400370000000001	-0.5678770000000000
Se	-0.4367320000000000	-3.3834179999999998	-1.3103170000000000
Se	3.8740220000000001	-3.8425620000000000	0.0443090000000000
W	4.3043089999999999	-1.7789680000000001	-1.2180759999999999
Se	1.3639310000000000	-1.6398429999999999	1.5694120000000000
Se	6.0855439999999996	-2.1147490000000002	-2.5993339999999998
W	1.6797660000000001	-0.1238030000000000	-0.4534170000000000
Se	4.3127409999999999	0.1775800000000000	0.1064570000000000
Se	2.3544879999999999	-1.3524820000000000	-2.6218849999999998

W₈Se₁₆; $E_{tot} = -4\,686\,330.095\,613\,00$ eV; $E_{rel} = 37.873\,656\,375\,0$ meV/f.u.

W	-1.3250770000000001	-2.9307699999999999	1.6861950000000001
Se	0.9546300000000000	-3.4900730000000002	2.1567880000000001
Se	-1.5964760000000000	-1.0632960000000000	3.2718120000000002
W	-1.6441880000000000	2.6497720000000000	-0.1177170000000000
Se	0.5574249999999999	3.4486990000000000	0.0337120000000000
Se	-2.9770050000000001	4.2390080000000001	-1.0185610000000000
W	-1.7676950000000000	-0.2735820000000000	0.8275000000000000
Se	-1.5504119999999999	0.7873030000000000	-1.6458729999999999
Se	-2.3731100000000001	2.0097640000000001	2.1574629999999999
W	0.9796130000000000	-1.6656860000000000	0.1979790000000000
Se	-1.3250690000000001	-2.3912760000000000	-0.6730280000000000
Se	3.4603419999999998	-2.0093030000000001	0.5732470000000000
W	3.2431960000000002	-0.6009400000000000	-1.3541740000000000
Se	0.6854000000000000	0.3238220000000000	1.6159150000000000
Se	4.7816859999999997	-1.0748489999999999	-2.9627750000000002
W	0.8410590000000000	0.9382230000000000	-0.7258940000000000
Se	3.2305259999999998	1.7305960000000000	-0.7694780000000000
Se	1.0817810000000001	-1.0758570000000001	-2.3045900000000001
W	-3.7242510000000002	-1.8200719999999999	2.3079540000000001
Se	-3.3460730000000001	-4.2681950000000004	1.9969319999999999

Se	-4.1732870000000002	-0.8868490000000000	0.0676970000000000
W	-4.5406789999999999	0.8287110000000000	1.7697950000000000
Se	-6.4297540000000000	1.9371000000000000	1.1503030000000001
Se	-4.9801029999999997	-0.3163620000000000	3.8452320000000002

W₈Se₁₆; $E_{tot} = -4\,686\,330.398\,602\,25$ eV; $E_{rel} = 0$ meV/f.u.

W	-5.2573829999999999	1.9437120000000001	0.7759210000000000
Se	-7.2611819999999998	2.1901809999999999	1.8326039999999999
Se	-5.0618069999999999	0.1147010000000000	-0.7168570000000000
W	-2.6001180000000002	2.9069870000000000	0.6292560000000000
Se	-4.5859490000000003	4.0689029999999997	-0.2384740000000000
Se	-0.5506030000000000	3.4882640000000000	1.7008909999999999
W	-2.6224900000000000	0.3287770000000000	0.3213020000000000
Se	-3.5723289999999999	1.4318880000000000	2.4532460000000000
Se	-2.2980139999999998	-1.7731669999999999	-1.0837019999999999
W	0.0447360000000000	1.3025329999999999	0.1587270000000000
Se	2.2959510000000001	1.7699840000000000	1.0817280000000000
Se	-1.8134180000000000	1.9480670000000000	-1.4790060000000000
W	-0.0473260000000000	-1.3143050000000001	-0.1506670000000000
Se	0.8258320000000000	0.2227460000000000	-1.9766330000000001
Se	-0.8357390000000000	-0.2367500000000000	1.9811140000000000
W	2.6060479999999999	-2.9124180000000002	-0.6181480000000000
Se	0.5526500000000000	-3.5098870000000000	-1.6752220000000000
Se	4.6070570000000002	-4.0537450000000002	0.2447590000000000
W	5.2583609999999998	-1.9317550000000001	-0.7881980000000000
Se	1.8190130000000000	-1.9465120000000000	1.4865349999999999
Se	7.2572840000000003	-2.1640160000000002	-1.8572130000000000
W	2.6193130000000000	-0.3335780000000000	-0.3225660000000000
Se	5.0616640000000004	-0.0966820000000000	0.6972790000000000
Se	3.5584479999999998	-1.4439270000000000	-2.4566750000000002

W₉Se₁₈; $E_{tot} = -5\,272\,121.852\,813\,44$ eV; $E_{rel} = 84.912\,525\,666\,6$ meV/f.u.

W	4.751808999999997	-4.220019999999999	-0.834411000000000
Se	5.991177999999997	-6.045020000000001	-0.259645000000000
Se	2.722917999999999	-4.608900000000002	-1.974227000000000
W	-5.757304000000004	2.710618999999999	0.764855000000000
Se	-7.751618999999998	3.007737000000001	1.828451000000000
Se	-5.589770999999998	0.885781000000000	-0.720793000000000
W	-3.116785999999998	3.614469000000002	0.673234000000000
Se	-5.037073999999996	4.848694000000001	-0.206362000000000
Se	-1.060190000000000	4.096172000000001	1.814599000000001
W	-3.101656000000002	1.009844000000000	0.340019000000000
Se	-4.108854000000000	2.089611000000001	2.454412000000000
Se	-2.843030000000002	-1.063226999999999	-1.016429000000000
W	-0.513460999999999	1.990423000000001	0.239021000000000
Se	1.781824000000001	2.437828000000001	1.139856000000000
Se	-2.320764000000000	2.667570000000000	-1.431467000000000
W	-0.482764000000000	-0.718510000000000	-0.059326000000000
Se	0.298592000000000	0.886488000000001	-1.865193000000001
Se	-1.367718000000000	0.386392000000000	2.027861000000001
W	2.137344999999998	-2.446187000000001	-0.455684000000000
Se	-0.120196000000000	-2.862660000000000	-1.426007999999999
Se	3.937743000000002	-3.202780999999999	1.229657000000000
W	4.567491000000004	-1.453043000000001	-0.508451000000000
Se	1.284535000000000	-1.356958000000001	1.624495000000000
Se	6.207133999999999	-2.576187000000000	-1.935317000000000
W	2.041461000000000	0.305507000000000	-0.154384000000000
Se	4.481562000000003	0.448642000000000	0.955648000000001
Se	2.967592999999999	-0.832287000000000	-2.244413999999999

W₉Se₁₈; $E_{tot} = -5\ 272\ 122.617\ 026\ 17\ \text{eV}$; $E_{rel} = 0\ \text{meV}/\mathbf{f.u.}$

W	32.782471000000010	12.755525999999997	2.667466999999998
W	31.398828999999992	15.281000000000006	3.058317000000002
W	29.971128000000002	18.059497000000004	3.552303000000002

W	34.166170000000010	15.281110999999992	3.0589160000000000
W	32.781993999999974	18.029275999999994	3.3917280000000001
W	31.364695000000011	20.718292000000017	3.8463759999999998
W	35.594988999999982	18.059736000000009	3.5527700000000002
W	34.200456000000026	20.718706999999984	3.8460320000000001
W	32.782758000000012	23.271498000000011	4.2325290000000004
Se	32.782631000000021	13.966284999999992	4.7610820000000000
Se	31.178488000000015	16.718081999999990	5.1479670000000004
Se	28.972145000000011	19.857804999999990	4.715678999999997
Se	34.386197000000028	16.718126000000016	5.1483600000000003
Se	32.782285000000017	19.610517999999990	5.4927950000000001
Se	30.735347000000009	22.663116999999997	5.3351590000000000
Se	36.593373999999972	19.857838000000010	4.714705999999996
Se	34.829751999999992	22.663350999999987	5.335265999999998
Se	32.782718000000027	25.463992999999985	3.6301660000000000
Se	32.782685000000007	10.555203999999998	3.2600600000000002
Se	30.742639000000005	13.396278999999998	1.5417240000000001
Se	29.025037999999986	16.349019999999994	2.2088310000000000
Se	34.822960000000019	13.396255000000000	1.5415010000000000
Se	32.782707000000020	16.428453000000011	1.3831580000000001
Se	31.140263999999984	19.253513999999991	1.7686400000000000
Se	36.539824000000030	16.349101999999985	2.209023999999999
Se	34.425075999999971	19.253308000000005	1.768014999999999
Se	32.782828999999996	22.023026999999990	2.158386999999998

W₁₀Se₂₀; $E_{tot} = -5\ 857\ 913.420\ 393\ 40\ \text{eV}$; $E_{rel} = 6.039\ 706\ 100\ 0\ \text{meV}/\mathbf{f.u.}$

W	3.2986810000000002	1.6166970000000001	1.4219200000000001
Se	5.260362999999999	1.1198020000000000	0.1959590000000000
Se	3.779446999999998	2.920999999999998	3.2114440000000002
W	4.702468999999998	-3.8304140000000002	-0.8142030000000000
Se	5.958492999999998	-5.7110750000000001	-0.5705290000000000
Se	3.130329999999998	-4.007705999999998	-2.6004730000000000

W	-6.2569920000000003	2.1878329999999999	0.5962330000000000
Se	-8.1362710000000007	2.5521370000000001	1.8375040000000000
Se	-6.1277629999999998	0.2360380000000000	-0.7256490000000000
W	-3.7222900000000001	3.1957800000000001	0.2615540000000000
Se	-5.7275369999999999	4.2267130000000002	-0.6792160000000000
Se	-1.5830510000000000	3.9147150000000002	1.2330939999999999
W	-3.5568170000000001	0.5767060000000001	0.0949380000000000
Se	-4.4531530000000004	1.7531829999999999	2.2023060000000001
Se	-3.3525369999999999	-1.5821460000000001	-1.2489830000000000
W	-1.1533650000000000	1.8262480000000001	-0.1261090000000000
Se	1.4688099999999999	2.5838709999999998	0.1195830000000000
Se	-3.0167160000000002	2.0855169999999998	-1.8275239999999999
W	-0.9768150000000000	-1.1977519999999999	-0.7463460000000000
Se	-0.0983930000000000	0.6784289999999999	-2.1138279999999998
Se	-1.6434180000000000	0.0648620000000000	1.5871350000000000
W	1.9377400000000000	-2.5763940000000001	-0.8042260000000000
Se	-0.1134580000000000	-2.8265940000000001	-2.3859599999999999
Se	3.3256429999999999	-3.5435099999999999	1.1425719999999999
W	3.9882279999999999	-1.1811449999999999	0.2213400000000000
Se	0.3221250000000000	-2.2723860000000000	1.0719790000000000
Se	6.0497189999999996	-1.8711850000000001	-1.0991670000000000
W	1.2566020000000000	0.0304510000000000	0.0422030000000000
Se	2.6340740000000000	-0.5119830000000000	2.3238129999999999
Se	2.8058519999999998	-0.4576920000000000	-1.8213630000000001

W₁₀Se₂₀; $E_{tot} = -5\ 857\ 913.480\ 790\ 46\ \text{eV}$; $E_{rel} = 0\ \text{meV}/\mathbf{f.u.}$

W	6.4142080000000004	-3.3104879999999999	-0.4445810000000000
Se	6.2107479999999997	-1.5324130000000000	1.0938859999999999
Se	8.4917490000000004	-3.6730640000000001	-1.3075190000000001
W	3.6995680000000002	-4.0655029999999996	-0.6056390000000000
Se	5.4858120000000001	-5.4183269999999997	0.3936010000000000
Se	1.7378960000000001	-4.4320579999999996	-1.9034519999999999

W	-6.419524000000000	3.2944070000000001	0.4480560000000000
Se	-8.502335999999997	3.6191520000000001	1.3131550000000001
Se	-6.200116999999997	1.5437820000000000	-1.1187170000000000
W	-3.7066940000000002	4.0635159999999999	0.6246890000000000
Se	-5.5023660000000003	5.421675999999997	-0.3523260000000000
Se	-1.7489980000000001	4.4184700000000001	1.9314730000000000
W	-3.8620239999999999	1.4960270000000000	0.1918040000000000
Se	-4.9603370000000000	2.5739209999999999	2.2614640000000001
Se	-3.6045400000000001	-0.5616719999999999	-1.2329410000000001
W	-1.1370720000000001	2.2590119999999998	0.3606710000000000
Se	1.0589510000000000	2.6216210000000002	1.3528780000000000
Se	-2.7481460000000002	3.1318090000000001	-1.4242690000000000
W	-1.3881859999999999	-0.3698870000000000	-0.0676040000000000
Se	-0.2331470000000000	1.1716290000000000	-1.7173339999999999
Se	-2.3216899999999998	0.7202140000000000	2.0017980000000000
W	1.1414350000000000	-2.2498279999999999	-0.3593240000000000
Se	-1.0538520000000000	-2.6117729999999999	-1.3574440000000001
Se	2.7539699999999998	-3.1044800000000001	1.4346960000000000
W	3.8657360000000001	-1.4921599999999999	-0.2048620000000000
Se	0.2399630000000000	-1.1504690000000000	1.7099150000000001
Se	4.9542339999999996	-2.6021850000000000	-2.2636219999999998
W	1.3956210000000000	0.3822140000000000	0.0533590000000000
Se	3.6179999999999999	0.5803650000000000	1.2026060000000001
Se	2.3211409999999999	-0.7235050000000000	-2.0144169999999999

$\mathbf{W}_{11}\mathbf{Se}_{22}$; $E_{tot} = -6\,443\,704.948\,266\,86\text{ eV}$; $E_{rel} = 11.935\,118\,272\,7\text{ meV/f.u.}$

W	-6.467597999999997	3.3270659999999999	0.4716520000000000
W	-3.7740520000000002	4.052292999999997	0.6510880000000000
W	-3.8968210000000001	1.4740949999999999	0.1841800000000000
W	-1.2419890000000000	2.2822230000000001	0.3312890000000000
W	-1.3595240000000000	-0.3966240000000000	-0.1169160000000000
W	1.2912450000000000	0.4620480000000000	0.0148260000000000

W	1.2495130000000001	-2.2960690000000001	-0.3825760000000000
W	3.8088660000000001	-1.3858090000000001	-0.2770480000000000
W	3.8078910000000001	-4.1444679999999998	-0.6141880000000000
W	6.2736789999999996	-3.2570770000000002	-0.5276690000000001
W	6.3543269999999996	-6.0297770000000002	-0.8766510000000000
Se	-8.5276800000000001	3.7210230000000002	1.3647890000000000
Se	-5.5287369999999996	5.4534940000000001	-0.3185850000000000
Se	-5.0126220000000004	2.5159989999999999	2.2589260000000002
Se	-6.2852090000000000	1.5706979999999999	-1.0912590000000000
Se	-1.8015260000000000	4.3642779999999997	1.9685600000000001
Se	-2.8620749999999999	3.1542110000000001	-1.4321600000000001
Se	-2.3422679999999998	0.6530490000000000	1.9590879999999999
Se	-3.6598039999999998	-0.5560250000000000	-1.2393149999999999
Se	0.9911660000000000	2.6161680000000000	1.3461559999999999
Se	-0.3204190000000000	1.2395270000000000	-1.7574710000000000
Se	0.2593430000000000	-1.1933650000000000	1.6555460000000000
Se	-1.0621370000000001	-2.5558139999999998	-1.3899670000000000
Se	3.6233860000000000	0.7416030000000000	0.9871230000000000
Se	2.2110919999999998	-0.6523940000000000	-2.0593370000000002
Se	1.5883959999999999	-4.4558439999999999	-1.7107260000000000
Se	6.2221650000000004	-1.3652650000000000	0.9384550000000000
Se	2.8697200000000000	-3.0409940000000000	1.4175570000000000
Se	4.7901790000000002	-2.5400019999999999	-2.3327900000000001
Se	4.3731520000000002	-6.3154139999999996	-2.1268120000000001
Se	5.4822259999999998	-4.9911870000000000	1.1549780000000001
Se	7.9297100000000000	-4.4402270000000001	-1.8851979999999999
Se	7.4902069999999998	-7.9106670000000001	-0.2696410000000000

W₁₁Se₂₂; $E_{tot} = -6\,443\,705.079\,553\,16$ eV; $E_{rel} = 0$ meV/f.u.

W	-5.8715669999999998	4.3906549999999998	1.3685920000000000
Se	-7.3080309999999997	6.1200089999999996	0.9804480000000000
Se	-3.7629920000000001	4.8444250000000002	2.3505029999999998

W	3.954032999999999	0.816696000000000	1.385574000000000
Se	5.837032999999999	0.465317000000000	-0.001768000000000
Se	4.546495000000000	1.873408000000000	3.299926000000000
W	5.142399000000000	-4.300332000000000	-1.608460999999999
Se	6.382359000000000	-6.206417000000000	-1.646852000000000
Se	3.498759999999999	-4.224149999999998	-3.332863999999998
W	-5.551418000000000	1.690120000000000	0.833095999999999
Se	-7.076214000000000	2.586743999999999	2.521563000000000
Se	-5.562567999999997	-0.123195000000000	-0.736417000000000
W	-3.217855999999998	2.834471000000000	0.652772000000000
Se	-5.183085000000000	3.567666000000000	-0.828032000000000
Se	-0.856930000000000	3.319615999999999	1.478278000000000
W	-3.010389000000000	0.113117000000000	0.124104000000000
Se	-3.745553000000000	1.046091000000000	2.376170000000000
Se	-2.872275999999998	-1.951626000000000	-1.354490000000000
W	-0.622285000000000	1.337943000000000	0.059886000000000
Se	2.089761999999999	1.963071999999999	0.305074000000000
Se	-2.461870999999999	1.895241000000000	-1.560273999999999
W	-0.461438000000000	-1.649547000000000	-0.975831000000000
Se	0.376747000000000	0.415430000000000	-2.068503000000000
Se	-1.077858999999999	-0.667455000000000	1.491527000000000
W	2.397063000000000	-3.025803999999999	-1.311453000000000
Se	0.291023000000000	-3.038797999999999	-2.845775000000000
Se	3.847687000000000	-4.255772000000000	0.424489000000000
W	4.521842999999996	-1.804302000000000	-0.208065000000000
Se	0.875347000000000	-2.936227999999998	0.665377000000000
Se	6.516254000000000	-2.339763000000000	-1.687089000000000
W	1.813062000000000	-0.547647000000000	-0.094562000000000
Se	3.287338000000000	-1.404299000000000	2.026241000000000
Se	3.265127999999998	-0.804684000000000	-2.083181000000000

$\mathbf{W}_{12}\mathbf{Se}_{24}$; $E_{tot} = -7\,029\,496.521\,113\,23$ eV; $E_{rel} = 136.598\,508\,416\,6$ meV/f.u.

W	-6.4612930000000004	3.3317990000000002	0.4511080000000000
W	-3.7512989999999999	4.0757700000000003	0.6282900000000000
W	-3.9030689999999999	1.5034179999999999	0.1911560000000000
W	-1.2006850000000000	2.2740809999999998	0.3556350000000000
W	-1.4020480000000000	-0.3669840000000000	-0.0949240000000000
W	1.3422490000000000	0.3903990000000000	0.0828800000000000
W	1.1504080000000001	-2.2816310000000000	-0.3958810000000000
W	3.8923340000000000	-1.5243420000000001	-0.1986220000000000
W	3.6995300000000002	-4.1636340000000001	-0.6604290000000000
W	6.3990729999999996	-3.3891300000000002	-0.4575450000000000
W	6.2577439999999998	-5.9609110000000003	-0.9056650000000001
W	8.9647089999999992	-5.2134650000000002	-0.6857780000000000
Se	-8.5371819999999996	3.6989589999999999	1.3173699999999999
Se	-5.5266950000000001	5.4505030000000003	-0.3543260000000000
Se	-5.0067360000000001	2.5788750000000000	2.2587799999999998
Se	-6.2607980000000003	1.5739980000000000	-1.1080820000000000
Se	-1.7962240000000000	4.4144470000000000	1.9488040000000000
Se	-2.8067790000000001	3.1430140000000000	-1.4278810000000000
Se	-2.3610150000000001	0.7004970000000000	1.9858330000000000
Se	-3.6640259999999998	-0.5455960000000000	-1.2260080000000000
Se	1.0043500000000001	2.6395780000000002	1.3439710000000000
Se	-0.2488190000000000	1.2168850000000000	-1.7113080000000001
Se	0.1812170000000000	-1.2194170000000000	1.6723619999999999
Se	-1.0751390000000001	-2.5246369999999998	-1.4494600000000000
Se	3.5629840000000002	0.6344950000000000	1.1494650000000000
Se	2.3197980000000000	-0.6709770000000000	-1.9789540000000001
Se	1.5072010000000000	-4.5143060000000004	-1.6811560000000001
Se	6.1391890000000000	-1.3496729999999999	0.9664950000000000
Se	2.7281179999999998	-3.1183299999999998	1.4021699999999999
Se	4.8794709999999997	-2.5819770000000002	-2.2697180000000001
Se	4.3190059999999999	-6.2992499999999998	-2.2503579999999999
Se	5.2849550000000001	-5.0376310000000002	1.1405390000000000
Se	8.7401780000000002	-3.4587080000000001	0.8734240000000000

Se	7.5347650000000002	-4.4567490000000003	-2.5117630000000002
Se	8.0198959999999992	-7.3337170000000000	0.1041880000000000
Se	11.0532620000000001	-5.5808130000000000	-1.5198140000000000

W₁₂Se₂₄; $E_{tot} = -7\,029\,498.160\,295\,33$ eV; $E_{rel} = 0$ meV/f.u.

W	34.3946650000000034	9.8587760000000006	2.7686750000000000
W	33.0310589999999991	12.5082070000000005	2.9429099999999999
W	31.3958860000000008	15.1742209999999993	3.1531419999999999
W	29.9051000000000009	18.1477210000000007	3.4506880000000000
W	35.8035190000000014	12.4319570000000006	3.1242580000000002
W	34.6724969999999999	15.0431299999999997	3.3227030000000002
W	32.5268709999999999	18.1779970000000013	3.5916489999999999
W	31.3959140000000012	20.7886969999999991	3.7891810000000001
W	37.2941190000000020	15.0735399999999995	3.4642279999999999
W	35.8036710000000014	18.0470480000000002	3.7619520000000000
W	34.1679200000000023	20.7130690000000008	3.9703279999999999
W	32.8045520000000010	23.3627280000000006	4.1419160000000002
Se	34.2783140000000017	11.1917240000000007	4.7811890000000004
Se	32.7096639999999965	14.0189649999999997	4.9077140000000004
Se	30.9848360000000014	16.7589870000000012	5.1530610000000001
Se	29.0055119999999995	19.9415319999999987	4.6920570000000001
Se	36.0628230000000016	13.9099780000000006	5.2317000000000000
Se	34.2369449999999986	16.8808779999999992	5.1360669999999997
Se	32.6628309999999971	19.6951819999999991	5.6372530000000003
Se	30.7673850000000009	22.7692949999999996	5.2460149999999999
Se	38.1684699999999992	17.1250490000000006	4.4354760000000004
Se	36.4557390000000012	20.0259350000000005	4.9731920000000001
Se	34.7164190000000019	22.7518640000000012	5.4342280000000001
Se	32.8128329999999977	25.5527920000000002	3.5226709999999999
Se	34.3864159999999970	7.6681299999999997	3.3844420000000000
Se	32.4828130000000002	10.4710889999999992	1.4763700000000000
Se	30.7437250000000013	13.1961080000000006	1.9410250000000000

Se	29.030780000000000	16.0960320000000010	2.4800789999999999
Se	36.4319220000000001	10.4532889999999998	1.6644450000000000
Se	34.5367669999999976	13.5274260000000002	1.2765890000000000
Se	32.9624540000000010	16.3403700000000001	1.7787160000000000
Se	31.1360290000000006	19.3097929999999991	1.6826260000000000
Se	38.1940099999999987	13.2798940000000005	2.2214049999999999
Se	36.2148979999999980	16.4622740000000007	1.7615590000000001
Se	34.4899369999999976	19.2016010000000001	2.0061789999999999
Se	32.9209960000000024	22.0281319999999994	2.1302569999999998

W₁₃Se₂₆; $E_{tot} = -7\,615\,288.018\,755\,50$ eV; $E_{rel} = 119.424\,446\,230\,7$ meV/f.u.

W	-6.5065429999999997	3.3666909999999999	0.4611540000000000
W	-3.8117850000000000	4.0791930000000001	0.6544980000000000
W	-3.9459130000000000	1.5042130000000000	0.1689610000000000
W	-1.2842300000000000	2.2900209999999999	0.3527620000000000
W	-1.4212149999999999	-0.3744780000000000	-0.1294410000000000
W	1.2474590000000001	0.4456520000000000	0.0654260000000000
W	1.1793870000000000	-2.2839909999999999	-0.4244520000000000
W	3.8105470000000001	-1.4242030000000001	-0.2089590000000000
W	3.7891219999999999	-4.1923170000000001	-0.6126520000000000
W	6.3381239999999996	-3.2853530000000002	-0.4506430000000000
W	6.3398859999999999	-6.0450780000000002	-0.7990830000000000
W	8.8081519999999998	-5.1686150000000000	-0.6500720000000000
W	8.8795140000000004	-7.9407860000000001	-1.0026040000000001
Se	-8.5638070000000006	3.7671559999999999	1.3591480000000000
Se	-5.5555190000000003	5.4933750000000003	-0.3152230000000000
Se	-5.0619030000000000	2.5422289999999998	2.2488320000000002
Se	-6.3292089999999996	1.6203580000000000	-1.1131240000000000
Se	-1.8506680000000000	4.3771950000000004	1.9902210000000000
Se	-2.8819230000000000	3.1864710000000001	-1.4233320000000000
Se	-2.4141070000000000	0.6555860000000000	1.9509570000000001
Se	-3.7072490000000000	-0.5084630000000000	-1.2788029999999999

Se	0.9205690000000000	2.5989749999999998	1.4142589999999999
Se	-0.3258950000000000	1.2671960000000000	-1.7280040000000001
Se	0.1560510000000000	-1.2405230000000000	1.6358919999999999
Se	-1.1178779999999999	-2.5123240000000000	-1.4470930000000000
Se	3.5362179999999999	0.7285140000000000	1.0638000000000001
Se	2.2483680000000001	-0.6019490000000000	-1.9990630000000000
Se	1.4948420000000000	-4.4565619999999999	-1.6584399999999999
Se	2.7462770000000001	-3.0921940000000001	1.3948600000000000
Se	4.7788209999999998	-2.5365929999999999	-2.2642730000000002
Se	4.1469790000000000	-6.3440789999999998	-1.9480960000000000
Se	6.1483330000000000	-1.1634249999999999	0.7993390000000000
Se	5.3641930000000002	-4.9436590000000002	1.2176650000000000
Se	7.3685140000000002	-4.4344039999999998	-2.4859320000000000
Se	6.9334220000000002	-8.2140920000000008	-2.3055759999999998
Se	8.7303359999999994	-3.2850869999999999	0.8225710000000001
Se	7.9664809999999999	-6.9024000000000001	1.0091630000000000
Se	10.4921220000000002	-6.3595759999999997	-1.9660510000000000
Se	9.9885769999999994	-9.8273419999999998	-0.3635660000000000

$\mathbf{W}_{13}\mathbf{Se}_{26}$; $E_{tot} = -7\,615\,289.569\,732\,55$ eV; $E_{rel} = 0.118\,519\,307\,6$ meV/f.u.

W	2.2143000000000002	-6.2780480000000001	-1.4760340000000001
Se	1.7453760000000000	-8.0040750000000003	-2.8857240000000002
Se	0.4203250000000000	-5.4929170000000003	-0.1891530000000000
W	-1.1205060000000000	4.6607279999999998	1.1934890000000000
Se	-2.8002419999999999	6.0325590000000000	0.2487040000000000
Se	0.7841990000000000	5.0526530000000003	2.6491560000000001
W	1.5446679999999999	3.0244580000000001	1.2282940000000000
Se	0.1663440000000000	3.9169969999999998	-0.7317810000000000
Se	2.7850290000000002	2.0134020000000001	-0.7462150000000000
W	3.9218169999999999	1.2626720000000000	1.2869060000000001
Se	5.8508639999999996	0.3229890000000000	0.2097170000000000
Se	3.6321580000000000	3.1959010000000001	2.7026029999999999

W	4.1568160000000001	-4.4310330000000002	-0.6365300000000000
Se	4.2117019999999998	-6.8394149999999998	-0.1630250000000000
Se	2.7589890000000001	-4.2877200000000002	-2.7717139999999998
W	-6.4185309999999998	2.4877310000000001	-0.2822630000000000
Se	-8.6137040000000002	2.5499939999999999	0.3078680000000000
Se	-5.9561219999999997	0.8432190000000001	-1.9401960000000000
W	-3.7715339999999999	3.5521600000000002	0.4351380000000000
Se	-5.6356200000000003	4.6665880000000000	-0.8769540000000000
Se	-2.3817390000000001	3.0892840000000001	2.5727980000000001
W	-3.8933849999999999	0.8324279999999999	-0.3771280000000000
Se	-5.1664149999999998	1.7506240000000000	1.6543420000000000
Se	-3.4591219999999998	-1.2121630000000001	-1.8788279999999999
W	-1.2890219999999999	2.0949550000000001	0.4409830000000000
Se	0.4012620000000000	1.1422110000000001	2.1623060000000001
Se	-2.7412150000000000	2.6039889999999999	-1.6211070000000001
W	-1.3952490000000000	-0.9930010000000000	-0.6591430000000000
Se	-0.0052730000000000	0.7386870000000000	-1.4779320000000000
Se	-2.4677699999999998	-0.1222940000000000	1.4472280000000000
W	1.8596770000000000	-3.1611199999999999	-0.6174170000000000
Se	-0.4349960000000000	-2.8184220000000000	-1.9914499999999999
Se	3.2880620000000000	-3.7152050000000001	1.5227370000000000
W	4.0671830000000000	-1.6314070000000001	0.3389360000000000
Se	0.2221800000000000	-2.0813880000000000	1.0846309999999999
Se	5.8199880000000004	-2.7944640000000001	-1.2342089999999999
W	1.8185570000000000	-0.1499270000000000	0.3353010000000000
Se	3.1199360000000000	-0.6791540000000000	2.5186920000000002
Se	2.7610079999999999	-1.1424810000000001	-1.7830269999999999

$W_{14}Se_{28}$; $E_{tot} = -8\,201\,079.566\,448\,13\text{ eV}$; $E_{rel} = 177.343\,202\,214\,2\text{ meV/f.u.}$

W	-6.4925750000000004	3.3634189999999999	0.4532600000000000
W	-3.7874379999999999	4.0973269999999999	0.6285849999999999
W	-3.9325709999999998	1.5219579999999999	0.1883420000000000

W	-1.2467420000000000	2.2947340000000001	0.3582220000000000
W	-1.4270879999999999	-0.3583250000000000	-0.1029510000000000
W	1.2850130000000000	0.4136440000000000	0.1000190000000000
W	1.1376230000000001	-2.2781579999999999	-0.4209840000000000
W	3.8367510000000000	-1.5182890000000000	-0.1277560000000000
W	3.7040440000000001	-4.2030310000000002	-0.6717350000000000
W	6.4071579999999999	-3.4242149999999998	-0.4056570000000000
W	6.2576890000000001	-6.0672069999999998	-0.9104360000000000
W	8.9354089999999999	-5.2745249999999997	-0.6664410000000000
W	8.8246120000000001	-7.8461499999999997	-1.1403669999999999
W	11.5191700000000008	-7.0861409999999996	-0.9008020000000000
Se	-8.5603429999999996	3.7415500000000002	1.3334740000000000
Se	-5.5535430000000003	5.4815389999999997	-0.3539680000000000
Se	-5.0374900000000000	2.5934750000000002	2.2552910000000002
Se	-6.3020009999999997	1.6022989999999999	-1.1031340000000001
Se	-1.8293539999999999	4.4243040000000002	1.9543280000000001
Se	-2.8467120000000001	3.1690689999999999	-1.4296240000000000
Se	-2.3966129999999999	0.7024560000000000	1.9790070000000000
Se	-3.7043439999999999	-0.5185580000000000	-1.2338350000000000
Se	0.9530820000000000	2.6290439999999999	1.3928179999999999
Se	-0.2818430000000000	1.2444759999999999	-1.7060360000000001
Se	0.1415750000000000	-1.2403210000000000	1.6582490000000001
Se	-1.1203590000000001	-2.4929540000000001	-1.4608449999999999
Se	3.5222380000000002	0.6663559999999999	1.1552810000000000
Se	2.3197190000000001	-0.6170620000000000	-1.9435060000000000
Se	1.4744139999999999	-4.4369940000000003	-1.7461130000000000
Se	2.6521029999999999	-3.1960660000000001	1.3786579999999999
Se	4.8728899999999999	-2.5301969999999998	-2.1941970000000000
Se	4.0872770000000003	-6.3813680000000002	-2.0104570000000002
Se	6.0676079999999999	-1.3162529999999999	0.9794030000000000
Se	5.2376050000000003	-5.0614280000000003	1.1473590000000000
Se	8.6560799999999993	-3.2631039999999998	0.7833560000000001
Se	7.4346269999999999	-4.4428400000000003	-2.4799920000000002

Se	6.8954420000000001	-8.1772320000000001	-2.5078809999999998
Se	7.8271980000000001	-6.9495430000000002	0.9044320000000000
Se	11.2818980000000000	-5.3396059999999999	0.6657780000000000
Se	10.0927030000000002	-6.3128349999999998	-2.7246229999999998
Se	10.5839549999999996	-9.2176410000000004	-0.1283230000000000
Se	13.6069940000000003	-7.4386780000000003	-1.7433940000000001

W₁₄Se₂₈; $E_{tot} = -8\,201\,082.049\,252\,96$ eV; $E_{rel} = 0$ meV/f.u.

W	36.2567519999999988	1.4524220000000001	3.4479080000000000
W	34.8748750000000030	3.8476520000000001	3.4441649999999999
W	39.5455949999999987	1.2290950000000000	3.6208309999999999
W	37.5203190000000006	3.7792710000000000	3.4799829999999998
W	36.3243790000000004	6.8085589999999998	3.6168740000000001
W	42.4849880000000013	1.1508309999999999	3.8416720000000000
W	41.3386560000000003	3.7551130000000001	3.6526679999999998
W	39.4089719999999986	7.0972949999999999	3.6525810000000001
W	37.7262490000000028	9.3921679999999999	3.8416280000000000
W	45.5010290000000026	1.0346820000000001	3.9715720000000001
W	43.9677000000000007	3.7475630000000000	3.8495720000000002
W	42.4741890000000026	6.6383029999999996	3.7601879999999999
W	40.7187600000000032	9.3776080000000004	3.8517210000000000
W	39.1334159999999969	12.0613600000000005	3.9740530000000001
Se	37.5334100000000035	-0.3251670000000000	4.4931250000000000
Se	36.0381259999999983	2.9250609999999999	5.4321229999999998
Se	33.9710759999999965	5.8434939999999997	4.4880950000000004
Se	40.8466740000000001	-0.5954100000000000	4.5752160000000002
Se	39.3497920000000008	2.9641899999999999	5.2290760000000001
Se	37.7277569999999969	5.7724399999999996	5.2274859999999999
Se	35.3940809999999999	8.8466850000000008	4.5709920000000004
Se	44.0512519999999981	-0.4827020000000000	5.0873460000000001
Se	42.5564699999999974	2.7729279999999998	5.6806140000000003
Se	40.9026509999999988	5.7317689999999999	5.3198770000000000

Se	39.164949999999975	8.643276999999994	5.680953999999998
Se	37.094383999999980	11.564403000000004	5.087437999999997
Se	47.366379999999995	-0.030258000000000	3.239405999999998
Se	46.059809999999988	2.935121999999998	5.257068000000003
Se	44.674061000000018	5.969966999999996	4.783648000000003
Se	42.994947000000034	8.875866999999995	4.787262000000001
Se	41.058888000000032	11.595098000000001	5.259972000000003
Se	39.143270999999986	14.209374999999996	3.242157000000002
Se	34.116242999999972	1.811647000000000	2.276406999999998
Se	37.932518999999992	1.916403000000001	1.710707999999999
Se	36.115485999999971	5.066643000000000	1.707794000000000
Se	41.131127999999968	1.972888999999999	1.833537999999999
Se	39.493389999999980	4.917932999999997	2.207155000000002
Se	37.763404999999988	7.809255000000003	1.832627999999999
Se	44.318055000000011	1.944458999999999	2.061611000000001
Se	42.896977999999972	4.975756999999998	1.929048000000001
Se	41.246490000000014	7.836691000000001	1.930344000000001
Se	39.332067999999996	10.583498999999998	2.064973000000002

$\mathbf{W}_{15}\mathbf{Se}_{30}$; $E_{tot} = -8\,786\,871.085\,215\,88$ eV; $E_{rel} = 162.622\,492\,066\,6$ meV/f.u.

W	-6.534473000000002	3.363008999999999	0.459076000000000
W	-3.839971999999999	4.080822999999996	0.679729000000000
W	-3.968054000000000	1.508750000000000	0.179871000000000
W	-1.306362000000000	2.296181999999999	0.383658000000000
W	-1.442250999999999	-0.364311000000000	-0.115362000000000
W	1.233004999999999	0.448844000000000	0.093425000000000
W	1.150517000000000	-2.267796999999998	-0.417917000000000
W	3.797763000000002	-1.429738000000000	-0.186820000000000
W	3.755946999999999	-4.171044000000002	-0.677675000000000
W	6.373993999999997	-3.298013999999998	-0.462424000000000
W	6.359793999999999	-6.067287000000003	-0.898605000000000
W	8.905620000000008	-5.162077000000000	-0.707037000000000

W	8.9068079999999998	-7.9162160000000004	-1.1234470000000001
W	11.3742990000000006	-7.0506200000000003	-0.9296710000000000
W	11.4401240000000008	-9.8144880000000008	-1.3682110000000001
Se	-8.5998540000000006	3.7527599999999999	1.3412660000000001
Se	-5.5801749999999997	5.4954799999999997	-0.2968720000000000
Se	-5.1018470000000002	2.5328040000000001	2.2552409999999998
Se	-6.3398209999999997	1.6269899999999999	-1.1241099999999999
Se	-1.8891020000000001	4.3768710000000004	2.0284030000000000
Se	-2.8932620000000000	3.2004570000000001	-1.3959960000000000
Se	-2.4457800000000001	0.6532800000000000	1.9668650000000001
Se	-3.7227839999999999	-0.4976890000000000	-1.2746109999999999
Se	0.8932200000000000	2.6105890000000000	1.4444210000000000
Se	-0.3354780000000000	1.2865759999999999	-1.6981320000000000
Se	0.1328960000000000	-1.2406670000000000	1.6506390000000000
Se	-1.1402550000000000	-2.4915330000000000	-1.4496780000000000
Se	3.5006879999999998	0.7217130000000000	1.1130370000000001
Se	2.2405160000000000	-0.5805840000000000	-1.9733010000000000
Se	1.4471270000000001	-4.4376350000000002	-1.6668630000000000
Se	2.7153520000000002	-3.1284559999999999	1.3712850000000001
Se	4.8062279999999999	-2.4749050000000001	-2.2503120000000001
Se	4.0668430000000004	-6.3266450000000001	-1.9411300000000000
Se	6.1107500000000003	-1.1539390000000000	0.8014960000000000
Se	5.3241139999999998	-4.9850630000000002	1.1293679999999999
Se	7.3566729999999998	-4.3843300000000003	-2.5202220000000000
Se	6.7214580000000002	-8.1856810000000007	-2.2888229999999998
Se	8.7178850000000008	-3.0614669999999999	0.5645730000000000
Se	7.9252950000000002	-6.8629810000000004	0.9179270000000000
Se	11.2910559999999993	-5.2060380000000004	0.5882080000000000
Se	9.9534280000000006	-6.2618900000000002	-2.7573420000000000
Se	9.5047730000000001	-10.0359300000000005	-2.6971959999999999
Se	10.5161650000000009	-8.8339680000000005	0.6684880000000000
Se	13.0654219999999999	-8.2089140000000000	-2.2657810000000000
Se	12.5323910000000005	-11.7301730000000006	-0.7897140000000000

W₁₅Se₃₀; $E_{tot} = -8\,786\,873.524\,553\,26$ eV; $E_{rel} = 0$ meV/f.u.

W	5.434720999999997	-0.601981000000000	0.949646000000000
Se	5.254713999999999	0.952773000000000	2.718376999999998
Se	7.309391999999999	-1.479754000000000	-0.173244000000000
W	5.332042999999996	-5.970353000000002	-1.705032000000001
Se	6.094661999999996	-8.101839999999993	-1.488348999999999
Se	3.739421999999998	-5.702567000000002	-3.454143999999999
W	5.377848000000002	-3.371770999999999	-0.414605000000000
Se	4.423237000000003	-2.640683000000001	1.835077000000001
Se	7.182218999999999	-4.431172000000001	-1.784465000000000
W	-2.362670000000000	4.658501000000002	1.957597000000000
Se	-4.022199999999998	6.189993000000003	1.282270000000000
Se	-0.447163000000000	4.796438000000002	3.390902000000001
W	0.416762000000000	2.971499999999998	1.587731999999999
Se	-1.025446000000001	4.289669000000000	-0.060344000000000
Se	1.669856999999999	2.499826999999998	-0.518751000000000
W	2.903783999999999	1.342295999999999	1.316511000000000
Se	4.299268999999998	0.747892000000000	-0.735958000000000
Se	2.449936999999998	3.058679999999998	3.018622999999998
W	2.894966000000002	-4.175709000000003	-1.528583000000000
Se	4.110269999999999	-5.489474000000004	0.322307000000000
Se	0.895828000000000	-4.151684999999996	-3.133691999999999
W	-7.698443000000001	2.865266000000001	-0.047419000000000
Se	-9.902062000000008	2.805019999999998	0.513394000000000
Se	-7.201825000000004	1.625423000000001	-2.020119999999999
W	-5.061377000000002	3.723514000000002	0.944334000000000
Se	-6.899532999999999	5.119258999999996	-0.103389000000000
Se	-3.699072000000001	2.874934000000001	2.959144000000002
W	-5.167321000000003	1.271566999999999	-0.458896000000000
Se	-6.489124999999996	1.728694000000000	1.713811999999999
Se	-4.639319999999997	-0.326740000000000	-2.402028000000001
W	-2.588473000000000	2.324679999999999	0.676932000000000

Se	-0.9030560000000000	1.0709860000000000	2.2272490000000000
Se	-3.9869990000000000	3.2695630000000002	-1.2559020000000001
W	-2.6993350000000000	-0.4207970000000000	-0.9890460000000000
Se	-1.2516910000000001	1.3936379999999999	-1.4613039999999999
Se	-3.7926720000000000	-0.0069340000000000	1.2019850000000001
W	0.3984740000000000	-2.5221410000000000	-1.4308970000000001
Se	-1.8715999999999999	-2.2585470000000001	-2.5301279999999999
Se	1.5322220000000000	-3.5769989999999998	0.5029960000000000
W	3.0059429999999998	-1.4513149999999999	-0.0401040000000000
Se	-1.1010620000000000	-1.8088700000000000	0.5062090000000000
Se	4.2095680000000000	-2.2431820000000000	-2.2368549999999998
W	0.5493160000000000	0.3106600000000000	0.2271020000000000
Se	1.8247260000000001	-0.6899670000000000	2.1349459999999998
Se	1.5012570000000001	-0.4682960000000000	-2.0138899999999998

W₁₆Se₃₂; $E_{tot} = -9\,372\,662.617\,667\,02$ eV; $E_{rel} = 201.621\,371\,312\,5$ meV/f.u.

W	-6.5312739999999998	3.3929220000000000	0.4571990000000000
W	-3.8304279999999999	4.1194509999999998	0.6367170000000000
W	-3.9707189999999999	1.5442760000000000	0.1882570000000000
W	-1.2927280000000001	2.3192759999999999	0.3630120000000000
W	-1.4584410000000001	-0.3352040000000000	-0.1090250000000000
W	1.2387319999999999	0.4407500000000000	0.1084750000000000
W	1.1109789999999999	-2.2574299999999998	-0.4262310000000000
W	3.7909750000000000	-1.4812460000000001	-0.1263020000000000
W	3.6902180000000002	-4.1814970000000002	-0.6907510000000000
W	6.3647640000000001	-3.3965869999999998	-0.3636260000000000
W	6.2654280000000000	-6.0868549999999999	-0.9255949999999999
W	8.9525889999999997	-5.2836429999999996	-0.6469020000000000
W	8.8337020000000006	-7.9322759999999999	-1.1525680000000000
W	11.4995229999999999	-7.1154840000000004	-0.9094130000000000
W	11.4126980000000007	-9.6875630000000008	-1.3854550000000001
W	14.0974269999999997	-8.9105360000000005	-1.1412439999999999

Se	-8.5951769999999996	3.7819639999999999	1.3420090000000000
Se	-5.5884169999999997	5.5098269999999996	-0.3493360000000000
Se	-5.0793400000000002	2.6099990000000002	2.2565130000000000
Se	-6.3459580000000004	1.6316320000000000	-1.1000790000000000
Se	-1.8699520000000001	4.4427420000000000	1.9630369999999999
Se	-2.8904890000000001	3.1974119999999999	-1.4253140000000000
Se	-2.4367700000000001	0.7144200000000001	1.9755750000000001
Se	-3.7431260000000002	-0.4902270000000000	-1.2374320000000001
Se	0.9070500000000000	2.6447720000000001	1.4090240000000001
Se	-0.3183130000000000	1.2823800000000001	-1.7012879999999999
Se	0.1007340000000000	-1.2333220000000000	1.6521090000000000
Se	-1.1539310000000000	-2.4546800000000002	-1.4783350000000000
Se	3.4722300000000001	0.6799570000000000	1.1836050000000000
Se	2.2800880000000001	-0.5807690000000000	-1.9390220000000000
Se	1.4296249999999999	-4.4074190000000000	-1.7406090000000001
Se	2.6266120000000002	-3.1826240000000001	1.3674170000000001
Se	4.8613939999999998	-2.4773179999999999	-2.1751860000000001
Se	4.0495200000000002	-6.3151390000000003	-2.0390090000000001
Se	6.0399950000000002	-1.2521929999999999	0.9500860000000000
Se	5.1870779999999996	-5.0973980000000001	1.1199200000000000
Se	7.4202250000000003	-4.3890900000000004	-2.4323359999999998
Se	6.6594449999999998	-8.2662720000000007	-2.2505519999999999
Se	8.6043880000000001	-3.1891340000000001	0.7435610000000000
Se	7.7984530000000003	-6.9365839999999999	0.9017030000000000
Se	11.2111909999999995	-5.1024050000000001	0.5320060000000000
Se	9.9900090000000006	-6.2943740000000004	-2.7222770000000001
Se	9.4838210000000007	-10.0311880000000002	-2.7533099999999999
Se	10.4098140000000008	-8.8011470000000003	0.6618680000000000
Se	13.8473530000000000	-7.1674069999999999	0.4264410000000000
Se	12.6691739999999999	-8.1410830000000001	-2.9649169999999998
Se	13.1766150000000000	-11.0500109999999996	-0.3710810000000000
Se	16.1881670000000000	-9.2508119999999998	-1.9830129999999999

W₁₆Se₃₂; $E_{tot} = -9\,372\,665.843\,608\,96$ eV; $E_{rel} = 0$ meV/f.u.

W	32.8526219999999967	7.0109779999999997	2.8033939999999999
W	31.3669049999999991	9.6860060000000008	3.0797770000000000
W	29.7368349999999992	12.3143969999999996	3.3266890000000000
W	28.1992709999999995	15.1510949999999998	3.4918369999999999
W	34.1783500000000018	9.6440889999999992	2.9555440000000002
W	32.4555069999999972	12.2139460000000000	3.2227739999999998
W	30.7858079999999994	15.0758759999999992	3.4309729999999998
W	29.7920720000000010	18.0861559999999990	3.7021269999999999
W	35.7731319999999968	12.3045810000000007	3.2108940000000001
W	34.7792269999999988	15.3145710000000008	3.4823210000000002
W	33.1088540000000009	18.1764879999999991	3.6903419999999998
W	31.3869320000000016	20.7469199999999994	3.9567510000000001
W	37.3660100000000028	15.2398609999999994	3.4215879999999999
W	35.8284629999999993	18.0765120000000010	3.5859209999999999
W	34.1983239999999995	20.7051710000000000	3.8321630000000000
W	32.7130969999999976	23.3802209999999988	4.1098699999999999
Se	32.7961439999999982	8.3907469999999993	4.7846419999999998
Se	31.0120259999999988	11.1295739999999999	5.1078080000000003
Se	29.3563800000000015	13.9420889999999993	5.3038670000000003
Se	27.3491980000000012	17.2654180000000004	4.2786419999999996
Se	34.3678930000000022	11.2279470000000003	4.9203780000000004
Se	32.8179500000000033	14.1392070000000007	4.8367339999999999
Se	31.2769210000000015	16.9270090000000017	5.1871440000000000
Se	29.0841430000000010	20.0674799999999998	4.8827780000000001
Se	36.1841750000000033	13.9356120000000008	5.1716280000000001
Se	34.5596699999999970	16.9659340000000007	5.3994109999999997
Se	32.8004200000000026	19.7456829999999997	5.6869030000000000
Se	30.7816839999999985	22.7784289999999991	5.3745180000000001
Se	38.2153240000000025	17.1102319999999999	4.5747540000000004
Se	36.5025479999999973	20.0927429999999987	4.8013990000000000
Se	34.6920360000000016	22.8203229999999984	5.2893999999999997

Se	32.648167999999983	25.566314999999995	3.4909460000000001
Se	32.9189980000000020	4.8263220000000002	3.4271550000000000
Se	30.873145999999984	7.5697580000000002	1.6240110000000001
Se	29.0623070000000006	10.2981700000000007	2.1112750000000000
Se	27.3494810000000008	13.280737999999995	2.3389020000000000
Se	34.7840190000000007	7.612377999999996	1.5383270000000000
Se	32.764859999999988	10.6452220000000004	1.2254250000000000
Se	31.005276999999995	13.4250460000000000	1.5130960000000000
Se	29.380814999999983	16.455066999999997	1.7416240000000001
Se	36.4812640000000030	10.3236290000000004	2.0297070000000001
Se	34.2879030000000000	13.463746999999997	1.7260830000000000
Se	32.747110999999967	16.2513730000000010	2.0761360000000000
Se	31.197358999999987	19.1627480000000006	1.9921480000000000
Se	38.2160900000000012	13.125553999999993	2.6348460000000000
Se	36.208737999999968	16.4484180000000002	1.6093200000000001
Se	34.5526660000000021	19.2609850000000016	1.8048130000000000
Se	32.7691310000000016	22.000907999999990	2.1278079999999999

W₃₆Se₇₂; $E_{tot} = -21\,088\,493.176\,152\,86\text{ eV}$; $E_{rel} = 302.459\,197\,250\,0\text{ meV/f.u.}$

W	33.787196999999990	25.9560500000000012	3.1119279999999998
W	34.889865999999978	28.5251470000000005	2.9560919999999999
W	35.248969999999999	23.200766999999990	3.2128000000000001
W	36.4007440000000031	25.7356520000000017	3.0883430000000001
W	36.782921999999992	20.437488999999994	3.3233269999999999
W	37.9470010000000002	22.989958999999989	3.2079149999999998
W	38.369194999999977	17.650414999999989	3.4416620000000000
W	39.534979999999973	20.1871790000000004	3.3142049999999998
W	39.9649410000000032	14.8563440000000000	3.5404629999999999
W	41.1311990000000023	17.3871350000000007	3.4293950000000000
W	41.5685160000000025	12.064619999999997	3.6111030000000000
W	42.726297999999999	14.593780999999999	3.5000170000000002
W	43.179842999999982	9.2716440000000002	3.6498230000000000

W	44.3319150000000022	11.8047489999999993	3.5447839999999999
W	44.7988089999999985	6.4855119999999999	3.6723479999999999
W	45.9443380000000019	9.0188150000000000	3.5716250000000000
W	46.4234489999999980	3.7031360000000002	3.6882990000000002
W	47.5660170000000022	6.2370570000000001	3.5921759999999998
W	48.0479740000000035	0.9213610000000000	3.7036889999999998
W	49.1905270000000030	3.4554130000000001	3.6076229999999998
W	49.6691679999999991	-1.8603140000000000	3.7247100000000000
W	50.8150509999999969	0.6729450000000000	3.6238809999999999
W	51.2810819999999978	-4.6464049999999997	3.7523119999999999
W	52.4337239999999980	-2.1135799999999998	3.6470729999999998
W	52.8860919999999979	-7.4358550000000001	3.7982360000000002
W	54.0444499999999977	-4.9069390000000004	3.6865690000000000
W	54.4806379999999990	-10.2293210000000006	3.8696730000000001
W	55.6475760000000008	-7.6993470000000004	3.7582789999999999
W	56.0768890000000013	-13.0296140000000005	3.9853610000000002
W	57.2422889999999995	-10.4930620000000001	3.8574739999999998
W	57.6645370000000028	-15.8324669999999994	4.0920860000000001
W	58.8283869999999993	-13.2811839999999997	3.9760030000000000
W	59.2108320000000035	-18.5787650000000006	4.2107520000000003
W	60.3621740000000031	-16.0437539999999998	4.0867250000000004
W	60.7214150000000004	-21.3680780000000006	4.3434489999999997
W	61.8233719999999991	-18.7988919999999986	4.1875910000000003
Se	32.9980699999999985	24.1213489999999986	4.4266459999999999
Se	35.1832589999999996	27.0903799999999997	4.9108120000000000
Se	34.4655600000000035	21.1050700000000013	4.2327690000000002
Se	36.7116389999999981	24.2070849999999993	5.0424270000000000
Se	36.0546050000000022	18.2664529999999985	4.3056840000000003
Se	38.2858769999999993	21.4006760000000007	5.1394940000000000
Se	37.6656570000000031	15.4524299999999997	4.4175550000000001
Se	39.8792660000000012	18.6010719999999985	5.2543300000000004
Se	39.2833779999999990	12.6451250000000002	4.5187080000000002
Se	41.4903669999999991	15.7927330000000001	5.3491640000000000

Se	40.8985630000000029	9.8376680000000007	4.5712130000000002
Se	43.1111050000000020	12.9919510000000002	5.4098179999999996
Se	42.5166430000000020	7.0373440000000000	4.5972039999999996
Se	44.7295420000000021	10.1958470000000005	5.4463359999999996
Se	44.1402879999999982	4.2460589999999998	4.6125449999999999
Se	46.3496850000000009	7.4052980000000002	5.4684999999999997
Se	45.7656700000000001	1.4630660000000000	4.6304259999999999
Se	47.9733039999999988	4.6210760000000004	5.4858960000000003
Se	32.8217780000000019	27.8120319999999985	1.8429650000000000
Se	34.6338670000000022	30.6661859999999997	3.6957979999999999
Se	34.8905730000000034	24.8007239999999989	1.2587420000000000
Se	36.8351669999999984	28.0326279999999990	1.7211460000000001
Se	36.4796750000000003	22.0150809999999986	1.3753439999999999
Se	38.5840490000000003	25.1779240000000009	2.0343100000000001
Se	38.0315099999999973	19.2270520000000005	1.5021000000000000
Se	40.2196720000000028	22.3826169999999998	2.2836590000000001
Se	39.6174200000000027	16.4492219999999989	1.6132370000000000
Se	41.8497460000000032	19.6163029999999985	2.4969600000000001
Se	41.1934290000000018	13.6612779999999994	1.6947900000000000
Se	43.4200590000000020	16.8196429999999992	2.5424180000000001
Se	42.7859479999999976	10.8788680000000006	1.7468750000000000
Se	45.0129629999999992	14.0367899999999999	2.5968580000000001
Se	44.3933899999999966	8.0982380000000003	1.7759229999999999
Se	46.6106100000000012	11.2532680000000003	2.6193979999999999
Se	46.0146299999999968	5.3187360000000004	1.7942210000000001
Se	48.2248919999999970	8.4746039999999994	2.6451630000000002
Se	47.3886380000000003	-1.3158989999999999	4.6508409999999998
Se	49.5992260000000016	1.8399410000000000	5.5018539999999998
Se	47.6407510000000016	2.5374330000000000	1.8100499999999999
Se	49.2642560000000032	-0.2470210000000000	1.8277260000000000
Se	49.0024019999999965	-4.0944560000000001	4.6772099999999996
Se	51.2200739999999968	-0.9396210000000000	5.5204399999999998
Se	50.8840569999999985	-3.0378940000000001	1.8503250000000000

Se	49.8481730000000027	5.6954430000000000	2.6654599999999999
Se	51.4737060000000000	2.9121939999999999	2.6834340000000001
Se	53.0972039999999978	0.1204860000000000	2.6992829999999999
Se	50.5994409999999988	-6.8781800000000004	4.7006720000000000
Se	52.8270649999999975	-3.7205659999999998	5.5503119999999999
Se	52.5019789999999986	-5.8343429999999996	1.8877999999999999
Se	54.7149140000000003	-2.6802359999999998	2.7260640000000000
Se	52.1918560000000014	-9.6614369999999994	4.7559790000000000
Se	54.4189679999999996	-6.5033969999999997	5.6033010000000001
Se	54.1221600000000009	-8.6356160000000006	1.9495600000000000
Se	56.3295590000000033	-5.4882640000000000	2.7794620000000001
Se	53.7615809999999996	-12.4583370000000002	4.8026530000000003
Se	55.9943260000000009	-9.2912929999999996	5.6859570000000001
Se	55.7327239999999975	-11.4441009999999999	2.0447750000000000
Se	57.9468910000000008	-8.2955729999999992	2.8814839999999999
Se	55.3921149999999969	-15.2251539999999999	5.0161429999999996
Se	57.5797099999999986	-12.0692070000000005	5.7974360000000003
Se	57.3255359999999996	-14.2433049999999994	2.1600619999999999
Se	59.5570740000000001	-11.1094869999999997	2.9940319999999998
Se	57.0270590000000013	-18.0207949999999997	5.2650800000000002
Se	59.1316690000000023	-14.8579390000000000	5.9242640000000000
Se	58.8997999999999990	-17.0499860000000005	2.2570169999999998
Se	61.1462539999999990	-13.9480889999999995	3.0671339999999998
Se	58.7756559999999979	-20.8753419999999998	5.5786300000000004
Se	60.7209829999999968	-17.6437460000000002	6.0405509999999998
Se	60.4285970000000034	-19.9329579999999993	2.3884020000000001
Se	62.6128640000000019	-16.9650609999999986	2.8735800000000000
Se	60.9775989999999979	-23.5092070000000000	3.6037309999999998
Se	62.7895120000000020	-20.6545120000000004	5.4568050000000001

W₃₆Se₇₂; $E_{tot} = -21\,088\,494.614\,603\,22$ eV; $E_{rel} = 262.502\,242\,805\,5$ meV/f.u.

W	14.5624599999999997	15.3821119999999993	4.5128430000000002
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W	13.457739000000001	18.267147999999998	3.792689000000002
W	11.917562999999995	20.906566999999990	3.400115000000000
W	9.874193999999992	24.051556000000015	3.033987000000002
W	18.324995999999987	15.417002999999993	4.003839000000001
W	16.224267999999986	18.141103000000011	3.759103999999998
W	15.156295999999993	20.866960999999999	3.522955000000001
W	13.278390999999992	24.145253000000003	3.267957000000000
W	11.761437000000008	26.679368000000002	3.367897999999998
W	21.399188999999998	15.381629000000002	3.576226000000001
W	19.977160000000014	18.142063000000003	3.422362000000001
W	17.907818999999999	20.402377000000013	3.434457999999998
W	16.223113000000014	23.720279000000014	3.228205000000000
W	14.597502000000004	26.637028999999983	3.012169000000001
W	13.194471000000001	29.211442999999992	3.339897000000001
W	24.470103999999992	14.856654999999999	2.970483000000002
W	22.876923000000015	17.704612000000009	3.266903999999998
W	21.750018000000007	20.317727000000014	3.152042999999999
W	17.962666999999997	26.722532999999985	3.286964000000002
W	16.049731999999988	29.125263000000003	3.239675999999998
W	14.458290999999991	32.100222999999997	2.963655999999998
W	26.257972999999998	18.198996999999985	3.033227000000001
W	24.587158999999998	21.026744000000008	3.194747000000000
W	23.466712999999986	23.525839999999988	3.212699999999999
W	21.469183000000010	26.967151999999987	3.474645000000002
W	19.837731999999990	29.204819000000005	3.515120000000000
W	18.209164999999987	31.942954000000003	3.377227000000000
W	27.700907999999983	20.766702999999997	3.062199999999998
W	26.166577000000002	23.691580999999993	3.315217000000001
W	24.600104999999992	26.213487000000006	3.448751000000001
W	22.720152999999998	29.519559999999985	3.766888999999999
W	21.286546999999988	31.891538000000006	3.777077999999999
W	29.632256999999992	23.991161999999992	3.111917000000000
W	27.579454999999994	26.435189999999986	3.703513000000001

W	26.086694999999989	28.987528999999985	3.9686430000000001
W	24.325375000000011	32.312111999999991	4.455601999999998
Se	16.607206999999989	13.924206999999991	5.026550000000003
Se	14.751827000000005	17.370132999999992	5.841205999999997
Se	13.251390999999999	20.209679999999988	5.372346000000003
Se	11.413401000000004	22.983194000000010	4.845602999999997
Se	9.669964999999995	25.868306000000005	4.629067000000000
Se	19.865390000000014	13.869281000000009	4.988406999999996
Se	18.246338999999990	17.376740999999991	5.345609999999998
Se	16.572302000000005	20.053028999999987	5.466497000000004
Se	14.794624999999999	22.979670999999997	5.012311999999997
Se	13.229587999999997	25.793001000000003	5.110757000000004
Se	10.982943000000006	28.754339999999991	4.435477999999998
Se	23.059661999999994	13.900890999999997	4.740513000000000
Se	21.443463999999987	17.150224000000015	5.274669000000003
Se	19.967058999999990	20.474194000000007	4.862987999999996
Se	18.286884000000006	24.515643000000007	4.213261000000001
Se	14.647688000000005	28.309345000000004	5.096447000000004
Se	12.768122999999992	31.377462999999988	4.570375000000003
Se	24.894624000000003	16.767407999999996	4.698681999999998
Se	23.259052000000005	19.647297999999993	4.908903999999997
Se	17.836437000000001	28.399059999999986	4.998016999999999
Se	16.144614000000007	31.319539999999999	4.803009999999996
Se	26.334997000000013	19.853176999999987	4.907129000000003
Se	24.736063000000015	22.633651000000004	5.135399999999997
Se	22.406517999999984	25.078437000000010	4.832679999999999
Se	21.191680999999991	28.325782000000002	5.490058000000003
Se	19.476503999999985	31.149215999999991	5.360216999999996
Se	28.130860999999994	22.608034000000000	4.770984999999996
Se	26.118819999999995	25.360929999999998	5.301013000000002
Se	24.376107000000011	28.094591000000012	5.357090999999996
Se	22.697243000000003	31.201187999999984	5.826403000000000
Se	29.675746000000002	25.615584999999994	4.924991999999996

Se	28.298415999999996	28.488706000000005	4.866965999999997
Se	26.598568000000002	31.2242430000000013	4.948522999999998
Se	12.840536999999994	16.0105140000000006	2.8800400000000002
Se	11.2434030000000007	18.758406999999983	2.5841360000000000
Se	9.601853999999994	21.528414999999990	2.7280050000000000
Se	16.2207380000000008	15.788959999999994	2.532986999999999
Se	14.7809430000000006	18.9557320000000011	1.8468240000000000
Se	13.3700720000000004	21.897311999999994	1.7882380000000000
Se	11.4950930000000007	24.878652999999999	1.454140999999999
Se	19.5946290000000012	15.901042999999996	1.9086790000000000
Se	17.9427480000000017	18.568633999999994	1.8709560000000001
Se	16.8361720000000012	21.833249999999996	1.708083999999999
Se	14.886711999999993	24.700959999999985	1.3731800000000001
Se	12.984109999999994	27.6227570000000000	1.3583130000000001
Se	22.8318820000000002	15.7475220000000000	1.4610140000000000
Se	21.3981010000000005	18.6626450000000013	1.3757580000000000
Se	16.457751999999993	27.4102110000000003	1.4207110000000001
Se	14.6010570000000008	30.2805140000000002	1.3900340000000000
Se	26.765185999999999	15.865178999999995	2.3493430000000002
Se	24.576492999999993	18.903684999999994	1.5136170000000000
Se	22.6534550000000010	21.936444999999991	1.4815170000000000
Se	19.783554999999998	27.2927290000000013	1.6949510000000001
Se	18.0590800000000016	30.1911850000000008	1.768942999999999
Se	16.495826999999985	33.6141730000000010	2.6821920000000001
Se	28.5058310000000006	18.6417220000000015	2.1468120000000002
Se	26.300747999999987	21.832402999999993	1.4126580000000000
Se	24.6923640000000013	24.663267999999986	1.4257930000000001
Se	23.123674999999986	27.7506750000000011	1.908844999999999
Se	21.3397210000000008	30.405207999999982	1.8289510000000000
Se	19.7534770000000002	33.5964150000000004	2.5956280000000000
Se	30.0156090000000013	21.537736999999999	2.4892970000000001
Se	27.9609650000000016	24.920162999999987	1.6474050000000000
Se	26.232172999999995	27.585014999999985	1.9070050000000001

Se	24.7554149999999993	30.6321620000000010	2.4905450000000000
Se	22.9455999999999989	33.5151060000000030	2.8222870000000002
Se	25.0905319999999996	34.0921700000000030	5.6642409999999996
Se	31.6689749999999997	24.3685560000000017	2.1602109999999999
Se	25.2448020000000000	12.9246529999999993	2.0322460000000002
Se	13.3718120000000003	13.8710810000000002	5.7417369999999996
Se	7.8341719999999997	24.1776130000000009	2.0115530000000001
Se	13.2933880000000002	33.7641520000000028	1.9168970000000001

W₃₆Se₇₂; $E_{tot} = -21\,088\,494.778\,584\,56$ eV; $E_{rel} = 257.947\,205\,583\,3$ meV/f.u.

W	-5.6247680000000004	27.7057099999999998	-11.7959270000000007
W	-3.7588729999999999	28.6503359999999994	-9.3962620000000001
W	-1.7813369999999999	29.4949709999999996	-6.8591949999999997
W	0.2556670000000000	29.9135659999999994	-4.3122299999999996
W	2.1832769999999999	30.4586790000000001	-2.0552619999999999
W	4.2274580000000004	30.8992010000000015	0.3615000000000000
W	-5.5932380000000004	24.8620429999999999	-13.1883800000000004
W	-3.8178030000000001	26.0399630000000002	-10.7640170000000008
W	-2.0556100000000002	26.8905679999999982	-8.3514309999999998
W	-0.2604370000000000	27.5115650000000009	-5.8949490000000004
W	1.6106320000000001	27.5906149999999997	-3.5260250000000002
W	4.1503410000000001	28.4075200000000017	-0.6140880000000000
W	5.8651790000000004	28.9779680000000006	1.3415410000000001
W	-5.6371490000000000	22.1769169999999995	-14.5688340000000007
W	-3.6913770000000001	23.0402130000000014	-12.3137360000000005
W	4.0416189999999999	24.7524659999999983	-2.1032210000000000
W	6.0183989999999996	25.9710940000000008	0.1981390000000000
W	-5.5711529999999998	19.1562529999999995	-15.7714079999999992
W	-3.8853100000000000	20.0129240000000017	-13.8163850000000004
W	4.4840159999999996	21.9461629999999985	-3.0705339999999999
W	6.0182060000000002	23.1252199999999988	-0.9373060000000000
W	-5.3925570000000000	16.1727470000000011	-16.6396739999999994

W	-3.7325490000000001	17.1724290000000011	-14.7895500000000002
W	4.5059040000000001	19.0660360000000004	-4.3666960000000001
W	6.2206039999999998	20.1295129999999993	-2.1478229999999998
W	-3.4704999999999999	14.1099669999999993	-15.7159600000000008
W	-1.4290280000000000	14.2354780000000005	-13.2947530000000000
W	0.3508200000000000	14.7804120000000001	-10.7037239999999994
W	2.4288599999999999	15.4654710000000009	-8.2858900000000002
W	4.3843459999999999	16.2463809999999995	-5.8360040000000000
W	6.2145510000000002	17.1763650000000005	-3.5594410000000001
W	-1.5442389999999999	11.9862079999999995	-14.7340309999999999
W	0.4555190000000000	12.4749260000000000	-12.3449290000000005
W	2.2863370000000001	12.9969509999999993	-9.9654889999999998
W	4.1333979999999997	13.5543060000000004	-7.4201530000000000
W	6.0424210000000000	14.3242130000000003	-4.9736539999999998
Se	-7.5444540000000000	26.6783779999999986	-12.7075049999999994
Se	-5.7694660000000004	27.0771119999999996	-9.4146040000000006
Se	-3.8677199999999998	27.9931519999999985	-6.9693500000000004
Se	-1.9852700000000001	28.7373179999999984	-4.4652430000000001
Se	0.1319760000000000	28.9933410000000009	-1.9816430000000000
Se	2.1041859999999999	29.6784469999999985	0.3956990000000000
Se	-7.4455340000000003	23.8743680000000005	-14.4741119999999999
Se	-5.4847190000000001	24.0308419999999998	-10.8765319999999992
Se	-3.1208589999999998	24.7266690000000011	-8.6109639999999992
Se	-0.7645870000000000	25.2889589999999984	-6.6702269999999997
Se	-0.0433640000000000	25.9120020000000011	-3.7243550000000001
Se	2.3448750000000000	26.5707740000000001	-1.1919390000000001
Se	4.2740460000000002	27.1460270000000001	1.6755279999999999
Se	-7.4216319999999998	20.8113959999999985	-15.8045460000000002
Se	-5.6076709999999999	21.2235890000000005	-12.3069089999999992
Se	2.2353679999999998	23.2399969999999989	-2.3410410000000001
Se	4.2061109999999999	24.2394120000000015	0.4101060000000000
Se	-7.4103260000000004	17.4083159999999992	-16.7004090000000005
Se	-5.5692230000000000	18.2513210000000008	-13.4146210000000004

Se	2.779955999999999	21.0741070000000015	-4.5435049999999997
Se	4.4760470000000003	21.1484079999999999	-0.6414150000000000
Se	-5.3689910000000003	15.1795659999999994	-14.4036799999999996
Se	-2.8186369999999998	16.2695399999999992	-12.3613409999999995
Se	2.4929700000000001	17.9456009999999999	-5.0551550000000001
Se	4.5393960000000000	18.2164099999999998	-1.9843210000000000
Se	-3.5205739999999999	12.8140149999999995	-13.5085180000000005
Se	-1.5456420000000000	13.2043040000000005	-10.9617030000000000
Se	0.4739700000000000	13.7052250000000004	-8.4156540000000000
Se	2.3896820000000001	14.5931599999999992	-5.9717430000000000
Se	4.4316649999999997	15.3408309999999997	-3.4106860000000001
Se	-0.7590479999999999	10.2394610000000004	-13.3420839999999998
Se	1.4468449999999999	10.7900869999999998	-10.8073540000000001
Se	3.4990320000000001	11.3888409999999993	-8.2718209999999992
Se	5.2139810000000004	12.1503080000000008	-5.3378810000000003
Se	-4.9979380000000004	29.9461089999999999	-11.4900319999999994
Se	-3.0475970000000001	30.8679589999999990	-8.7358849999999997
Se	-0.8285940000000001	31.5780940000000001	-6.1256930000000001
Se	1.3241510000000001	32.0810280000000034	-3.6886060000000001
Se	-3.8712830000000000	26.7613510000000012	-13.2481729999999995
Se	-1.8617340000000000	27.6628299999999996	-10.7230010000000000
Se	0.0025900000000000	28.4171920000000000	-8.2466620000000006
Se	1.9369570000000000	28.7274740000000008	-5.7513949999999996
Se	3.8383680000000000	29.1536539999999995	-3.1289180000000001
Se	-3.7647510000000000	23.8731860000000005	-14.6577540000000006
Se	-1.8532180000000000	24.2430090000000007	-11.4449839999999998
Se	3.6236660000000001	26.1448619999999998	-4.2174519999999998
Se	5.7861890000000002	26.8637850000000000	-1.9831240000000001
Se	-3.9906079999999999	21.0534070000000000	-16.1430679999999995
Se	-2.3803730000000001	20.9167270000000016	-12.0204699999999995
Se	6.0618670000000003	23.8843829999999997	-3.3353150000000000
Se	7.8860599999999996	24.3928870000000018	0.1798320000000000
Se	-3.8636010000000001	18.0142850000000010	-17.2427780000000013

Se	-1.8036970000000001	18.8627129999999994	-14.5781340000000004
Se	6.2903019999999996	20.9345150000000011	-4.5204630000000003
Se	7.9751779999999997	21.3410960000000003	-1.0024700000000000
Se	-4.4606789999999998	14.4448760000000007	-18.0453629999999983
Se	-1.6913080000000000	15.6727740000000004	-15.5884350000000005
Se	-0.4019950000000000	16.4696929999999995	-12.5589139999999997
Se	0.5676990000000000	16.8698079999999990	-9.4258080000000000
Se	3.4882659999999999	17.5844239999999985	-8.0237079999999992
Se	6.1960139999999999	18.0709650000000011	-5.8978739999999998
Se	8.0211670000000002	18.1887630000000016	-2.3428710000000001
Se	-2.3816929999999998	12.0981290000000001	-16.9727500000000013
Se	0.5149520000000000	13.3288779999999996	-14.7450039999999998
Se	2.3070400000000002	14.1664549999999991	-12.2000989999999998
Se	4.2697229999999999	14.5320850000000004	-9.7423669999999998
Se	6.1746790000000003	15.0825010000000006	-7.3118540000000003
Se	8.0261189999999996	15.1580739999999992	-4.0442419999999997
Se	6.1690899999999997	30.0034370000000017	-0.9037650000000000
Se	3.6051620000000000	32.5416529999999966	-1.3266490000000000
Se	7.8514759999999999	27.5663519999999984	1.1865120000000000
Se	4.9380980000000001	30.7986119999999985	2.7229800000000002

W₃₆Se₇₂; $E_{tot} = -21\,088\,496.812\,146\,12\text{ eV}$; $E_{rel} = 201.459\,384\,472\,2\text{ meV/f.u.}$

W	11.7186149999999998	15.5107959999999991	3.4604180000000002
W	10.0177899999999998	18.2023709999999994	3.6059040000000002
W	8.4718110000000006	20.9377479999999991	3.6155499999999998
W	6.7802650000000000	23.7180010000000010	3.4023119999999998
W	5.3339470000000002	26.5747919999999986	3.1167300000000000
W	14.9002070000000000	15.3815620000000006	3.3084210000000001
W	13.0401030000000002	17.7942479999999996	3.4514649999999998
W	11.3758780000000002	20.4529059999999987	3.6989730000000001
W	9.4268230000000006	23.7741870000000013	3.6627990000000001
W	7.9887569999999997	26.3428940000000011	3.3668890000000000

W	6.8022809999999998	29.2518209999999996	3.0854810000000001
W	18.0468149999999987	15.4136760000000006	3.2961800000000001
W	16.1704620000000006	17.6835160000000009	3.2024379999999999
W	11.2793460000000003	26.6688830000000010	3.7443450000000000
W	9.9148130000000005	29.6747019999999999	3.3678140000000001
W	8.3884190000000007	31.8586910000000003	3.1153209999999998
W	21.2978950000000005	15.3419790000000003	3.5102699999999998
W	20.0243870000000008	17.6625340000000008	3.2468129999999999
W	12.8582040000000006	29.7107950000000010	3.6662910000000002
W	11.5843989999999994	32.0314660000000018	3.4029010000000000
W	24.4940210000000000	15.5144020000000005	3.7978070000000002
W	22.9676819999999999	17.6985689999999991	3.5451750000000000
W	21.6031820000000003	20.7043929999999996	3.1687210000000001
W	16.7122369999999982	29.6901359999999990	3.7111619999999998
W	14.8357460000000003	31.9598930000000010	3.6170789999999999
W	26.0803680000000000	18.1215289999999989	3.8273410000000001
W	24.8942650000000008	21.0308129999999984	3.5457679999999998
W	23.4557989999999990	23.5990460000000013	3.2501159999999998
W	21.5067260000000005	26.9201659999999983	3.2141989999999998
W	19.8420519999999989	29.5791359999999983	3.4623029999999999
W	17.9823820000000012	31.9918240000000011	3.6051799999999998
W	27.5484590000000011	20.7982359999999993	3.7958740000000000
W	26.1022829999999999	23.6549930000000010	3.5103119999999999
W	24.4111529999999988	26.4353680000000004	3.2971710000000001
W	22.8650060000000011	29.1709759999999996	3.3072859999999999
W	21.1641680000000001	31.8625669999999985	3.4533659999999999
Se	12.9969239999999999	13.7328829999999993	4.3586999999999998
Se	11.4573470000000004	17.0505819999999986	5.3723089999999996
Se	9.7229510000000001	19.8425769999999986	5.5020369999999996
Se	7.9135759999999999	22.6408430000000003	5.3867260000000003
Se	6.2532230000000002	25.5230940000000004	5.1443810000000001
Se	4.4049449999999997	28.6638149999999996	3.8792550000000001
Se	16.4467449999999999	13.6517280000000003	4.1468259999999999

Se	14.790407999999993	17.038347000000017	5.179958000000001
Se	13.443709000000001	20.095306000000008	4.821429000000002
Se	11.478692999999998	22.776184000000007	4.978113999999997
Se	9.642614999999993	25.619688000000000	5.357249000000004
Se	8.115474000000007	28.491734999999985	4.906512000000002
Se	6.113127999999997	31.622817999999988	3.875433999999998
Se	19.710124000000004	13.720224999999992	4.402702999999998
Se	18.050491999999984	17.267144999999993	4.909842000000003
Se	11.365258000000007	28.605747000000009	5.361275000000000
Se	9.756093999999992	31.587679000000014	5.144487999999999
Se	23.239612000000010	13.743938000000000	4.711541000000004
Se	21.257336999999997	17.052820000000005	5.330898000000004
Se	19.277343999999994	20.236775999999990	3.782696000000001
Se	14.750678999999999	28.437716000000018	4.984218000000003
Se	13.083192000000004	31.591020000000003	5.388397999999996
Se	24.502245999999995	17.180561000000009	5.582063999999999
Se	22.913327999999999	19.952663999999986	5.008602999999999
Se	20.849463000000001	22.958558000000000	3.781534000000002
Se	18.058398000000004	28.095818999999988	4.856988000000003
Se	16.414539000000013	31.438023000000012	5.504251000000000
Se	26.110661000000003	19.958819999999993	5.581724000000004
Se	24.602301000000006	22.834839999999998	5.332385999999996
Se	22.813634000000004	25.503892000000005	4.917066000000002
Se	21.382203000000005	28.446076999999989	5.186748999999998
Se	19.703202000000010	31.333771999999997	5.372499999999996
Se	28.459306999999990	22.768063000000015	4.706977000000002
Se	26.719384999999991	25.841205999999997	4.392057000000003
Se	25.138933000000015	28.700572999999986	4.142944000000000
Se	23.346389999999995	31.647642999999986	4.344655999999996
Se	9.536303000000002	15.725410999999994	2.569232000000000
Se	7.744003000000002	18.672616999999989	2.769746000000000
Se	6.163789999999997	21.531925999999986	2.519833000000002
Se	4.423478000000002	24.604859000000011	2.205003000000000

Se	13.179354999999993	16.039428999999984	1.5412930000000000
Se	11.500432000000000	18.926984000000009	1.7261970000000000
Se	10.069495999999991	21.869308000000002	1.9957030000000000
Se	8.280632999999999	24.538560000000004	1.5804110000000000
Se	6.772198000000004	27.414472000000000	1.3309850000000001
Se	16.467767999999995	15.935539000000003	1.4092620000000000
Se	14.824115000000008	19.277933000000009	2.0570650000000001
Se	12.033372000000000	24.414732000000008	3.1317640000000000
Se	9.969523999999998	27.420560999999993	1.9043019999999999
Se	8.380489000000007	30.192703000000016	1.3307739999999999
Se	19.799088999999986	15.782495000000008	1.5247470000000001
Se	18.131934999999986	18.935860999999992	1.9290980000000000
Se	13.605363999999998	27.136531999999990	3.1306180000000001
Se	11.625313000000002	30.320425000000002	1.5823280000000000
Se	9.642635000000003	33.629330000000031	2.2016119999999999
Se	23.126270999999991	15.785396000000004	1.7686660000000001
Se	21.517264000000008	18.767510999999989	1.5518080000000001
Se	14.832269000000001	30.106391999999996	2.0036060000000000
Se	13.172385000000002	33.653084999999973	2.5103130000000000
Se	26.769196999999984	15.750133999999992	3.0376829999999999
Se	24.766870999999983	18.881367999999984	2.0063800000000001
Se	23.239886999999995	21.753441999999997	1.5556230000000000
Se	21.403915000000014	24.596821999999995	1.9348200000000000
Se	19.438517000000009	27.278106000000011	2.0920850000000000
Se	18.092258999999985	30.335363000000010	1.7335680000000000
Se	16.435997000000004	33.721752000000022	2.7668260000000000
Se	28.477565999999995	18.709177000000004	3.0328240000000002
Se	26.629187000000017	21.849879000000014	1.7680240000000000
Se	24.968939999999999	24.732285000000010	1.5258989999999999
Se	23.159604000000016	27.530864000000011	1.4112790000000000
Se	21.425005999999998	30.322880000000014	1.5414060000000001
Se	19.885888999999988	33.640545000000030	2.5553889999999999

$W_{36}Se_{72}$; $E_{tot}=-21\,088\,500.923\,118\,43\text{ eV}$; $E_{rel}=87.265\,709\,194\,4\text{ meV/f.u.}$

W	20.0042860000000005	1.2202500000000001	3.5274770000000002
W	22.6384310000000006	1.1371340000000001	3.7737069999999999
W	21.2775019999999984	3.5459939999999999	3.6806930000000002
W	26.3988650000000007	1.1425780000000001	3.7781080000000000
W	24.6062879999999993	3.8394189999999999	3.6593179999999998
W	23.1587560000000003	6.7911140000000003	3.7110219999999998
W	29.5917610000000018	1.1390750000000001	3.5421849999999999
W	27.8312039999999996	3.4368400000000001	3.6438860000000002
W	25.8761359999999989	6.9182259999999998	3.6218400000000002
W	24.7264729999999986	9.5546229999999994	3.4715600000000002
W	32.8225100000000012	1.0909409999999999	3.4403039999999998
W	30.9924870000000006	3.4561440000000001	3.5665670000000000
W	29.9090419999999995	6.7388510000000004	3.4786800000000002
W	27.4270339999999990	9.7483050000000002	3.5643950000000002
W	26.3092669999999984	12.3062260000000006	3.4155650000000000
W	36.0904049999999970	1.1953670000000001	3.4676019999999999
W	34.2504920000000013	3.3965429999999999	3.5973940000000000
W	32.7987910000000014	6.9932770000000000	3.4854379999999998
W	31.4573180000000008	9.3867370000000001	3.4373580000000001
W	29.0544599999999988	12.4982780000000009	3.5853619999999999
W	27.9851640000000010	15.0571699999999993	3.5158100000000001
W	39.3089239999999975	1.3290540000000000	3.6846950000000001
W	38.0232469999999978	3.6179130000000002	3.6795920000000000
W	35.9140969999999982	7.0334620000000001	3.6236700000000002
W	34.4360029999999995	9.5122959999999992	3.6401940000000002
W	33.0617179999999991	12.1147440000000000	3.5691730000000002
W	31.1086010000000002	15.6345410000000005	3.6682530000000000
W	29.7167640000000013	17.8846719999999983	3.7567349999999999
W	42.4536119999999997	1.3459479999999999	3.7763849999999999
W	40.8402900000000031	3.9172530000000001	3.8772850000000001
W	39.3950269999999989	6.4552680000000002	3.8590339999999999

W	37.481177999999999	9.712521999999999	3.912380000000002
W	36.053212000000020	12.196256999999992	3.847831999999999
W	34.253236000000011	15.396053000000002	3.788357000000000
W	32.761650000000030	17.898863999999997	3.859402999999999
W	31.333701000000014	20.615511000000015	3.823861000000000
Se	21.040317000000017	-0.594500000000000	4.709410000000001
Se	18.951823999999984	3.115781999999998	4.568031000000004
Se	24.448268999999998	-0.151153000000000	4.914774000000004
Se	22.840980999999993	2.897724999999999	5.466870000000001
Se	21.126808000000005	5.756284000000000	4.890734000000001
Se	27.832553000000008	-0.617003000000000	4.497842000000003
Se	26.154550000000004	2.905921000000002	5.486938999999996
Se	24.561007000000000	5.717774000000004	5.439934000000000
Se	22.333541000000003	8.930312000000007	4.388979000000000
Se	31.116395000000007	-0.562020000000000	4.462421000000000
Se	29.456047999999991	2.754922999999998	5.457090000000000
Se	27.884487000000000	5.750439000000001	4.915359999999997
Se	26.064762999999992	8.681556999999997	5.418543999999998
Se	24.040098000000004	11.750159000000000	4.434173999999996
Se	34.490403000000006	-0.652428000000000	4.107218999999997
Se	32.700212000000005	2.621611000000001	5.390039999999999
Se	31.275952000000002	5.637238000000000	5.161976000000001
Se	29.429628000000010	8.677184000000005	4.963550999999998
Se	27.641269000000012	11.524744999999994	5.409825999999998
Se	25.686056000000007	14.661996000000003	4.261746999999997
Se	37.774574000000012	-0.396966000000000	4.563163000000003
Se	36.109907999999972	2.819141000000001	5.285733999999997
Se	34.395927999999978	5.637673000000004	5.082455000000004
Se	32.818415000000017	8.610846999999997	5.421033000000004
Se	31.064412999999983	11.440086000000009	5.016408000000002
Se	29.489366000000004	14.352738000000004	5.305564000000004
Se	27.493719999999997	17.431923999999986	4.598475999999998
Se	41.102159999999978	-0.192818000000000	4.943174000000000

Se	39.485512999999974	2.885053999999998	5.639681000000004
Se	37.679918999999982	5.724168999999998	5.327854000000003
Se	36.066552999999990	8.648853000000008	5.557134999999997
Se	34.485736000000028	11.403425000000004	5.518319000000000
Se	32.774858999999993	14.275551999999994	5.273030999999996
Se	31.209143999999984	17.252324000000015	5.651494999999997
Se	29.358733000000009	20.215406000000015	5.036007999999998
Se	44.311469999999999	0.342852000000000	2.946013000000002
Se	43.050328999999978	3.249556999999998	5.060371000000000
Se	41.552824000000011	6.091147000000003	4.892172999999997
Se	39.803342000000007	8.876580999999998	4.525897999999998
Se	38.190215999999995	11.751599000000006	5.077670000000003
Se	36.588540000000018	14.599655999999995	4.402878000000003
Se	35.002265000000013	17.438455000000011	4.860379000000000
Se	33.308813999999981	20.154136999999986	5.048104999999996
Se	31.395624000000015	22.733245000000001	3.016528999999998
Se	21.300468999999997	1.894085999999999	1.631724000000000
Se	24.538843000000000	1.702717000000000	2.127033000000000
Se	22.736710999999997	4.871209000000003	2.065998000000000
Se	27.847439000000014	1.624468000000000	1.760544000000001
Se	26.194230000000010	4.795739000000002	2.047725999999999
Se	24.341238000000006	7.773760000000002	1.700611000000001
Se	31.166727999999991	1.695970000000000	1.660706000000000
Se	29.430097000000000	4.681409999999996	1.977873999999999
Se	27.822561000000003	7.675457999999999	2.079092999999999
Se	25.968921000000017	10.632123999999992	1.587164000000000
Se	34.454796000000018	1.736471000000001	1.624301999999999
Se	32.779190999999973	4.731910000000001	2.086840000000000
Se	31.206990000000011	7.648596999999996	1.575634999999999
Se	29.467611000000016	10.510930000000001	2.064849999999999
Se	27.660308000000006	13.442156999999999	1.614320999999999
Se	37.758488999999973	1.863680000000000	1.754366000000001
Se	36.105704000000029	4.768231000000001	2.308840000000000

Se	34.501080000000017	7.700936999999997	1.7307610000000000
Se	32.903353000000027	10.520346000000000	1.704256999999999
Se	31.153135999999999	13.399653000000007	2.291408999999998
Se	29.375886999999987	16.288142000000006	1.817531999999999
Se	41.064109000000020	2.088175999999998	1.938220000000001
Se	39.443877999999980	4.874772000000001	1.947340000000001
Se	37.949675999999966	7.806059000000003	2.186887000000000
Se	36.195264000000017	10.579402999999992	1.972331000000001
Se	34.683360999999979	13.499396000000008	2.079984000000001
Se	32.878087000000007	16.245155000000005	1.910830000000000
Se	31.245160999999995	19.042490000000008	1.986945000000000

W₃₆Se₇₂; $E_{tot} = -21\,088\,500.984\,693\,52$ eV; $E_{rel} = 85.555\,290\,027\,7$ meV/f.u.

W	21.411968999999991	-1.176789000000001	3.175628000000001
W	19.944145999999999	1.464831999999999	3.175937999999999
W	18.348001000000000	4.051842999999999	3.037970000000001
W	16.429466000000015	7.326012999999997	3.086116000000001
W	15.009866000000006	9.900024999999994	3.240286999999999
W	13.396440999999994	12.583885000000004	3.200998999999999
W	11.482215999999993	15.805747999999995	3.206823000000000
W	10.052343999999997	18.237434000000004	3.162442000000000
W	8.190896000000004	21.478598999999991	3.158157000000001
W	6.807223999999997	23.958853000000013	3.061106999999998
W	4.951168000000000	27.239316999999998	3.022071000000000
W	3.528074000000002	29.932363999999997	3.138560000000000
W	1.995039000000000	32.537360999999971	3.116007999999999
W	22.558050999999990	1.310894999999999	4.275761000000001
W	21.288873999999999	3.870414999999999	4.387692000000004
W	19.309146999999994	7.124353000000002	4.371753000000000
W	17.896626000000013	9.400482999999995	4.447887999999998
W	16.015802999999982	12.703637999999998	4.471745000000003
W	14.604478000000003	15.163624999999997	4.483831000000003

W	12.6109130000000000	18.4777869999999993	4.5158009999999997
W	11.3099489999999996	20.7996349999999985	4.4815459999999998
W	9.3769449999999992	24.1881480000000018	4.4458810000000000
W	8.1056830000000009	26.5258469999999988	4.3683240000000003
W	6.2734759999999996	29.8785370000000015	4.3728740000000004
W	4.7081369999999998	32.2672389999999965	4.2433949999999996
W	23.7717379999999991	3.8111400000000000	5.3896540000000002
W	22.2436819999999997	6.7054530000000003	5.5496010000000000
W	20.7997629999999987	9.1859359999999999	5.7384800000000000
W	18.8804839999999992	12.4566049999999997	5.7692360000000003
W	17.2876219999999989	15.1225020000000008	5.6696600000000004
W	15.7531180000000006	17.7406949999999988	5.7523030000000004
W	13.8745940000000001	21.0291120000000014	5.8372029999999997
W	12.4808810000000001	23.5079829999999994	5.7814490000000003
W	10.6269939999999998	26.7912700000000008	5.7531809999999997
W	9.1985840000000003	29.2742329999999988	5.5606559999999998
W	7.4680369999999998	32.0538200000000018	5.3852240000000000
Se	20.5646529999999998	-0.0688730000000000	5.1545920000000001
Se	18.9527639999999984	2.7605580000000001	5.0801040000000004
Se	17.2169820000000016	5.5672699999999997	4.8104570000000004
Se	15.6444960000000002	8.4168730000000007	5.1986660000000002
Se	13.9843700000000002	11.2233079999999994	5.1848440000000000
Se	12.2606190000000002	14.0520200000000006	4.9609730000000001
Se	10.6505650000000003	16.9833800000000004	5.2614489999999998
Se	8.9318150000000003	19.7705839999999995	4.9511360000000000
Se	7.3929780000000003	22.7281399999999998	5.1746949999999998
Se	5.6984300000000001	25.5092059999999989	4.8057090000000002
Se	4.1290500000000003	28.4240910000000007	5.0505180000000003
Se	2.5012420000000000	31.2497219999999984	5.1038500000000004
Se	23.6887229999999995	-0.5078900000000000	2.9070589999999998
Se	22.0091040000000007	2.5298129999999999	6.4886390000000000
Se	20.2956479999999999	5.4802119999999999	6.1910119999999997
Se	18.7315299999999993	8.2707189999999997	6.5985449999999997

Se	17.0227150000000016	11.1127230000000008	6.3690720000000001
Se	15.3589529999999996	13.9548109999999994	6.6109429999999998
Se	13.6708010000000009	16.7731670000000008	6.3664930000000002
Se	12.0341260000000005	19.7093810000000005	6.6897029999999997
Se	10.3910140000000002	22.5356270000000016	6.3476100000000004
Se	8.7923270000000002	25.4579290000000000	6.6002700000000001
Se	7.1547900000000002	28.2062510000000017	6.1812709999999997
Se	5.4624660000000000	31.1798269999999995	6.4654330000000000
Se	24.2171239999999983	5.5663830000000001	6.9730410000000003
Se	22.6279520000000005	8.5011910000000004	7.2079930000000001
Se	20.7798529999999992	11.3750250000000008	7.0568980000000003
Se	19.1923800000000000	14.3385639999999999	7.2171230000000000
Se	17.5580560000000006	17.0965769999999999	7.2244630000000001
Se	15.7744830000000000	19.8939330000000005	7.1046500000000004
Se	14.2024600000000003	22.8679290000000002	7.4154749999999998
Se	12.5490619999999993	25.7258250000000004	7.0361070000000003
Se	10.9117420000000003	28.7049319999999994	7.2498440000000004
Se	9.2004049999999999	31.5645640000000007	6.9774880000000001
Se	18.1128590000000003	2.1829749999999999	1.5391610000000000
Se	16.4666519999999998	5.1210909999999998	1.7531490000000001
Se	14.6862610000000000	8.0091300000000007	1.5743849999999999
Se	13.1652869999999993	10.7544360000000001	1.6446149999999999
Se	11.4963130000000007	13.6557089999999999	1.8834880000000001
Se	9.7888870000000008	16.4242990000000013	1.5425750000000000
Se	8.0701769999999993	19.2590420000000009	1.9326900000000000
Se	6.5076159999999996	22.1221490000000003	1.4816480000000001
Se	4.8805019999999999	25.0580229999999986	1.7640180000000001
Se	3.2378239999999998	27.9854050000000001	1.5040780000000000
Se	1.9297940000000000	30.9353529999999992	1.3591519999999999
Se	-0.0123250000000000	33.5529340000000005	3.4529519999999998
Se	21.9118700000000004	2.5975690000000000	2.2450770000000002
Se	20.1974310000000017	5.4114990000000001	2.4610390000000000
Se	18.4844700000000017	8.2551249999999996	2.2211370000000001

Se	16.979120999999992	11.077954000000001	2.6276730000000001
Se	15.236933999999998	13.886186000000004	2.3339080000000001
Se	13.566335000000005	16.801769000000002	2.6482679999999998
Se	11.886039000000002	19.566758000000001	2.3102399999999998
Se	10.282631999999996	22.452843000000014	2.5917150000000002
Se	8.667149999999995	25.248829000000006	2.2153040000000002
Se	7.061971999999999	28.153113999999986	2.4576750000000001
Se	5.508836999999998	31.054444000000002	2.2221030000000002
Se	3.728645000000002	34.159008999999975	2.8569460000000002
Se	25.098396999999985	2.1425160000000001	4.3788729999999996
Se	23.264873000000015	5.3773410000000004	3.5880580000000002
Se	21.545552000000007	8.1141020000000008	3.5963900000000000
Se	20.010390000000010	10.937756999999995	4.0061650000000002
Se	18.303869999999999	13.826679999999996	3.7585329999999999
Se	16.644992999999995	16.595393999999989	3.7209590000000001
Se	14.982113999999993	19.515415999999983	4.0395760000000003
Se	13.273016999999994	22.286414000000006	3.7429779999999999
Se	11.755871000000008	25.223124999999996	3.9996010000000002
Se	10.076553999999998	27.971077000000011	3.6081360000000000
Se	8.576558000000003	30.824974000000010	3.5925680000000000
Se	6.709157000000003	34.038876000000019	4.3609109999999998
Se	19.996279000000012	-0.4362980000000000	1.4130940000000001
Se	21.264361000000010	-3.4182610000000002	3.5300240000000001

W₃₆Se₇₂; $E_{tot}=-21\ 088\ 501.190\ 420\ 91\ \text{eV}$; $E_{rel}=79.840\ 640\ 305\ 5\ \text{meV/f.u.}$

W	14.933109999999992	15.324362000000007	3.4147340000000002
W	13.140314000000000	18.159908000000015	3.5636640000000002
W	11.575805000000008	20.871971999999995	3.6070630000000001
W	10.131816000000006	23.737007999999994	3.4958860000000000
W	18.161712000000014	15.277920999999992	3.3268399999999998
W	16.345973000000008	17.519691999999992	3.4531930000000002
W	14.264127999999995	20.676542000000013	3.4394610000000001

W	12.7571150000000006	23.4361420000000003	3.4238879999999998
W	11.6718750000000000	26.5626430000000013	3.3886799999999999
W	21.2740040000000015	15.2739469999999997	3.3931979999999999
W	19.4123610000000006	17.7301900000000003	3.4286669999999999
W	18.3418279999999996	20.8198180000000015	3.4464210000000000
W	16.7838540000000016	23.6336469999999998	3.5557370000000001
W	14.7429810000000003	26.9159490000000012	3.4268779999999999
W	13.2124640000000007	29.2171750000000010	3.3384890000000000
W	24.4802129999999991	15.3878760000000003	3.4920610000000001
W	23.4021930000000005	17.7992319999999999	3.4071180000000001
W	21.2078290000000003	21.1568289999999983	3.5316429999999999
W	17.9433100000000003	26.2316259999999986	3.4368289999999999
W	16.1860169999999997	29.6824779999999997	3.4397319999999998
W	14.9001959999999993	31.9877460000000013	3.4334220000000002
W	26.2202120000000001	18.0895900000000012	3.5718990000000002
W	25.0259059999999991	20.5341529999999999	3.3966099999999999
W	22.5985809999999994	23.6962420000000016	3.4625290000000000
W	21.1629719999999999	26.2151710000000016	3.4763320000000002
W	19.5999249999999989	29.8405710000000006	3.4363470000000000
W	18.1787659999999995	32.1628169999999969	3.5453830000000002
W	27.7677760000000013	20.7570709999999998	3.5220229999999999
W	26.6316999999999986	23.9676439999999999	3.4940449999999998
W	25.0824309999999997	26.7848089999999992	3.5346890000000002
W	23.4419480000000000	29.5435359999999996	3.4999229999999999
W	21.2066510000000008	32.1287450000000021	3.5494849999999998
W	29.2843459999999993	23.7204669999999993	3.3938030000000001
W	27.7834959999999995	26.5703659999999999	3.3501509999999999
W	26.2376739999999984	29.2610150000000004	3.3435950000000001
W	24.5097069999999988	31.9789560000000002	3.3943690000000002
Se	16.2207790000000003	13.5799090000000007	4.3378220000000001
Se	14.5707470000000008	16.9312460000000016	5.2828860000000004
Se	12.8719649999999994	19.7860699999999987	5.4398520000000001
Se	11.2574860000000001	22.6379979999999996	5.4022069999999998

Se	9.312222999999995	25.806042999999990	4.3740300000000003
Se	19.7065190000000001	13.541859999999998	4.2353009999999998
Se	17.9738429999999987	16.8070899999999988	5.2881660000000004
Se	16.3270389999999992	19.7632629999999985	4.7992600000000003
Se	14.7042420000000007	22.6870229999999999	4.9768770000000000
Se	13.0752530000000000	25.5854520000000001	5.0313179999999997
Se	10.9176939999999991	28.7974500000000013	4.1758490000000004
Se	23.1096159999999990	13.6414360000000006	4.3909640000000003
Se	21.4064049999999995	16.9989789999999985	5.0227570000000004
Se	19.7482010000000017	19.7435520000000011	5.1595170000000001
Se	18.0663249999999991	22.6080150000000017	5.2939990000000003
Se	16.2802630000000015	25.5974010000000014	5.1557420000000000
Se	14.6656420000000001	28.6459389999999985	5.2549229999999998
Se	12.7243650000000006	31.7607940000000006	4.3111439999999996
Se	24.8698090000000001	16.9261119999999998	5.3820759999999996
Se	23.0647829999999985	19.8599050000000013	4.9336110000000000
Se	21.3261509999999994	22.7874109999999988	5.3527839999999998
Se	19.6511209999999998	25.5570929999999983	5.1988469999999998
Se	18.0198150000000012	28.4784779999999991	4.8869879999999997
Se	16.4497609999999987	31.5005810000000004	5.2981199999999999
Se	26.4882060000000017	19.7462069999999983	5.4066440000000000
Se	24.6929109999999987	22.7502320000000005	4.7860699999999996
Se	23.1391440000000017	25.6824310000000011	5.0110489999999999
Se	21.4045120000000004	28.4984329999999986	4.7981460000000000
Se	19.6850659999999991	31.4828520000000012	5.4212470000000001
Se	28.0398969999999998	22.6444890000000001	5.2496359999999997
Se	26.4925899999999999	25.6715139999999984	5.3213559999999998
Se	24.8346440000000008	28.5566400000000016	5.3267620000000004
Se	22.9730799999999995	31.4079170000000012	5.2606299999999999
Se	30.2083900000000014	25.6868519999999982	4.3071289999999998
Se	28.4204280000000011	28.7189450000000015	4.4894910000000001
Se	26.6836319999999994	31.7937869999999982	4.3066490000000002
Se	12.7341909999999991	15.6331299999999995	2.5630839999999999

Se	10.8990770000000001	18.6161910000000006	2.6414010000000001
Se	9.1958289999999998	21.7551220000000001	2.5967419999999999
Se	16.4503079999999997	15.7604009999999999	1.5078830000000001
Se	14.6758120000000005	18.7756280000000011	1.7824460000000000
Se	12.8625729999999994	21.6933690000000006	1.5977220000000001
Se	11.4109339999999992	24.7335889999999985	1.6243810000000001
Se	19.7525559999999984	15.9995390000000004	1.5412969999999999
Se	17.9301430000000011	18.8622809999999994	1.8014220000000001
Se	16.2637129999999992	21.7120989999999985	2.0151960000000000
Se	14.7342420000000001	24.6112199999999994	2.1743370000000000
Se	13.0860889999999994	27.4804490000000001	1.5427569999999999
Se	22.9686279999999989	15.9706580000000002	1.6181559999999999
Se	21.3885199999999998	18.8985729999999990	2.1421220000000001
Se	19.7209450000000004	21.8062170000000002	1.6982210000000000
Se	18.1008050000000011	24.5430330000000012	1.6835970000000000
Se	16.4717610000000008	27.6156900000000007	1.8054060000000001
Se	14.5376630000000002	30.4283880000000018	1.5414450000000000
Se	26.6545349999999992	15.5840270000000007	2.5655239999999999
Se	24.8367949999999986	18.7750130000000013	1.5791649999999999
Se	23.1175280000000001	21.6919980000000017	1.9064719999999999
Se	21.2930670000000006	24.6251980000000010	1.5936729999999999
Se	19.6863509999999984	27.6212869999999988	1.9665459999999999
Se	17.9571520000000007	30.5880919999999996	1.6750689999999999
Se	16.1885210000000015	33.7578499999999977	2.5283180000000001
Se	28.5003349999999998	18.6140849999999993	2.5798939999999999
Se	26.4728299999999983	21.8270480000000013	1.7730950000000001
Se	24.6442160000000001	24.6639559999999989	2.0306090000000001
Se	23.0604149999999990	27.4867680000000014	2.0241829999999998
Se	21.4736319999999985	30.4551039999999986	1.8136790000000000
Se	19.7148240000000001	33.9225819999999985	2.7091020000000001
Se	30.1440270000000012	21.6948879999999988	2.5216820000000002
Se	28.1222940000000001	24.8284090000000006	1.5231619999999999
Se	26.5358969999999985	27.6410879999999999	1.4971969999999999

Se	24.9070360000000015	30.4328590000000005	1.5190999999999999
Se	23.1561219999999999	33.7283990000000031	2.5391119999999998

W₃₆Se₇₂; $E_{tot} = -21\,088\,501.284\,784\,41$ eV; $E_{rel} = 77.219\,431\,972\,2$ meV/f.u.

W	20.0429950000000012	1.2933660000000000	3.3783080000000001
W	18.2540760000000013	4.0407549999999999	3.2988819999999999
W	16.7594490000000000	6.4859650000000002	3.1475469999999999
W	14.8936469999999996	9.7486250000000005	3.1185459999999998
W	13.4582949999999997	12.1970200000000002	3.0495549999999998
W	11.5851889999999997	15.4292730000000002	3.0495009999999998
W	10.1500229999999991	17.8803969999999985	2.9763679999999999
W	8.2710100000000004	21.1165430000000001	2.9768100000000000
W	6.8457650000000001	23.5742100000000008	2.9016389999999999
W	4.9633710000000004	26.8428350000000009	2.9135890000000000
W	3.5607739999999999	29.5487670000000016	3.0441739999999999
W	2.0134379999999998	32.1425219999999996	3.0954079999999999
W	23.0284140000000015	1.2165919999999999	3.5954039999999998
W	21.4212659999999993	3.5808230000000001	3.5837340000000002
W	19.5791180000000011	6.9279940000000000	3.6145220000000000
W	18.2690260000000002	9.2442340000000005	3.5462929999999999
W	16.3126959999999990	12.6215659999999996	3.5184709999999999
W	14.9755699999999994	14.9158019999999993	3.4672079999999998
W	13.0045420000000007	18.3057540000000003	3.4460999999999999
W	11.6670200000000008	20.5993400000000015	3.3935719999999998
W	9.7110079999999996	23.9771390000000011	3.3656969999999999
W	8.4014869999999995	26.2933629999999994	3.2986059999999999
W	6.5590149999999996	29.6404509999999988	3.3301219999999998
W	4.9522360000000001	32.0046719999999993	3.3189160000000002
W	25.9670990000000010	1.0791919999999999	3.8189519999999999
W	24.4195940000000000	3.6726130000000001	3.8694540000000002
W	23.0167970000000004	6.3787310000000002	3.9995660000000002
W	21.1343209999999999	9.6476039999999994	4.0109990000000000

W	19.7090549999999993	12.1049819999999997	3.9350139999999998
W	17.8298279999999991	15.3407339999999994	3.9354529999999999
W	16.3943000000000012	17.7917969999999990	3.8637850000000000
W	14.5217969999999994	21.0241669999999985	3.8634879999999998
W	13.0867290000000001	23.4725959999999993	3.7934320000000001
W	11.2210029999999996	26.7352269999999983	3.7653660000000002
W	9.7262599999999999	29.1801700000000004	3.6146690000000001
W	7.9378440000000001	31.9280639999999991	3.5367590000000000
Se	21.1550909999999988	-0.5049930000000000	4.4240599999999999
Se	19.5148890000000002	2.8288600000000002	5.1990090000000002
Se	17.9874809999999989	5.6742910000000002	5.1804040000000002
Se	16.1764639999999993	8.3566710000000004	4.8715619999999999
Se	14.7047329999999992	11.3295220000000008	5.0517870000000000
Se	12.8806569999999994	14.0393369999999997	4.7988359999999997
Se	11.3953389999999999	17.0128899999999987	4.9792699999999996
Se	9.5700970000000005	19.7238760000000006	4.7239350000000000
Se	8.0910010000000003	22.7050060000000009	4.9033990000000003
Se	6.2857870000000000	25.4159049999999986	4.6262679999999996
Se	4.7875170000000002	28.3597590000000004	4.8796530000000002
Se	3.1724019999999999	31.1898079999999993	4.9956209999999999
Se	24.4638129999999983	-0.4421880000000000	4.8806490000000000
Se	22.8690120000000014	2.7629630000000001	5.5401040000000004
Se	21.2196210000000001	5.6178629999999998	5.3406960000000003
Se	19.6653540000000007	8.5605139999999995	5.5928370000000003
Se	17.9152060000000013	11.2951040000000003	5.2665459999999999
Se	16.3609420000000014	14.2355370000000008	5.5127059999999997
Se	14.6040620000000008	16.9710569999999983	5.1895490000000004
Se	13.0539799999999993	19.9180929999999989	5.4407959999999997
Se	11.2965049999999998	22.6521009999999983	5.1191800000000001
Se	9.7809500000000007	25.6052859999999995	5.3511689999999996
Se	8.0163589999999996	28.2732659999999996	5.0139279999999999
Se	6.4110790000000000	31.2881840000000011	5.3293879999999998
Se	27.7958789999999993	-0.0156750000000000	3.0251649999999999

Se	26.534542999999993	2.945879000000001	5.180133999999998
Se	25.146453000000011	5.856565999999999	4.990896000000002
Se	23.401977999999997	8.734597000000008	4.804890999999996
Se	21.847774000000011	11.717314000000000	5.090270000000003
Se	20.111729000000004	14.494737000000006	4.687508000000002
Se	18.515198999999991	17.406712999999999	5.044373000000002
Se	16.809664000000015	20.188307999999993	4.599248000000002
Se	15.205099000000006	23.093303999999998	4.974516999999996
Se	13.483313000000008	25.879177999999996	4.539880000000001
Se	11.893371999999994	28.866887999999994	4.758079999999996
Se	10.103630000000008	31.677789000000006	4.547399000000004
Se	17.876702000000016	1.542627000000000	2.367734000000000
Se	16.087243999999983	4.353880000000002	2.155691000000000
Se	14.497139000000007	7.341783000000004	2.372641999999999
Se	12.775066000000007	10.127834000000000	1.938375000000000
Se	11.170738000000001	13.032890999999993	2.312246000000000
Se	9.464487000000001	15.814209999999992	1.868022000000001
Se	7.867735999999998	18.726779000000005	2.225096000000002
Se	6.132091000000000	21.504495999999996	1.821974000000000
Se	4.578278000000001	24.486699999999990	2.107794000000002
Se	2.833615000000000	27.365304999999993	1.922420999999999
Se	1.446226000000000	30.276178000000016	1.733654999999999
Se	0.184568000000000	33.237155000000013	3.889467999999999
Se	21.569019999999983	1.933024000000001	1.585275000000000
Se	19.963826999999984	4.947415000000003	1.899483000000000
Se	18.199422999999995	7.615508000000002	1.561237000000000
Se	16.683600999999995	10.569188000000005	1.793293000000000
Se	14.925976999999996	13.303281000000001	1.471862000000000
Se	13.375486999999997	16.250112000000014	1.722758999999999
Se	11.618883999999995	18.985434999999990	1.399898000000001
Se	10.064828000000003	21.926373000000017	1.645771000000001
Se	8.314778999999997	24.660924000000014	1.319529000000000
Se	6.760633999999996	27.603978999999989	1.572503000000000

Se	5.1114220000000001	30.4590870000000002	1.3737450000000000
Se	3.5175749999999999	33.6635029999999986	2.0347620000000002
Se	24.8083789999999986	2.0314899999999998	1.9183390000000000
Se	23.1929330000000000	4.8609720000000003	2.0337239999999999
Se	21.6942990000000009	7.8052489999999999	2.2862030000000000
Se	19.8892969999999991	10.5163370000000000	2.0088390000000000
Se	18.4095900000000015	13.4974310000000006	2.1890489999999998
Se	16.5845359999999999	16.2083170000000010	1.9331769999999999
Se	15.0990389999999994	19.1819759999999988	2.1128930000000001
Se	13.2752970000000001	21.8914070000000009	1.8609830000000001
Se	11.8041250000000009	24.8647419999999997	2.0409920000000001
Se	9.9931099999999997	27.5473670000000013	1.7326360000000001
Se	8.4654840000000000	30.3931450000000005	1.7147699999999999
Se	6.8253219999999999	33.7259230000000017	2.4913669999999999

W₃₆Se₇₂; $E_{tot} = -21\,088\,502.714\,441\,44$ eV; $E_{rel} = 37.506\,736\,694\,4$ meV/f.u.

W	14.9499279999999999	15.4059320000000000	3.4342959999999998
W	13.3215050000000002	17.8085899999999988	3.4313110000000000
W	11.3077349999999992	20.9826590000000017	3.2737930000000000
W	18.1033890000000000	15.2647709999999996	3.3492970000000000
W	16.4595279999999988	17.5434100000000015	3.4689920000000001
W	14.7232819999999993	21.1420959999999987	3.3763070000000002
W	13.0504090000000001	23.7679949999999991	3.4516279999999999
W	11.3206070000000008	26.3858159999999984	3.7536010000000002
W	21.1946070000000013	15.2909659999999992	3.3780579999999998
W	19.5912089999999992	17.5220580000000012	3.4293170000000002
W	17.9139569999999999	21.2160170000000008	3.2820490000000002
W	16.0460710000000013	23.6499670000000002	3.3937460000000002
W	14.4818390000000008	26.2370739999999998	3.4581870000000001
W	13.3328769999999999	29.5301399999999994	3.4664640000000002
W	24.5142270000000018	15.4057899999999997	3.5018250000000002
W	23.3727890000000009	17.7850129999999993	3.3944860000000001

W	21.146274999999993	21.152957000000007	3.431979999999998
W	19.867774000000007	23.623698999999984	3.419708000000000
W	18.308222000000007	26.171026999999987	3.503231000000000
W	16.530467000000016	29.763725999999984	3.438372000000002
W	14.985068999999993	31.899567999999986	3.463293000000002
W	26.203808999999997	18.100764000000016	3.597465000000001
W	24.968142000000003	20.478180999999993	3.427220999999999
W	22.715851000000007	23.833771999999997	3.484754000000001
W	21.233236999999990	26.220527000000006	3.528786999999999
W	19.728760999999987	29.881259000000000	3.422280000000002
W	18.170902000000017	32.094683000000034	3.521964999999998
W	27.748490000000003	20.816469000000014	3.571242999999999
W	26.711007999999996	23.912234999999990	3.482609000000001
W	25.123646000000008	26.624577999999996	3.506850000000000
W	22.931965000000017	29.835785000000013	3.453333000000002
W	21.278224000000016	32.115707000000004	3.565507999999999
W	29.315564999999994	23.725200000000010	3.414235999999998
W	27.818529999999991	26.550993999999993	3.331951000000001
W	26.275634000000002	29.216574999999989	3.376088000000002
W	24.493345000000015	31.988596000000011	3.533137000000000
Se	16.240393000000010	13.757854999999993	4.612523000000004
Se	14.735127000000003	17.024757999999985	5.322470000000000
Se	12.923545000000007	19.822946000000017	4.970504000000000
Se	11.181335999999999	22.642126999999986	5.005880000000003
Se	9.373445999999995	26.139669999999989	4.940584000000003
Se	19.728290999999987	13.588214000000007	4.362008000000003
Se	18.031479999999984	16.849630999999987	5.309878999999996
Se	16.363541000000014	19.830563999999990	4.820992999999996
Se	14.577811999999998	22.742450999999991	5.271073000000003
Se	12.923246000000007	25.532713000000011	5.367376000000001
Se	10.975262000000007	28.913498000000006	4.026139999999998
Se	23.172034000000000	13.666292000000003	4.387615000000003
Se	21.436325000000001	16.987776000000002	5.099433000000003

Se	19.5646260000000005	19.7906610000000001	4.8344120000000004
Se	17.9308820000000004	22.8394070000000013	5.0680529999999999
Se	16.3164550000000013	25.6140770000000018	5.0941039999999997
Se	14.7573410000000003	28.4776139999999991	5.0458600000000002
Se	12.7471619999999994	31.7783419999999985	4.4083470000000000
Se	24.8307469999999988	16.9535079999999994	5.3958789999999999
Se	22.9986120000000014	19.8733280000000008	4.9274509999999996
Se	21.3881389999999989	22.7189799999999984	5.3395330000000003
Se	19.7786350000000013	25.4356930000000006	5.3951729999999998
Se	18.1437449999999991	28.4494159999999994	4.9390879999999999
Se	16.4900500000000001	31.5646330000000006	5.3633350000000002
Se	26.4633809999999983	19.7640269999999987	5.4348169999999998
Se	24.7400359999999999	22.7331779999999988	4.7885920000000004
Se	23.1804309999999987	25.6625650000000007	5.1324880000000004
Se	21.3585789999999989	28.4695859999999996	4.9467160000000003
Se	19.7165950000000016	31.5954979999999992	5.4153180000000001
Se	28.0898639999999986	22.6483080000000001	5.3007710000000001
Se	26.5670690000000000	25.6583159999999992	5.3304260000000001
Se	24.7026949999999985	28.5887990000000016	5.1012610000000000
Se	22.9568750000000001	31.5670369999999991	5.4111719999999996
Se	30.2039289999999987	25.6935140000000004	4.3770980000000002
Se	28.5249179999999996	28.7794039999999995	4.2729999999999997
Se	26.6937519999999999	31.6933459999999982	4.3793990000000003
Se	12.7056600000000000	15.5704049999999992	2.4949210000000002
Se	10.9996469999999995	18.4624500000000005	2.8404250000000002
Se	9.2620419999999992	21.1740789999999990	2.2613400000000001
Se	16.4302549999999989	15.7709290000000006	1.5195380000000001
Se	14.7570610000000002	18.8659919999999985	1.8448380000000000
Se	12.8975069999999992	21.8304480000000005	1.6505950000000000
Se	11.0672420000000002	24.7139640000000007	2.0386220000000002
Se	19.6704439999999998	15.8180560000000003	1.4754240000000001
Se	18.0180259999999990	18.8934519999999999	1.9062180000000000
Se	16.2415209999999988	21.8740290000000002	1.5125010000000001

Se	14.5585920000000009	24.6717440000000003	1.5720179999999999
Se	12.8920549999999992	27.5628250000000001	1.9085300000000001
Se	22.9691890000000001	15.9170719999999992	1.6258220000000001
Se	21.3630980000000008	18.8807459999999985	2.0576140000000001
Se	19.6796809999999986	21.8073569999999997	1.5433589999999999
Se	18.0063129999999987	24.5523910000000001	1.7643390000000001
Se	16.4316090000000017	27.4450620000000001	2.1496100000000000
Se	14.7950379999999999	30.2539769999999990	1.5941179999999999
Se	26.6909840000000003	15.6085010000000004	2.6078109999999999
Se	24.8454900000000016	18.7688160000000011	1.5793390000000000
Se	23.0997799999999991	21.6855939999999983	1.9566600000000001
Se	21.3202150000000010	24.6563389999999991	1.5574509999999999
Se	19.7281709999999997	27.6140049999999988	1.9836450000000001
Se	18.0775940000000013	30.4683589999999995	1.5992430000000000
Se	16.2318530000000010	33.5815440000000009	2.3029020000000000
Se	28.4891739999999984	18.6417430000000017	2.6580580000000000
Se	26.4155580000000008	21.8503800000000012	1.8182100000000001
Se	24.7031589999999994	24.6630849999999988	1.9498450000000001
Se	23.0473759999999999	27.5516530000000017	2.1596560000000000
Se	21.3850049999999996	30.5285970000000013	1.6096670000000000
Se	19.7263219999999997	33.7130590000000012	2.3872510000000000
Se	30.1307510000000001	21.6484440000000014	2.5767050000000000
Se	28.1772120000000008	24.8115820000000014	1.5123640000000000
Se	26.4756439999999991	27.5828039999999994	1.5011429999999999
Se	24.7576369999999990	30.3782670000000010	1.6686700000000001
Se	23.2496359999999989	33.7696699999999979	2.6002010000000002

W₃₆Se₇₂; $E_{tot} = -21\,088\,503.607\,691\,06$ eV; $E_{rel} = 12.694\,247\,250\,0$ meV/f.u.

W	19.9095750000000002	1.4184019999999999	3.5450249999999999
W	18.1627860000000005	4.1633490000000002	3.3539620000000001
W	16.6077410000000008	6.6764970000000003	3.0873469999999998
W	14.9868799999999993	9.2249389999999991	2.8536250000000001

W	23.129796999999999	1.2690980000000001	3.5843929999999999
W	21.460288999999995	3.6079699999999999	3.5273780000000001
W	19.4085980000000013	6.9161250000000001	3.2265950000000001
W	18.1207029999999989	9.2185819999999996	2.9229390000000000
W	26.3280490000000000	1.2060960000000001	3.6165370000000001
W	24.6178290000000004	3.5109629999999998	3.5931310000000001
W	23.1877519999999997	7.1825210000000004	3.2572869999999998
W	21.4928540000000012	9.4072540000000000	3.1644760000000001
W	29.5379509999999996	1.1708680000000000	3.6313510000000000
W	27.8618290000000002	3.4637080000000000	3.5908660000000001
W	26.3351259999999989	7.1738710000000001	3.2894040000000002
W	24.7314949999999989	9.4597180000000005	3.2727930000000001
W	32.7438050000000018	1.1367060000000000	3.6449989999999999
W	31.1177239999999991	3.4344700000000001	3.5942200000000000
W	29.5451529999999991	7.1435810000000002	3.3188439999999999
W	27.9190259999999988	9.4416239999999991	3.2681360000000002
W	35.9313629999999975	1.1186469999999999	3.6404120000000000
W	34.3277050000000017	3.4039199999999998	3.6235510000000000
W	32.8010930000000016	7.1147080000000003	3.3223360000000000
W	31.1249360000000017	9.4070780000000003	3.2816749999999999
W	39.1699690000000018	1.1709799999999999	3.7488130000000002
W	37.4750599999999991	3.3953970000000000	3.6556970000000000
W	36.0451759999999979	7.0674510000000001	3.3200370000000001
W	34.3347309999999979	9.3716050000000006	3.2964310000000001
W	42.5421830000000014	1.3597490000000001	3.9905469999999998
W	41.2543879999999987	3.6619030000000001	3.6867070000000002
W	39.2025349999999975	6.9701019999999998	3.3855870000000001
W	37.5329460000000026	9.3086780000000005	3.3284449999999999
W	45.6760080000000031	1.3530599999999999	4.0593959999999996
W	44.0548670000000016	3.9016060000000001	3.8259349999999999
W	42.4999690000000001	6.4147439999999998	3.5588810000000000
W	40.7532059999999987	9.1598020000000009	3.3677600000000001
Se	21.0555120000000002	-0.3316760000000000	4.5898750000000001

Se	19.576294999999982	3.1627710000000002	5.2616350000000001
Se	17.9725900000000003	5.9298529999999996	5.1053550000000003
Se	16.3856439999999992	8.7308699999999995	4.7694809999999999
Se	24.4973029999999987	-0.4214460000000000	4.6503560000000004
Se	22.9489079999999994	2.9593110000000000	5.4334009999999999
Se	21.3669839999999986	5.9573619999999998	4.6942719999999998
Se	19.7205100000000009	8.9340290000000007	4.8792299999999997
Se	27.7982879999999994	-0.4729140000000000	4.6471159999999996
Se	26.2280830000000016	2.9238610000000000	5.4529930000000002
Se	24.6628049999999988	5.8749099999999999	4.8700279999999996
Se	23.0554710000000007	8.9898650000000000	5.1005529999999997
Se	31.0594800000000006	-0.5076500000000000	4.6610420000000001
Se	29.4799889999999998	2.9036860000000000	5.4538300000000000
Se	27.8917460000000013	5.8233129999999997	4.8510309999999999
Se	26.3088979999999992	9.0174649999999996	5.1526430000000003
Se	34.3371509999999986	-0.5072790000000000	4.7214070000000001
Se	32.7107839999999968	2.8565250000000000	5.4810689999999997
Se	31.1491320000000016	5.7796890000000003	4.8498630000000000
Se	29.5190669999999997	9.0069420000000004	5.1622800000000000
Se	37.6784620000000032	-0.5585810000000000	4.5851769999999998
Se	35.9353809999999996	2.7863650000000000	5.5321680000000004
Se	34.3896719999999974	5.7460420000000001	4.8682429999999997
Se	32.7307720000000018	8.9641660000000005	5.1707159999999996
Se	41.0091809999999981	-0.2814780000000000	4.9738870000000004
Se	39.3210160000000002	2.9546239999999999	5.3826739999999997
Se	37.5807410000000033	5.7251010000000004	4.9477549999999999
Se	35.9373810000000020	8.9009250000000009	5.1892220000000000
Se	44.3319720000000004	0.0062140000000000	5.4411649999999998
Se	42.7052430000000030	3.1260960000000000	5.7360650000000000
Se	40.8622950000000031	5.8018869999999998	5.1703679999999999
Se	39.1733479999999972	8.8281799999999997	5.2288280000000000
Se	47.5240510000000000	0.2390140000000000	3.3539430000000001
Se	46.2840320000000034	3.4239340000000000	5.0506799999999998

Se	44.7185670000000002	6.2123400000000002	4.5391680000000001
Se	42.8970899999999986	8.9674540000000000	4.3600219999999998
Se	17.7656680000000016	1.6106600000000000	2.5528119999999999
Se	15.9441930000000003	4.3658320000000002	2.3738790000000001
Se	14.3787920000000007	7.1543479999999997	1.8626469999999999
Se	13.1386009999999995	10.3392260000000000	3.5599729999999998
Se	21.4894919999999985	1.7499439999999999	1.6840759999999999
Se	19.8005659999999999	4.7762729999999998	1.7427090000000001
Se	17.9574080000000009	7.4522760000000003	1.1772830000000001
Se	16.3308700000000009	10.5720259999999993	1.4726220000000001
Se	24.7255129999999994	1.6771689999999999	1.7237730000000000
Se	23.0820879999999988	4.8530160000000002	1.9652760000000000
Se	21.3417360000000009	7.6236620000000004	1.5305700000000000
Se	19.6536210000000011	10.8598979999999994	1.9393899999999999
Se	27.9321100000000015	1.6139150000000000	1.7423660000000001
Se	26.2732080000000003	4.8320220000000003	2.0446780000000002
Se	24.7274560000000001	7.7918719999999997	1.3809950000000000
Se	22.9843350000000015	11.1368379999999991	2.3280569999999998
Se	31.1438309999999987	1.5711370000000000	1.7508230000000000
Se	29.5137949999999982	4.7984020000000003	2.0631010000000001
Se	27.9520480000000013	7.7216659999999999	1.4320070000000000
Se	26.3256779999999999	11.0854929999999996	2.1916389999999999
Se	34.3540149999999969	1.5605920000000000	1.7604869999999999
Se	32.7711029999999965	4.7548349999999999	2.0620219999999998
Se	31.1828919999999989	7.6744100000000000	1.4591580000000000
Se	29.6034210000000009	11.0857670000000006	2.2520169999999999
Se	37.6073639999999969	1.5882140000000000	1.8127030000000000
Se	36.0000130000000027	4.7032140000000000	2.0431080000000001
Se	34.4347449999999995	7.6541689999999996	1.4599230000000001
Se	32.8646159999999981	11.0510389999999994	2.2659210000000001
Se	40.9422550000000003	1.6440450000000000	2.0340579999999999
Se	39.2957449999999966	4.6207079999999996	2.2187920000000001
Se	37.7138720000000021	7.6186829999999999	1.4794600000000000

Se	36.165469999999991	10.999454999999993	2.2625630000000001
Se	44.277282999999971	1.8472180000000000	2.1438370000000000
Se	42.690297999999985	4.6482429999999999	1.8078749999999999
Se	41.0864630000000020	7.4151530000000001	1.6513599999999999
Se	39.607174999999980	10.9096320000000002	2.3228040000000001

W₃₆Se₇₂; $E_{tot} = -21\,088\,504.064\,683\,96$ eV; $E_{rel} = 0$ meV/f.u.

W	29.633275999999986	1.2652530000000000	3.5064860000000002
W	27.873190999999985	3.9848509999999999	3.4627520000000001
W	26.286042999999994	6.7286409999999997	3.4146470000000000
W	24.7688190000000006	9.5482940000000003	3.2512520000000000
W	23.2039480000000005	12.4681940000000004	2.9291969999999998
W	21.5753780000000006	15.1309059999999995	2.8212989999999998
W	32.9845720000000000	1.1501370000000000	3.5402950000000000
W	30.728442999999986	3.6912600000000002	3.3899699999999999
W	29.0822870000000009	6.3803159999999997	3.3181479999999999
W	27.540048999999998	9.1566069999999993	3.2684510000000002
W	25.873235999999986	12.5709079999999993	3.1589580000000002
W	24.662728999999988	15.0017289999999992	2.9737890000000000
W	36.169593999999965	1.1782340000000000	3.5768290000000000
W	34.6464690000000033	3.6307450000000001	3.4980009999999999
W	32.9538340000000005	6.9521559999999996	3.5155940000000001
W	31.460705999999983	9.7336919999999996	3.5422050000000000
W	29.803067999999997	12.5504169999999995	3.3691000000000000
W	27.8538150000000009	15.0681469999999997	3.1787359999999998
W	39.3454550000000012	1.1707580000000000	3.7343810000000000
W	37.396335999999980	3.6884100000000002	3.5436749999999999
W	35.738003999999966	6.5053549999999998	3.3711679999999999
W	34.2458280000000030	9.2866090000000003	3.3976299999999999
W	32.552835999999992	12.6077019999999997	3.4156740000000001
W	31.029731999999992	15.0601590000000005	3.3367089999999999
W	42.536614999999976	1.2373810000000001	3.9395380000000002

W	41.3260840000000016	3.6676460000000000	3.7537669999999999
W	39.6590899999999991	7.0824710000000000	3.6444690000000000
W	38.1173709999999986	9.8584779999999999	3.5945670000000001
W	36.4707030000000003	12.5473230000000004	3.5233200000000000
W	34.2150389999999973	15.0884879999999999	3.3730069999999999
W	45.6247499999999988	1.1086980000000000	4.0911980000000003
W	43.9952040000000011	3.7709100000000002	3.9837080000000000
W	42.4301019999999980	6.6908740000000000	3.6614689999999999
W	40.9128830000000008	9.5100949999999997	3.4985590000000002
W	39.3262149999999977	12.2536869999999993	3.4502750000000000
W	37.5661879999999968	14.9732529999999997	3.4067780000000001
Se	30.9782170000000008	-0.4383680000000000	4.4725380000000001
Se	29.1852400000000003	2.8493360000000001	5.3411549999999997
Se	27.5211760000000005	5.6323850000000002	5.2926469999999997
Se	25.9433630000000015	8.4677030000000002	5.1914910000000001
Se	24.3631209999999996	11.3889610000000001	4.9221209999999997
Se	22.8282239999999987	14.3362169999999995	4.7410639999999997
Se	34.4044370000000015	-0.5853500000000000	4.3729019999999998
Se	32.6876999999999995	2.9149759999999998	5.1051000000000002
Se	31.0285280000000014	5.7487050000000002	4.9130450000000003
Se	29.4376530000000010	8.5278500000000008	4.8368180000000001
Se	27.7603790000000004	11.4199040000000007	4.6038769999999998
Se	26.1430900000000008	14.4273690000000006	4.9392630000000004
Se	37.7097809999999996	-0.5461250000000000	4.5137980000000004
Se	36.0189659999999989	2.7520940000000000	5.4815959999999997
Se	34.3316260000000000	5.6302089999999998	5.2100140000000001
Se	32.7929379999999995	8.6114909999999991	5.3899809999999997
Se	31.1092610000000001	11.5184909999999991	5.2701609999999999
Se	29.3404489999999996	14.4069970000000005	5.1024289999999999
Se	40.9593819999999980	-0.4978530000000000	4.7294970000000003
Se	39.2775949999999980	2.9633720000000001	5.2973759999999999
Se	37.6967110000000005	5.8242240000000001	4.9911339999999997
Se	36.1659480000000002	8.6244160000000001	4.9433299999999996

Se	34.4675530000000023	11.5017549999999993	4.8173250000000003
Se	32.6600449999999967	14.4882950000000008	5.2192059999999998
Se	44.1790639999999968	-0.3578940000000000	5.2426450000000004
Se	42.5983230000000006	2.8492020000000000	5.8161389999999997
Se	40.9893530000000013	5.7552380000000003	5.3787140000000004
Se	39.5034459999999967	8.7999749999999999	5.4699400000000002
Se	37.8560640000000035	11.6328530000000008	5.3948570000000000
Se	35.9315470000000019	14.4641400000000004	5.2011349999999998
Se	47.4958659999999995	0.0260980000000000	3.3993560000000000
Se	46.1557579999999987	3.0289590000000000	5.3427860000000003
Se	44.6908850000000015	5.9568899999999996	4.8022330000000002
Se	43.2078950000000006	8.8970120000000001	4.4406299999999996
Se	41.5088220000000021	11.8357869999999998	4.5027309999999998
Se	39.7055980000000019	14.8534810000000004	4.3599389999999998
Se	27.4940299999999986	1.3851199999999999	2.5531009999999998
Se	25.6905350000000006	4.4029600000000002	2.4107449999999999
Se	23.9915780000000005	7.3421909999999997	2.4722620000000002
Se	22.5086720000000007	10.2823469999999997	2.1100690000000002
Se	21.0433619999999983	13.2113080000000007	1.5698240000000001
Se	19.7040879999999987	16.2142030000000013	3.5133420000000002
Se	31.2680599999999984	1.7745029999999999	1.7120789999999999
Se	29.3433400000000013	4.6059049999999999	1.5183739999999999
Se	27.6958020000000005	7.4389799999999999	1.4435549999999999
Se	26.2099639999999994	10.4839859999999998	1.5340309999999999
Se	24.6012410000000017	13.3902959999999993	1.0968199999999999
Se	23.0209639999999993	16.5976450000000000	1.6701400000000000
Se	34.5393439999999998	1.7502920000000000	1.6941710000000001
Se	32.7317290000000014	4.7368709999999998	2.0960179999999999
Se	31.0335269999999994	7.6145990000000001	1.9701370000000000
Se	29.5023100000000014	10.4143209999999993	1.9222450000000000
Se	27.9216410000000010	13.2754340000000006	1.6161509999999999
Se	26.2402869999999986	16.7368699999999997	2.1839400000000002
Se	37.8589679999999973	1.8318639999999999	1.8107640000000000

Se	36.0899760000000001	4.7204610000000002	1.6432789999999999
Se	34.4064180000000022	7.6274569999999997	1.5230360000000001
Se	32.8674019999999985	10.6083020000000001	1.7035340000000001
Se	31.1807920000000003	13.4865949999999994	1.4312900000000000
Se	29.4895609999999984	16.7846370000000000	2.3998040000000000
Se	41.0557999999999979	1.8113750000000000	1.9735689999999999
Se	39.4388330000000025	4.8189929999999999	2.3090359999999999
Se	37.7610320000000002	7.7108800000000004	2.0763929999999999
Se	36.1709409999999991	10.4900179999999992	2.0000770000000001
Se	34.5116110000000020	13.3237439999999996	1.8079030000000000
Se	32.7953460000000021	16.8241039999999984	2.5405940000000000
Se	44.3710349999999991	1.9031780000000000	2.1711730000000000
Se	42.8358619999999988	4.8501899999999996	1.9907210000000000
Se	41.2557339999999968	7.7713460000000003	1.7217720000000001
Se	39.6779709999999994	10.6064849999999993	1.6201220000000001
Se	38.0141360000000006	13.3893509999999996	1.5721650000000000
Se	36.2210899999999967	16.6771029999999989	2.4410170000000000

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,239.021\,027\,68$ eV; $E_{rel} = 365.463\,760\,772\,7$ meV/f.u.

W	20.9139739999999996	-0.1989630000000000	3.4086509999999999
W	22.0205430000000000	2.1408480000000001	3.8230590000000002
W	19.2825950000000006	2.4581439999999999	3.4122810000000001
W	17.6765469999999993	5.1815490000000004	3.3982950000000001
W	16.0728159999999995	7.9566340000000002	3.3508969999999998
W	14.4641999999999999	10.7421249999999997	3.2894410000000001
W	12.8553250000000006	13.5348039999999994	3.2257479999999998
W	11.2382650000000002	16.3272280000000016	3.1835670000000000
W	9.6194559999999996	19.1214039999999983	3.1733690000000001
W	8.0023890000000009	21.9178320000000006	3.1904870000000001
W	6.3917760000000001	24.7153579999999984	3.2182070000000000
W	4.7850619999999999	27.5140799999999999	3.2398430000000000
W	3.1765560000000002	30.3105790000000006	3.2476490000000000

W	23.6551110000000016	-0.5816850000000000	3.8375949999999999
W	20.4373019999999990	4.8717530000000000	3.8176960000000002
W	18.8149489999999986	7.6650520000000002	3.8014679999999998
W	17.1994259999999990	10.4641110000000008	3.7305980000000001
W	15.5893429999999995	13.2568719999999995	3.6642800000000002
W	13.9755240000000001	16.0476920000000014	3.6196510000000002
W	12.3548960000000001	18.8357199999999985	3.6096499999999998
W	10.7374860000000005	21.6246259999999992	3.6244670000000001
W	9.1245259999999995	24.4185319999999990	3.6522649999999999
W	7.5165290000000002	27.2181509999999989	3.6778330000000001
W	5.9071730000000002	30.0191060000000007	3.6932209999999999
W	1.5625869999999999	33.1046210000000016	3.2439870000000002
W	2.6760530000000000	35.6141959999999997	3.6893940000000001
W	-0.0554250000000000	35.8980379999999997	3.2364809999999999
W	-1.6734130000000000	38.6931450000000012	3.2305489999999999
W	-3.2897409999999998	41.4896150000000006	3.2298119999999999
W	-4.9040749999999997	44.2861970000000014	3.2323390000000001
W	-6.5182209999999996	47.0819159999999997	3.2337699999999998
W	-8.1347690000000004	49.8768209999999996	3.2312479999999999
W	-9.7536070000000006	52.6704300000000032	3.2247020000000002
W	-11.3716200000000001	55.4668769999999967	3.2177099999999998
W	-12.9866960000000002	58.2661140000000017	3.2198600000000002
W	-14.5958530000000000	61.0680850000000035	3.2338629999999999
W	-16.2060139999999997	63.8689359999999979	3.2600099999999999
W	4.2935619999999997	32.8184510000000031	3.6955320000000000
W	1.0575159999999999	38.4078429999999997	3.6830259999999999
W	-0.5589210000000000	41.2015320000000003	3.6808450000000001
W	-2.1732770000000001	43.9972830000000030	3.6818360000000001
W	-3.7876200000000000	46.7939020000000028	3.6841390000000001
W	-5.4037780000000000	49.5909049999999993	3.6834730000000002
W	-7.0219509999999996	52.3861959999999982	3.6779910000000000
W	-8.6403890000000008	55.1809099999999972	3.6698640000000000
W	-10.2550279999999994	57.9748779999999968	3.6657790000000001

W	-11.864625999999995	60.7726510000000033	3.6727210000000001
W	-13.4717310000000001	63.5709360000000032	3.6945389999999998
W	-17.8168620000000004	66.6634279999999961	3.2865250000000001
W	-16.7001980000000003	69.1672300000000035	3.7407720000000002
W	-19.4358359999999983	69.4533700000000067	3.3018589999999999
W	-21.0550700000000006	72.2422849999999954	3.2908569999999999
W	-22.6709430000000012	75.0335850000000022	3.2473209999999999
W	-24.2820760000000000	77.8264410000000026	3.1813340000000001
W	-25.8979500000000016	80.6262159999999994	3.1094789999999999
W	-27.5205379999999984	83.4189520000000044	3.0931739999999999
W	-29.1046890000000005	86.1500929999999983	3.0862259999999999
W	-30.7387480000000011	88.8727810000000034	3.0714549999999998
W	-15.0831649999999993	66.3696630000000027	3.7227440000000001
W	-18.3205710000000010	71.9610919999999936	3.7332329999999998
W	-19.9368659999999984	74.7553259999999966	3.6905850000000000
W	-21.5477629999999998	77.5479870000000062	3.6271480000000000
W	-23.1560069999999989	80.3327450000000027	3.5652729999999999
W	-24.7614270000000012	83.1094570000000061	3.5166100000000000
W	-26.3657560000000011	85.8325990000000019	3.5015010000000002
W	-27.9995089999999998	88.4902220000000028	3.5030920000000001
Se	21.8857399999999984	-2.1141160000000001	4.5807039999999999
Se	20.2536149999999999	1.1255090000000001	5.3574970000000004
Se	18.6527290000000008	3.9193590000000000	5.3560720000000002
Se	17.0202719999999985	6.6841699999999999	5.3119600000000000
Se	15.4197690000000005	9.4780999999999995	5.2544570000000004
Se	13.8096560000000004	12.2649679999999996	5.1885610000000000
Se	12.1944529999999993	15.0416919999999994	5.1346900000000000
Se	10.5719949999999994	17.8122369999999997	5.1091290000000003
Se	8.9526819999999994	20.5901330000000016	5.1141769999999998
Se	7.3397880000000004	23.3809499999999986	5.1383939999999999
Se	5.7309089999999996	26.1824350000000017	5.1644090000000000
Se	4.1202170000000002	28.9865409999999990	5.1797209999999998
Se	25.4560730000000000	-1.8011640000000000	3.1532290000000001

Se	24.056281999999995	1.192110000000000	5.335925999999997
Se	22.500088999999991	4.177592999999999	5.170211000000001
Se	20.919253999999987	7.032739000000003	5.038708999999999
Se	19.332239000000013	9.855783000000006	4.935187000000000
Se	17.725291999999996	12.652751999999996	4.860307999999999
Se	16.121697999999985	15.444117999999996	4.795518000000004
Se	14.497213999999996	18.219098999999999	4.786883999999997
Se	12.874328999999995	20.994351999999992	4.802006000000004
Se	11.255763000000000	23.775897000000005	4.831927000000003
Se	9.644491000000004	26.569594999999996	4.860583000000001
Se	8.034188999999996	29.372704999999998	4.880472000000001
Se	19.098646999999997	0.202154000000000	1.908805000000001
Se	17.209979000000006	2.954546000000001	2.186459999999998
Se	15.564640000000007	5.744075999999997	2.201995999999998
Se	13.945928999999996	8.536839999999998	2.159932000000000
Se	12.341122999999996	11.339819000000003	2.085297000000002
Se	10.731517999999994	14.146214000000005	2.020830999999998
Se	9.114494000000005	16.953970999999992	1.984782000000000
Se	7.490318000000003	19.758144999999990	1.989255000000000
Se	5.870180999999996	22.559353000000015	2.015490999999999
Se	4.260131000000003	25.356880000000003	2.042203999999999
Se	2.655666000000001	28.150310000000011	2.055368000000001
Se	1.049393000000000	30.942340000000015	2.054104000000002
Se	22.788007000000003	0.614151000000000	1.894031999999999
Se	21.087417999999996	3.395319999999999	1.875164000000001
Se	19.470372000000011	6.165222000000000	1.880486000000001
Se	17.865196999999984	8.940644000000007	1.835363000000001
Se	16.245888000000008	11.729853999999996	1.764572000000000
Se	14.634090000000005	14.535443000000008	1.707338000000000
Se	13.019647000000009	17.346392000000016	1.679492999999999
Se	11.402397000000006	20.153822999999992	1.680879999999999
Se	9.786376999999999	22.954988000000002	1.703086000000001
Se	8.176895999999993	25.752738000000008	1.731271000000000

Se	6.571869999999997	28.548269999999987	1.7526430000000000
Se	4.9649660000000004	31.3425860000000007	1.7613129999999999
Se	2.5047269999999999	31.7870600000000003	5.1810369999999999
Se	0.8860040000000000	34.5827269999999984	5.1743829999999997
Se	-0.7327200000000000	37.3755319999999998	5.1672390000000004
Se	-2.3490869999999999	40.1684770000000029	5.1641040000000000
Se	-3.9632890000000001	42.9637760000000029	5.1652990000000001
Se	-5.5772830000000004	45.7608010000000007	5.1676140000000004
Se	-7.1935799999999999	48.5582939999999965	5.1669539999999996
Se	-8.8120940000000001	51.3544940000000025	5.1621610000000002
Se	-10.4302510000000002	54.1490179999999981	5.1547000000000001
Se	-12.0439779999999992	56.9430329999999998	5.1515370000000003
Se	-13.6518949999999997	59.7376000000000005	5.1595079999999998
Se	-15.2578390000000006	62.5339049999999972	5.1801870000000001
Se	6.4207760000000000	32.1787890000000019	4.8870690000000003
Se	4.8033400000000004	34.9808530000000033	4.8844750000000001
Se	3.1850730000000000	37.7766499999999965	4.8787300000000000
Se	1.5682400000000001	40.5689729999999997	4.8750679999999997
Se	-0.0468640000000000	43.3619160000000008	4.8750049999999998
Se	-1.6615810000000000	46.1575369999999978	4.8770540000000002
Se	-3.2778830000000001	48.9555509999999998	4.8777509999999999
Se	-4.8967070000000001	51.7536229999999975	4.8748719999999999
Se	-6.5151459999999997	54.5493510000000015	4.8676259999999996
Se	-8.1283100000000008	57.3432189999999977	4.8596139999999997
Se	-9.7357949999999995	60.1355649999999997	4.8580329999999998
Se	-11.3406199999999995	62.9295180000000016	4.8715669999999998
Se	-0.5632250000000000	33.7352330000000009	2.0460710000000000
Se	-2.1807859999999999	36.5305329999999984	2.0388679999999999
Se	-3.7991549999999998	39.3283050000000003	2.0360200000000002
Se	-5.4155430000000004	42.1263610000000028	2.0371779999999999
Se	-7.0305739999999997	44.9217360000000028	2.0396529999999999
Se	-8.6458990000000000	47.7148520000000005	2.0397590000000001
Se	-10.2625069999999994	50.5076880000000017	2.0353800000000000

Se	-11.880784999999995	53.304201999999965	2.029142999999999
Se	-13.498428999999998	56.106737000000025	2.025671000000000
Se	-15.112560000000002	58.913623999999987	2.031606000000000
Se	-16.723354000000005	61.717914000000004	2.051153999999999
Se	-18.335324000000000	64.512645000000062	2.078634000000001
Se	3.352002000000001	34.136048000000024	1.758664999999999
Se	1.734502999999999	36.929982000000025	1.751927000000000
Se	0.116463000000000	39.725836999999985	1.747052000000000
Se	-1.499654000000000	42.522891000000013	1.746798000000001
Se	-3.114023000000000	45.319710000000006	1.748823000000000
Se	-4.728491000000000	48.115062000000018	1.750304000000001
Se	-6.344781000000002	50.908580999999981	1.746934999999999
Se	-7.963376000000002	53.702075999999981	1.739878000000000
Se	-9.582539000000006	56.498201000000017	1.732625000000001
Se	-11.198753000000000	59.299466999999999	1.733984000000000
Se	-12.810150000000001	62.104306000000011	1.748564999999999
Se	-14.419168000000009	64.907098000000048	1.775142999999999
Se	-16.868245999999992	65.331789999999980	5.208693000000002
Se	-18.485371000000007	68.133598000000063	5.229946000000000
Se	-20.103988999999986	70.941322999999970	5.232067999999999
Se	-21.719644999999999	73.751897999999971	5.203070999999996
Se	-23.331956000000017	76.558491000000036	5.147382000000003
Se	-24.951979000000015	79.347104999999991	5.076061000000002
Se	-26.557304999999995	82.124630999999937	5.030292000000002
Se	-28.173120000000008	84.894800000000036	5.034775999999999
Se	-29.875150000000014	87.676129000000031	5.016149000000004
Se	-12.951534999999998	65.727230000000058	4.898105000000002
Se	-14.571989999999996	68.528785999999966	4.925620999999996
Se	-16.197555000000013	71.333431000000045	4.932440999999999
Se	-17.815719999999989	74.141465999999941	4.898185999999999
Se	-19.426926999999992	76.948685999999950	4.836379000000000
Se	-21.031752999999984	79.751981000000007	4.760354999999997
Se	-22.650956999999982	82.546223999999952	4.717514999999997

Se	-24.296472000000014	85.335548000000028	4.7301810000000000
Se	-26.184820999999995	88.088919000000042	5.0051550000000002
Se	-19.953185999999988	67.295261999999939	2.1082290000000001
Se	-21.575710999999983	70.071432000000015	2.1211069999999999
Se	-23.199794000000007	72.847843999999949	2.1109909999999998
Se	-24.804542999999989	75.638867000000047	2.0475129999999999
Se	-26.412268999999984	78.435713000000069	1.9728730000000001
Se	-28.000598000000001	81.258678000000033	1.8706520000000000
Se	-29.582429000000012	84.113258999999993	1.7371900000000000
Se	-31.139019999999986	87.098971000000059	1.5720190000000001
Se	-32.542000000000016	90.090484000000036	3.7541280000000001
Se	-16.031900000000003	67.699135999999958	1.7994619999999999
Se	-17.649737999999993	70.478502000000060	1.8062199999999999
Se	-19.272497000000013	73.250412999999947	1.7817799999999999
Se	-20.888068000000005	76.027698999999984	1.7287290000000000
Se	-22.498796999999997	78.814351999999995	1.6620600000000001
Se	-24.101092999999988	81.608390999999975	1.6038079999999999
Se	-25.734860999999987	84.372221999999936	1.5576019999999999
Se	-27.336808000000013	87.165558000000043	1.5554159999999999
Se	-28.970784999999993	90.406058000000016	2.3303440000000002

$\mathbf{W}_{66}\mathbf{Se}_{132}$; $E_{tot} = -38\,662\,254.387\,172\,96$ eV; $E_{rel} = 132.643\,377\,742\,4$ meV/f.u.

W	38.319733999999969	3.118590000000002	3.0885199999999999
W	41.509320999999999	2.9188950000000000	3.4705080000000001
W	39.558461999999987	6.3027420000000003	3.4576199999999999
W	36.443610999999971	6.3792640000000000	3.0705070000000001
W	35.079987000000027	8.9824500000000000	3.1320350000000001
W	33.449548999999975	11.6381320000000006	3.0672560000000000
W	31.520375999999988	14.861549999999994	3.0772900000000001
W	30.065971999999986	17.280387000000011	3.0540289999999999
W	28.196885999999992	20.516840999999994	3.0563359999999999
W	26.785119999999992	22.981892999999995	2.9574340000000001

W	24.9203510000000001	26.2616340000000008	2.9302700000000002
W	23.5254259999999995	28.9729719999999986	3.0387330000000001
W	21.9798480000000005	31.5656849999999984	3.0802839999999998
W	38.2075779999999980	8.6195149999999998	3.4995150000000002
W	36.3246669999999980	11.9340060000000001	3.4585439999999998
W	34.9073110000000000	14.3779249999999994	3.4492509999999998
W	32.9119639999999976	17.6898599999999995	3.4987089999999998
W	31.5881940000000014	19.9969239999999999	3.4595150000000001
W	29.6457610000000003	23.3787790000000015	3.4243990000000002
W	28.3523689999999995	25.7022039999999983	3.3359510000000001
W	26.5258959999999995	29.0578499999999984	3.3329170000000001
W	24.9199950000000001	31.4244960000000013	3.3040949999999998
W	44.6243460000000027	2.8820739999999998	3.8588819999999999
W	42.7585940000000022	6.1184180000000001	3.8212109999999999
W	41.3407839999999993	8.5853780000000004	3.8736340000000000
W	39.4644850000000034	11.8450220000000002	3.8470569999999999
W	37.8254820000000009	14.4931260000000002	3.7606350000000002
W	36.3062550000000002	17.1098770000000009	3.8350689999999998
W	34.4389650000000032	20.3971960000000010	3.9093730000000000
W	33.0244209999999967	22.8590429999999998	3.8486630000000002
W	31.1685209999999984	26.1328080000000007	3.8102299999999998
W	29.6896969999999989	28.5859869999999994	3.6335020000000000
W	27.9090330000000009	31.3426639999999992	3.5239370000000001
Se	39.6016139999999979	2.1942339999999998	5.0333880000000004
Se	37.7559979999999982	4.9545740000000000	4.8144460000000002
Se	36.3061700000000016	7.8842879999999997	5.0642199999999997
Se	34.6465889999999987	10.6731029999999993	5.0096930000000004
Se	32.8449430000000007	13.4295329999999993	4.7926570000000002
Se	31.3152469999999994	16.3989159999999998	5.0524750000000003
Se	29.4985770000000009	19.1290179999999985	4.8042069999999999
Se	28.0233390000000000	22.1213890000000006	4.9695660000000004
Se	26.2271110000000007	24.8413480000000000	4.6622000000000003
Se	24.7442489999999999	27.7932729999999992	4.8846140000000000

Se	23.138756999999982	30.621165999999988	4.984104999999996
Se	42.949342999999989	2.187472999999998	5.463772999999998
Se	41.169240999999995	4.995810999999998	5.184680000000002
Se	39.669102999999998	7.884756000000003	5.477551000000001
Se	37.908911000000034	10.700077999999995	5.221824999999999
Se	36.306097000000012	13.566338000000000	5.433254999999999
Se	34.535201000000007	16.319183999999999	5.209889000000004
Se	32.983134999999972	19.294985000000005	5.497651000000003
Se	31.234277999999998	22.055572000000015	5.184840000000003
Se	29.719863000000001	25.019038999999994	5.398798000000002
Se	27.969943000000007	27.697911000000013	5.032986000000002
Se	26.376984000000002	30.721965000000009	5.318889999999997
Se	46.768990999999998	2.463363999999999	4.952950999999997
Se	45.039186000000008	5.294260999999997	4.562583000000001
Se	43.502254000000006	8.180868000000003	4.934942999999996
Se	41.698765000000016	10.997429999999996	4.654655000000000
Se	40.135803000000028	13.955871000000001	4.761224999999996
Se	38.487859000000003	16.701118000000010	4.789780999999996
Se	36.673785999999998	19.469024999999985	4.709276000000000
Se	35.172178000000024	22.471140999999994	4.978386999999997
Se	33.421106000000018	25.261662000000012	4.602369000000004
Se	31.848988999999995	28.268397000000002	4.789245000000002
Se	30.074881999999988	31.091411999999983	4.537372999999997
Se	36.071213999999977	3.980484999999998	2.293698000000000
Se	34.324182999999979	6.831874000000000	2.019515999999999
Se	32.811757999999975	9.565270999999992	2.023604000000002
Se	31.216782999999995	12.516071999999994	2.199786000000000
Se	29.376477000000013	15.216632999999999	1.937843000000000
Se	27.774004999999989	18.122982000000004	2.330357999999999
Se	26.060981000000017	20.907032999999984	1.895618999999999
Se	24.526939999999997	23.902352000000005	2.141856000000002
Se	22.800474000000012	26.786235999999988	1.920677000000000
Se	21.415652999999989	29.696752000000000	1.720807999999999

Se	20.149723999999991	32.656939000000013	3.875579999999998
Se	39.912345000000020	4.241835000000000	1.733451000000001
Se	38.126170000000019	7.053333000000003	1.466971999999999
Se	36.743783999999980	9.961339000000006	1.751423000000000
Se	34.905599000000023	12.719314000000007	1.471741000000000
Se	33.310780999999986	15.688316999999996	1.751802000000001
Se	31.516127000000009	18.390368999999997	1.464933000000000
Se	29.987285000000000	21.320261999999996	1.715607000000001
Se	28.258324000000018	24.054662000000004	1.369993999999999
Se	26.725435999999984	27.006935999999996	1.591531999999999
Se	25.084095999999988	29.868749000000011	1.367489000000000
Se	23.486581000000010	33.083232000000024	2.017938000000000
Se	43.304023999999983	4.273297999999996	2.098047999999999
Se	41.462637999999983	7.048733999999996	1.891289000000000
Se	40.033143000000026	9.978533000000005	2.138058000000000
Se	38.260607000000003	12.844158999999994	1.896355999999999
Se	36.575372000000015	15.600035000000001	1.864622999999999
Se	34.995784000000004	18.567875000000008	2.151114000000002
Se	33.191040000000010	21.279775999999982	1.912203000000001
Se	31.744659999999997	24.251644999999999	2.097005999999999
Se	29.953405000000001	26.936928000000018	1.765409999999999
Se	28.442101000000010	29.789860000000009	1.718684000000001
Se	26.800959999999999	33.130543000000030	2.458092999999999
W	56.431767000000007	-27.810618000000016	3.386582000000002
W	59.421084999999979	-27.892500999999993	3.607314000000001
W	57.815497000000006	-25.526298000000006	3.580025000000000
W	54.651105999999986	-25.054200000000016	3.277489000000001
W	53.172047999999966	-22.601651000000004	3.101332000000002
W	51.316321999999995	-19.327801000000009	3.063645000000002
W	49.902445999999976	-16.865030999999983	3.001612999999999
W	48.034888999999997	-13.578029000000008	3.076735000000002
W	46.514772999999981	-10.961684000000000	3.152562999999998
W	44.875754999999981	-8.313337999999999	3.066669999999998

W	42.999836999999994	-5.053814000000000	3.039957999999999
W	41.582225999999986	-2.586688000000001	3.092001000000002
W	39.716586999999970	0.649492000000000	3.054806999999998
W	55.988872000000006	-22.169662999999999	3.576905000000000
W	54.694439000000027	-19.847139999999996	3.488170000000002
W	52.752335999999997	-16.465181000000012	3.453850000000001
W	51.428970999999971	-14.157498000000004	3.414258999999999
W	49.433714000000019	-10.846645000000005	3.463909000000001
W	48.015276000000001	-8.402281999999996	3.455219000000000
W	46.133183000000025	-5.088180999999996	3.414226999999999
W	44.782162999999971	-2.770956000000000	3.455658000000001
W	42.831457999999978	0.612705000000001	3.443020000000002
W	62.360838000000011	-28.033805000000010	3.832771000000002
W	60.814064000000019	-25.441676999999985	3.875144000000001
W	59.420239999999997	-22.729638000000013	3.983560999999999
W	57.555523999999984	-19.449788000000016	3.956799999999999
W	56.143658999999995	-16.985248999999996	3.857853000000000
W	54.274723999999991	-13.748820000000003	3.860174000000002
W	52.819417999999989	-11.329549999999993	3.836501999999999
W	50.890993999999992	-8.106529000000001	3.846667000000001
W	49.260300999999983	-5.451086000000001	3.782045000000001
W	47.897072000000014	-2.847572000000000	3.842887999999999
W	46.021237999999968	0.413166000000000	3.824848999999999
Se	57.539509000000025	-29.599855999999991	4.452469999999999
Se	55.897604000000012	-26.258562999999988	5.192648000000002
Se	54.386830000000033	-23.405941999999996	5.145768999999996
Se	52.595619999999967	-20.720328999999996	4.813629999999999
Se	51.148899000000001	-17.748477999999986	4.999437000000004
Se	49.344445000000003	-15.036766999999993	4.761466000000004
Se	47.765058000000033	-12.068870999999997	5.048148000000003
Se	46.079791000000002	-9.312875999999993	5.016949999999996
Se	44.307482000000003	-6.447020000000002	4.775508000000003
Se	42.877941999999973	-3.517068999999998	5.022285000000001

Se	41.036774999999987	-0.741560000000000	4.815710000000000
Se	60.854013999999994	-29.551538000000007	4.894380000000000
Se	59.255811000000013	-26.337562999999994	5.545201999999997
Se	57.614178000000026	-23.475630999999999	5.321134999999999
Se	56.081383000000024	-20.523870999999998	5.543168999999998
Se	54.353000999999990	-17.789345999999983	5.197845000000000
Se	52.823461999999993	-14.858914999999997	5.448334000000000
Se	51.029299000000017	-12.156973000000007	5.161800000000004
Se	49.434491999999988	-9.188183999999997	5.441849000000004
Se	47.596559999999966	-6.430036999999996	5.162329999999999
Se	46.214506000000001	-3.521805000000001	5.446551000000004
Se	44.428561000000020	-0.710070000000000	5.180157000000003
Se	64.191064999999947	-29.124817000000002	3.038151000000000
Se	62.924542000000024	-26.165268999999986	5.193038999999997
Se	61.539537000000028	-23.255047999999986	4.994359000000002
Se	59.813020000000016	-20.370836000000006	4.773581000000001
Se	58.278612000000025	-17.375941999999984	5.020222999999997
Se	56.565584999999987	-14.591597999999994	4.585739000000002
Se	54.963393000000035	-11.684853000000004	4.976739000000002
Se	53.123961999999988	-8.984391999999997	4.714262999999999
Se	51.528255999999989	-6.033801999999997	4.890884999999999
Se	50.016136000000030	-3.300422000000002	4.894518999999998
Se	48.269576000000007	-0.448954000000000	4.619970000000004
Se	54.266489999999975	-27.559535000000003	2.372478999999998
Se	52.492351999999968	-24.736062000000004	2.120070000000001
Se	50.920537000000030	-21.729378000000005	2.308103000000000
Se	49.169541999999999	-18.939112999999990	1.932345000000000
Se	47.667701999999985	-15.936861000000004	2.201410999999998
Se	45.853043999999970	-13.169316000000002	2.122138000000001
Se	44.204341999999969	-10.424241999999996	2.152296000000002
Se	42.641429000000022	-7.466114000000001	2.259167000000001
Se	40.838579000000028	-4.648975000000001	1.978380000000000
Se	39.301381999999967	-1.762615000000000	2.351192000000002

Se	37.571948999999965	1.068206999999999	1.9606060000000001
Se	57.9641530000000031	-27.1895449999999990	1.5925309999999999
Se	56.371653999999995	-24.1655070000000016	1.8787950000000000
Se	54.6218640000000022	-21.4865700000000004	1.5134700000000001
Se	53.1071400000000011	-18.5236249999999991	1.7276650000000000
Se	51.358384999999984	-15.7624080000000006	1.4149799999999999
Se	49.8058890000000005	-12.7868510000000004	1.7029740000000000
Se	48.034723999999971	-10.0345720000000007	1.4801310000000001
Se	46.4313470000000024	-7.1685549999999996	1.6917640000000000
Se	44.6716010000000026	-4.3531789999999999	1.4360649999999999
Se	43.171500999999992	-1.4640280000000001	1.7289250000000000
Se	41.3914510000000035	1.3441749999999999	1.4498450000000001
Se	61.203719999999970	-27.0889430000000004	1.9291689999999999
Se	59.5970560000000020	-24.2605059999999995	2.0289679999999999
Se	58.1139920000000032	-21.3092900000000007	2.2519819999999999
Se	56.3180090000000035	-18.5889239999999987	1.9445479999999999
Se	54.8427020000000027	-15.5967079999999996	2.1105670000000001
Se	53.0261690000000030	-12.8667470000000002	1.8616569999999999
Se	51.4957860000000025	-9.8975690000000007	2.1211180000000001
Se	49.6939660000000032	-7.1416060000000003	1.9041450000000000
Se	48.034494999999997	-4.3526850000000001	1.8496159999999999
Se	46.584828999999992	-1.4230719999999999	2.0994240000000000
Se	44.7392400000000023	1.3374320000000000	1.8802010000000000

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,255.815\,573\,15$ eV; $E_{rel} = 111.000\,950\,621\,2$ meV/f.u.

W	19.984847999999995	1.048133999999999	3.5776990000000000
W	18.1588740000000008	4.0164400000000002	3.5393150000000002
W	16.4938620000000000	6.7191869999999998	3.6159469999999998
W	14.911863999999996	9.4351830000000003	3.5472280000000000
W	13.326615999999996	12.167899999999995	3.4585689999999998
W	23.1630180000000010	1.0610050000000000	3.5315279999999998
W	21.3887560000000008	3.3594759999999999	3.5265019999999998

W	19.234780000000007	6.5218189999999998	3.4099230000000000
W	17.5992449999999998	9.2812210000000004	3.3853920000000000
W	16.0507470000000012	12.0702710000000000	3.4183919999999999
W	14.9834770000000006	15.2627500000000005	3.4458839999999999
W	26.3948259999999983	1.0402220000000000	3.4966740000000001
W	24.5996319999999997	3.3366090000000002	3.5582669999999998
W	23.1312029999999993	6.9584159999999997	3.4094920000000002
W	21.6719429999999988	9.7160159999999998	3.5373150000000000
W	20.0411779999999986	12.3310720000000007	3.4419400000000002
W	17.7124640000000007	15.4852840000000000	3.4832109999999998
W	16.5358389999999993	18.0398800000000001	3.3597139999999999
W	29.6048189999999991	1.0663220000000000	3.4382950000000001
W	27.8303140000000013	3.3504090000000000	3.5119590000000001
W	26.2589520000000007	7.0849529999999996	3.3312840000000001
W	24.3962509999999995	9.2352969999999992	3.4089160000000001
W	22.6542859999999990	12.3577919999999999	3.4316870000000002
W	21.7596470000000011	15.0384580000000003	3.3200829999999999
W	19.2663019999999996	18.2977099999999986	3.4902259999999998
W	18.1089190000000002	20.8224640000000001	3.4109349999999998
W	32.6392009999999999	0.6080200000000000	3.0056929999999999
W	31.0584759999999989	3.3371270000000002	3.4449550000000002
W	29.4166060000000016	6.9555660000000001	3.3994160000000000
W	28.1334559999999989	9.2236250000000002	3.4211950000000000
W	24.4939239999999998	15.3996680000000001	3.4264039999999998
W	23.2770200000000003	17.8371269999999988	3.3603489999999998
W	20.8721209999999999	21.1322769999999984	3.5069420000000000
W	19.6743430000000004	23.6480740000000011	3.3635660000000001
W	18.3709530000000001	26.6968110000000003	3.0714959999999998
W	34.4590729999999965	3.9668920000000001	3.5373199999999998
W	33.3040719999999979	6.5501990000000001	3.4176080000000000
W	30.8497459999999997	9.7032799999999995	3.5619130000000001
W	29.8503299999999996	12.3554890000000004	3.4482740000000001
W	28.0072849999999995	15.3831959999999999	3.4095330000000001

W	26.232497999999996	18.293034999999997	3.589437999999999
W	24.835367999999990	20.7237630000000017	3.5219680000000002
W	22.6459510000000002	23.9939500000000017	3.531051999999999
W	21.5109180000000002	26.4535920000000004	3.2773850000000002
W	36.0105969999999971	6.724016999999999	3.6609550000000000
W	34.9154229999999970	9.3241289999999992	3.4322580000000000
W	32.4639719999999983	12.3407429999999998	3.4710860000000001
W	30.7330770000000015	15.0337859999999992	3.3252799999999998
W	29.1985059999999983	17.8136639999999993	3.3414730000000001
W	27.7221970000000013	20.6018459999999983	3.4993789999999998
W	25.8775170000000010	23.9865369999999984	3.6290510000000000
W	24.5130519999999983	26.4299509999999991	3.591054999999999
W	37.5890289999999965	9.4491820000000004	3.6006209999999998
W	36.4473240000000018	12.1046479999999992	3.4568439999999998
W	34.7748360000000005	15.5052009999999996	3.497279999999999
W	33.2091470000000015	18.3142670000000010	3.4889000000000001
W	31.6053430000000013	21.1397410000000008	3.523442999999999
W	29.9690060000000003	23.9005299999999998	3.5647790000000001
W	28.0326090000000008	26.5213819999999991	3.6252350000000000
W	39.1648190000000014	12.1909810000000007	3.4983520000000001
W	37.5018889999999985	15.2896920000000005	3.4629460000000001
W	35.9355860000000007	18.0794420000000002	3.3681920000000001
W	34.3452410000000015	20.8756740000000001	3.4248789999999998
W	32.7737989999999968	23.6896640000000005	3.3818260000000002
W	30.9936839999999982	26.4475969999999982	3.3599790000000000
W	34.0892750000000007	26.7276160000000012	3.159972999999999
Se	21.2763869999999997	-0.6051490000000000	4.6241810000000001
Se	19.5605849999999997	2.7922560000000001	5.2898170000000002
Se	17.8586950000000009	5.6361790000000003	5.4317190000000002
Se	16.2001419999999996	8.4078239999999997	5.4188489999999998
Se	14.5508590000000009	11.1623789999999996	5.3661409999999998
Se	12.9144310000000004	14.2420290000000005	4.8896579999999998
Se	24.6015359999999994	-0.6929689999999999	4.3913510000000002

Se	22.9702410000000015	2.7272230000000000	5.4019310000000003
Se	21.2967830000000014	5.6709519999999998	4.7949299999999999
Se	19.6641919999999999	8.5703479999999992	4.8800650000000001
Se	18.0294589999999992	11.3495120000000007	4.9139710000000001
Se	16.3143150000000006	14.1631979999999995	5.1611440000000002
Se	14.1316290000000002	17.3480840000000001	4.2235160000000000
Se	27.9056229999999985	-0.5997510000000000	4.5073420000000004
Se	26.2770909999999986	2.6718730000000002	5.3815119999999999
Se	24.6859390000000012	5.6465339999999999	4.9189270000000000
Se	23.0081510000000016	8.5456590000000006	5.3597039999999998
Se	21.3709290000000003	11.4486539999999994	5.3807720000000003
Se	19.6667610000000010	14.3675560000000004	4.9067020000000001
Se	17.8702660000000009	17.1989340000000013	5.3261979999999998
Se	15.7652149999999995	20.2037620000000011	4.2897910000000001
Se	31.1655970000000018	-0.4582360000000000	4.6793600000000000
Se	29.5489940000000004	2.7107929999999998	5.3126189999999998
Se	27.8365189999999991	5.6340029999999999	4.8903829999999999
Se	26.2591320000000010	9.2155389999999997	5.0791350000000000
Se	23.3734859999999998	14.0304079999999995	5.1763050000000002
Se	21.2616399999999999	17.1197860000000013	4.8371950000000004
Se	19.5305889999999991	20.0156179999999999	5.3291269999999997
Se	17.5610980000000012	22.9303530000000002	4.6320430000000004
Se	32.9611080000000030	2.4953889999999999	4.9713919999999998
Se	31.2346910000000015	5.5988689999999997	4.7733290000000004
Se	29.5150509999999997	8.5171200000000002	5.3712590000000002
Se	24.6547069999999984	17.0702619999999996	5.2828309999999998
Se	22.8131920000000008	19.9646580000000000	4.9084289999999999
Se	21.1335259999999998	22.9015769999999996	5.2845829999999996
Se	34.6102279999999993	5.5742310000000002	5.4370539999999998
Se	32.8513790000000014	8.5499329999999993	4.9133469999999999
Se	31.1297280000000001	11.4413239999999998	5.4019209999999998
Se	29.0989709999999988	14.0124779999999998	5.1790630000000002
Se	27.8025519999999986	17.0361680000000000	5.2578100000000001

Se	26.260626999999995	19.9852670000000003	5.4575220000000000
Se	24.4179570000000012	22.8085859999999983	5.1794620000000000
Se	36.2916400000000010	8.4048590000000001	5.4723230000000003
Se	34.4717040000000026	11.3647620000000007	4.9568969999999997
Se	32.8214240000000004	14.3836189999999995	4.9199560000000000
Se	31.2021699999999989	17.1271909999999998	4.8281570000000000
Se	29.6543120000000009	19.9575460000000007	4.9414790000000002
Se	27.9032489999999989	22.8501660000000015	4.8606689999999997
Se	37.9381309999999985	11.1853309999999997	5.4101109999999997
Se	36.1746020000000001	14.1887950000000007	5.1833190000000000
Se	34.6065790000000035	17.2149590000000003	5.3307650000000004
Se	32.9451650000000029	20.0054690000000015	5.3349380000000002
Se	31.3547569999999993	22.8487280000000013	5.3598330000000001
Se	39.5710600000000028	14.2770309999999991	4.9153770000000003
Se	38.3531240000000011	17.3787410000000015	4.2231790000000000
Se	36.7203409999999977	20.2325760000000017	4.2750610000000000
Se	34.8864749999999972	22.9238210000000002	4.7023039999999998
Se	17.9816639999999985	1.7404040000000001	2.1041780000000001
Se	15.8892900000000008	4.3455260000000004	2.7523830000000000
Se	14.2037189999999995	7.2541370000000001	2.5982740000000000
Se	12.4992850000000004	10.1511049999999994	2.5627559999999998
Se	21.4977069999999983	1.5208969999999999	1.6677310000000001
Se	19.7538349999999987	4.6091970000000000	1.7849180000000000
Se	17.7839269999999985	7.4699619999999998	1.5817280000000000
Se	16.1836510000000011	10.3638999999999992	1.5791080000000000
Se	14.5972170000000006	13.3912940000000003	1.7178070000000001
Se	24.7325569999999999	1.5638200000000000	1.6489860000000001
Se	23.0416799999999995	4.6860749999999998	2.0089530000000000
Se	21.1794949999999993	7.6268140000000004	1.9453950000000000
Se	19.6029669999999996	10.3422400000000003	1.9625109999999999
Se	17.9723229999999994	13.2822200000000006	2.0851560000000000
Se	16.2165660000000003	16.3155639999999984	1.5272600000000001
Se	27.9437139999999999	1.5750560000000000	1.5952050000000000

Se	26.2651250000000012	4.7408169999999998	2.0537459999999998
Se	24.6110509999999998	7.6424420000000000	1.4813719999999999
Se	23.3100850000000008	10.6848460000000003	1.6661950000000001
Se	21.3289700000000018	13.3012409999999992	1.5129830000000000
Se	19.6991920000000000	16.1625100000000010	2.0159189999999998
Se	17.7732889999999983	19.1688480000000006	1.5178799999999999
Se	31.1265740000000015	1.6543850000000000	1.4440139999999999
Se	29.5227210000000007	4.6987750000000004	1.9825520000000001
Se	27.9203849999999996	7.6430059999999997	1.4859370000000001
Se	23.1153760000000013	16.1389980000000008	1.4889530000000000
Se	21.2737669999999994	18.9983940000000011	2.0256120000000002
Se	19.3784589999999994	21.9362940000000002	1.5534129999999999
Se	34.9210610000000017	1.5826610000000001	2.6682630000000001
Se	32.9178970000000035	4.5723240000000001	1.7979940000000001
Se	31.3662220000000005	7.6393550000000001	1.9439970000000000
Se	29.2163520000000005	10.6776199999999992	1.6816759999999999
Se	26.2280459999999991	14.1403199999999991	2.2282850000000001
Se	24.6497819999999983	19.0465869999999988	1.6528670000000001
Se	22.9276589999999985	21.8503989999999995	2.0874139999999999
Se	21.1348459999999996	24.7248069999999984	1.5788690000000001
Se	36.7213289999999972	4.3897240000000002	2.7950460000000001
Se	34.7669309999999996	7.4978530000000001	1.6169169999999999
Se	32.9180309999999992	10.3543740000000000	1.9938300000000000
Se	31.1765599999999985	13.2892489999999999	1.5280190000000000
Se	29.3961979999999983	16.1183419999999984	1.4733920000000000
Se	27.7718859999999985	18.9576600000000006	1.6000840000000001
Se	26.2484089999999988	22.0238769999999988	1.9000740000000000
Se	24.4492520000000013	24.8024589999999989	1.7472770000000000
Se	38.3225759999999980	7.2744689999999999	2.6753369999999999
Se	36.3447919999999982	10.3811219999999995	1.6249359999999999
Se	34.5272700000000015	13.2931380000000008	2.1094960000000000
Se	32.7924799999999976	16.1672249999999984	2.0221540000000000
Se	31.2001869999999997	19.0108980000000010	2.0254880000000002

Se	29.5703530000000008	21.8482039999999991	2.0526239999999998
Se	27.9154939999999989	24.7870099999999987	2.0119560000000001
Se	39.9933750000000003	10.1761820000000007	2.6020439999999998
Se	37.9049750000000003	13.4169309999999999	1.7468919999999999
Se	36.2650720000000035	16.3444859999999998	1.5431889999999999
Se	34.7000770000000003	19.2148879999999984	1.5294669999999999
Se	33.1047370000000001	21.9953210000000006	1.5664620000000000
Se	31.3207610000000010	24.8012470000000000	1.5842030000000000
Se	17.6631630000000008	24.8550070000000005	1.8150109999999999
Se	19.6132330000000010	25.8506779999999985	4.9724449999999996
Se	19.9187569999999994	28.0461939999999998	1.9067780000000001
Se	22.8875279999999997	25.8710549999999984	5.3505529999999997
Se	23.0730730000000008	28.0098599999999998	2.2340119999999999
Se	26.2589480000000002	25.8563620000000007	5.3675699999999997
Se	26.2285350000000008	28.2366059999999983	3.1985060000000001
Se	29.5717900000000000	25.7146189999999990	5.3694340000000000
Se	32.8466430000000003	25.8354560000000006	5.0510890000000002
Se	32.5476310000000026	28.0840859999999992	1.9947360000000001
Se	34.8187849999999983	24.8981260000000013	1.9003000000000001
Se	29.4496660000000006	28.2431589999999986	2.6115200000000001
Se	35.8300490000000025	28.0057730000000014	3.8328940000000000
Se	16.6213659999999983	27.9728549999999991	3.7225359999999998
Se	11.3161170000000002	13.6789749999999994	3.1918690000000001
Se	41.1776910000000029	13.6974920000000004	3.2310669999999999
Se	33.2980400000000003	-1.2790159999999999	1.9000600000000001
Se	17.6460709999999992	0.1106570000000000	3.8257029999999999

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,257.361\,483\,67$ eV; $E_{rel} = 87.578\,063\,954\,5$ meV/f.u.

W	19.8554649999999988	1.0675049999999999	3.4091450000000001
W	18.0904589999999992	3.8928729999999998	3.5586080000000000
W	16.4716020000000007	6.6223190000000001	3.6222840000000001
W	14.9341720000000002	9.3764140000000005	3.5628449999999998

W	13.462960000000007	12.238856000000002	3.501960000000000
W	23.077906999999997	0.894089000000000	3.347481999999998
W	21.371334000000009	3.227523999999998	3.480969000000000
W	19.205909999999994	6.431981999999996	3.438178999999999
W	17.600464999999998	9.216969000000006	3.416917000000002
W	16.116507999999996	12.022503000000004	3.434515999999999
W	15.000292999999992	15.207115999999992	3.373343000000002
W	26.246233000000001	0.833114000000000	3.328202999999998
W	24.603037000000005	3.104525999999999	3.454362999999999
W	23.116699000000006	6.853345000000000	3.382714000000000
W	21.664567999999992	9.612859000000003	3.529208000000001
W	20.127148999999993	12.228524999999994	3.479960000000002
W	17.720185000000007	15.475654000000005	3.498464999999999
W	16.516373999999990	17.964987000000007	3.344274000000000
W	29.414684000000012	0.894568999999999	3.347557000000001
W	27.889192000000013	3.105090000000001	3.454591000000002
W	26.245812000000008	6.721179000000002	3.325955000000000
W	24.769214999999991	9.098333000000002	3.440185000000000
W	22.883610000000009	12.543805000000008	3.512264000000001
W	21.603289000000002	14.999017000000003	3.434169999999999
W	19.287971999999999	18.308676999999994	3.514031999999998
W	18.013383000000010	20.743487999999993	3.597376000000001
W	32.636921000000010	1.068759000000000	3.409552999999998
W	31.120819000000009	3.228784000000001	3.481414000000000
W	29.374901000000013	6.853813999999999	3.383049000000002
W	27.721893000000015	9.098639999999996	3.440423000000000
W	24.353034999999984	15.190035000000000	3.523034000000000
W	23.154676999999995	18.442081000000017	3.443773999999999
W	21.331391000000000	20.747619000000003	3.557218999999999
W	19.584672999999987	24.383192000000011	3.281727000000001
W	18.452277999999997	26.690757000000014	3.123343000000002
W	34.401150000000012	3.894359999999998	3.559391999999999
W	33.285164999999992	6.433462999999997	3.438779999999999

W	30.826333999999992	9.6136230000000005	3.5298080000000001
W	29.6065709999999989	12.5443219999999993	3.5128910000000002
W	28.1365170000000013	15.1899789999999992	3.5236120000000000
W	26.2446009999999994	18.5597430000000010	3.4320909999999998
W	24.6030130000000007	20.8270780000000002	3.5502850000000001
W	22.9359989999999989	24.4391350000000003	3.3759670000000002
W	21.4641869999999990	26.6790009999999995	3.3429579999999999
W	36.0197100000000034	6.6240810000000003	3.6235409999999999
W	34.8899720000000002	9.2187970000000004	3.4178839999999999
W	32.3631870000000035	12.2296239999999994	3.4810449999999999
W	30.8864020000000004	14.9999459999999996	3.4353940000000001
W	29.3348389999999988	18.4430839999999989	3.4446750000000002
W	27.8859229999999982	20.8275189999999988	3.5511100000000000
W	26.2441589999999998	24.4646960000000000	3.4174069999999999
W	24.6435479999999991	26.7156039999999990	3.4559720000000000
W	37.5565080000000009	9.3785819999999998	3.5645289999999998
W	36.3735980000000012	12.0244979999999995	3.4362040000000000
W	34.7694990000000033	15.4772169999999996	3.5003929999999999
W	33.2012280000000004	18.3100909999999999	3.5161539999999998
W	31.1574589999999993	20.7485509999999991	3.5593569999999999
W	29.5523109999999996	24.4402399999999993	3.3783370000000001
W	27.8444609999999990	26.7157659999999986	3.4572349999999998
W	39.0271079999999984	12.2413170000000004	3.5040950000000000
W	37.4893459999999976	15.2092089999999995	3.3756990000000000
W	35.9728410000000025	17.9667589999999997	3.3469159999999998
W	34.4754209999999972	20.7450119999999991	3.6004160000000001
W	32.9035069999999976	24.3846090000000011	3.2857630000000002
W	31.0238879999999995	26.6797709999999988	3.3467030000000002
W	34.0361570000000029	26.6923829999999995	3.1296689999999998
Se	21.0548690000000001	-0.7339000000000000	4.3281720000000004
Se	19.5517180000000010	2.6882510000000002	5.2746519999999997
Se	17.8204360000000008	5.5177050000000003	5.4348280000000004
Se	16.1957279999999990	8.3192389999999996	5.4329340000000004

Se	14.612318999999994	11.136625999999997	5.385012999999998
Se	12.602220000000009	14.253037000000008	4.377669000000000
Se	24.543268000000012	-0.813374000000000	4.353587000000001
Se	22.950942000000013	2.497202999999998	5.288634000000001
Se	21.291789000000014	5.533462000000001	4.780541999999996
Se	19.654363000000000	8.456972999999996	4.898987000000000
Se	18.083847999999997	11.273224000000008	4.931892999999996
Se	16.292465000000000	14.144023000000007	5.129480000000000
Se	14.167180999999994	17.307970000000010	4.231026000000000
Se	27.949445000000008	-0.813038000000000	4.353575000000002
Se	26.246105000000000	2.445535000000000	5.266347999999998
Se	24.603759000000002	5.377354999999997	4.853756999999999
Se	23.066482000000006	8.458137000000007	5.302201000000002
Se	21.556274999999994	11.368529999999998	5.368513000000001
Se	19.613520000000012	14.264309000000008	4.975209000000004
Se	17.879946000000003	17.208531000000007	5.331376999999998
Se	15.714610999999997	20.269439999999995	4.221635000000000
Se	31.437661999999996	-0.732837000000000	4.328376999999997
Se	29.541181000000017	2.497876999999999	5.288778999999999
Se	27.887875000000011	5.377679999999998	4.853904000000000
Se	26.245480000000006	8.303276999999996	5.311874000000004
Se	24.920733999999995	11.311073999999996	4.817985000000002
Se	23.004084999999999	14.233669000000008	5.406462999999996
Se	21.274597000000000	17.185490000000015	4.826736000000004
Se	19.610447000000006	20.073591000000004	5.344394999999996
Se	17.914799999999996	22.962429000000002	4.758047000000004
Se	32.940111000000017	2.689553999999998	5.275248999999996
Se	31.199723999999998	5.534421000000000	4.781102999999999
Se	29.424420000000014	8.458548000000004	5.302589000000002
Se	27.569745000000011	11.311170000000006	4.818259000000003
Se	26.244751999999983	14.381669000000005	5.034539999999998
Se	24.652250999999997	17.295642999999983	5.086274999999997
Se	22.934561999999997	20.141695999999996	5.359091000000003

Se	21.2152220000000007	23.0993490000000001	4.8278420000000004
Se	34.6706250000000011	5.5192430000000003	5.4356429999999998
Se	32.8363900000000015	8.4580939999999991	4.8999370000000004
Se	30.9338879999999996	11.3692170000000008	5.3692469999999997
Se	29.4854330000000004	14.2339889999999993	5.4072519999999997
Se	27.8368989999999989	17.2959220000000009	5.0864960000000004
Se	26.2441269999999989	20.2607700000000008	5.3874820000000003
Se	24.5659419999999997	23.1198119999999996	4.9012169999999999
Se	36.2946730000000031	8.3210440000000006	5.4342059999999996
Se	34.4062920000000005	11.2746359999999992	4.9332659999999997
Se	32.8761510000000001	14.2653409999999994	4.9766120000000003
Se	31.2144730000000017	17.1863150000000005	4.8282689999999997
Se	29.5536980000000007	20.1422489999999996	5.3605159999999996
Se	27.9218229999999998	23.1200609999999998	4.9020500000000000
Se	37.8775449999999978	11.1387190000000000	5.3868380000000000
Se	36.1971180000000032	14.1456579999999992	5.1314690000000001
Se	34.6090459999999993	17.2097750000000005	5.3335640000000000
Se	32.8779910000000015	20.0745420000000010	5.3468859999999996
Se	31.2725089999999994	23.0999139999999983	4.8305400000000001
Se	39.8873180000000005	14.2555589999999999	4.3801550000000002
Se	38.3219870000000000	17.3101419999999990	4.2337879999999997
Se	36.7741389999999981	20.2712970000000006	4.2248109999999999
Se	34.5733859999999993	22.9636800000000001	4.7618440000000000
Se	17.6667389999999997	1.3831720000000001	2.5542220000000002
Se	15.8265069999999994	4.2733010000000000	2.7622770000000001
Se	14.1789860000000001	7.2462840000000002	2.5910690000000001
Se	12.5027399999999993	10.2964409999999997	2.5998399999999999
Se	21.3872000000000000	1.4951340000000000	1.5257730000000000
Se	19.6662689999999998	4.5116209999999999	1.8151820000000001
Se	17.7731430000000010	7.4016140000000004	1.6105510000000001
Se	16.2117420000000010	10.3047389999999996	1.6041319999999999
Se	14.7124450000000007	13.3289899999999992	1.6506230000000000
Se	24.6384550000000004	1.3849790000000000	1.4771330000000000

Se	22.986269000000001	4.5704669999999998	1.9867030000000001
Se	21.1630520000000004	7.5297530000000004	1.9637309999999999
Se	19.6142609999999991	10.2827999999999999	1.9915620000000001
Se	18.0535020000000017	13.2350030000000007	2.1415560000000000
Se	16.2636220000000016	16.2867519999999999	1.5033470000000000
Se	27.8539980000000007	1.3853670000000000	1.4772850000000000
Se	26.2459780000000009	4.4800760000000004	1.9532849999999999
Se	24.6258440000000007	7.3941600000000003	1.4886919999999999
Se	23.1246270000000003	10.4868380000000005	1.8075300000000001
Se	21.3484710000000000	13.2880929999999999	1.5792759999999999
Se	19.6743750000000013	16.1864530000000002	2.0044580000000001
Se	17.8006029999999988	19.2162310000000005	1.5859559999999999
Se	31.1052110000000006	1.4963670000000000	1.5261100000000001
Se	29.5056219999999989	4.5711800000000000	1.9868720000000000
Se	27.8657550000000001	7.3944739999999998	1.4888690000000000
Se	26.2455269999999992	10.1620450000000009	1.6864589999999999
Se	24.7717039999999997	13.3831070000000008	1.9222729999999999
Se	22.9602870000000010	16.3135270000000006	1.7535620000000001
Se	21.2158599999999993	19.0661230000000010	1.7865789999999999
Se	19.4952180000000013	22.0533299999999990	1.9987459999999999
Se	34.8255120000000034	1.3851150000000001	2.5547960000000001
Se	32.8255180000000024	4.5130670000000004	1.8157420000000000
Se	31.3283139999999989	7.5308289999999998	1.9642660000000001
Se	29.3663279999999993	10.4874440000000000	1.8079719999999999
Se	27.7186589999999988	13.3833219999999997	1.9224559999999999
Se	26.2449919999999999	16.3459590000000006	2.0949230000000001
Se	24.6226799999999990	19.2335209999999996	1.5711800000000000
Se	22.8816619999999986	22.1312989999999985	2.0530450000000000
Se	21.2638630000000006	24.9587590000000006	1.5021370000000001
Se	36.6650309999999990	4.2754510000000003	2.7632129999999999
Se	34.7181339999999992	7.4034279999999999	1.6116690000000000
Se	32.8765319999999974	10.2842000000000002	1.9925480000000000
Se	31.1419919999999983	13.2892700000000001	1.5803330000000000

Se	29.529574000000002	16.314282999999996	1.7547130000000000
Se	27.867000999999984	19.234045999999993	1.5718019999999999
Se	26.244637999999984	22.202864000000017	2.0650860000000000
Se	24.598299000000008	25.047536999999984	1.5658730000000001
Se	38.312038000000011	7.248795000000003	2.5925650000000000
Se	36.278916999999999	10.306921000000009	1.6056919999999999
Se	34.436689999999987	13.236784999999994	2.1431119999999999
Se	32.815404999999984	16.187972999999995	2.0062489999999999
Se	31.273801999999999	19.067527999999994	1.7882050000000000
Se	29.607623000000002	22.132386000000003	2.0546989999999998
Se	27.891095000000000	25.048140000000001	1.5669430000000000
Se	39.987712000000019	10.299241000000003	2.6018720000000002
Se	37.777669000000003	13.331440000000006	1.6527060000000000
Se	36.226118999999971	16.288976000000017	1.5056740000000000
Se	34.688800999999980	19.218336999999982	1.5886320000000000
Se	32.993887999999983	22.055223999999991	2.0018620000000000
Se	31.225502999999998	24.960723000000015	1.5053500000000000
Se	17.351039000000001	24.960190999999982	1.9912510000000001
Se	19.696608999999987	26.270241999999996	5.1825229999999998
Se	19.764752000000014	28.202693000000000	1.9061340000000000
Se	22.990553999999995	26.227382999999997	5.2813949999999998
Se	22.982589000000008	28.383324999999992	2.4302079999999999
Se	26.243301999999999	26.250368999999992	5.3325290000000001
Se	26.244126999999989	28.435514000000013	2.5342699999999998
Se	29.496155999999992	26.227705000000003	5.2840189999999998
Se	32.790289999999988	26.270382000000015	5.1876660000000001
Se	32.724283999999973	28.205276000000013	1.9130970000000000
Se	35.137267999999988	24.962831000000013	1.9958890000000000
Se	29.505718999999991	28.384093000000000	2.4330900000000000

$W_{66}Se_{132}$; $E_{tot} = -38\,662\,258.432\,320\,26$ eV; $E_{rel} = 71.353\,267\,136\,3$ meV/f.u.

W	33.074424000000005	1.074904000000001	3.2659919999999998
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W	31.3411100000000005	3.9046289999999999	3.2991320000000002
W	34.6705520000000007	3.2152110000000000	3.4277790000000001
W	29.7502679999999984	6.5708719999999996	3.3730389999999999
W	28.0602260000000001	9.3859340000000007	3.3723200000000002
W	26.4445380000000014	12.1448549999999997	3.1504720000000002
W	24.5475910000000006	15.4345079999999992	3.1821720000000000
W	23.0108099999999993	18.1380160000000004	3.2734200000000002
W	21.4519990000000007	20.9186860000000010	3.2035350000000000
W	19.8245049999999985	23.6942629999999994	3.0955509999999999
W	17.9371900000000011	26.9963720000000009	3.1013530000000000
W	16.4605180000000004	29.5594789999999996	3.2880170000000000
W	14.8932719999999996	32.3515760000000014	3.2906209999999998
W	36.2644790000000015	0.9140620000000000	3.2907790000000001
W	32.7054820000000035	6.6149920000000000	3.3844509999999999
W	31.1901750000000000	8.9387640000000008	3.4582099999999998
W	29.1695540000000015	12.3712090000000003	3.3572380000000002
W	28.0716719999999995	14.9555330000000009	3.2406980000000001
W	25.7632100000000008	18.0498410000000007	3.3056980000000000
W	24.2534500000000008	20.9529730000000001	3.3540350000000001
W	22.9914220000000000	23.4192010000000010	3.3534540000000002
W	21.2103509999999993	26.9873529999999988	3.2609530000000002
W	19.7959239999999994	29.3132570000000001	3.3215780000000001
W	17.4728299999999983	32.3976809999999986	3.4311690000000001
W	39.3519310000000004	0.9151060000000000	3.4307859999999999
W	37.8447850000000017	3.1442470000000000	3.5246140000000001
W	36.4012669999999972	6.7961250000000000	3.3974859999999998
W	34.4448950000000025	8.9294300000000000	3.5742490000000000
W	33.0499030000000005	12.6092969999999998	3.4071699999999998
W	30.8237309999999987	15.0342210000000005	3.4373840000000002
W	29.8483149999999995	17.8153819999999996	3.3142849999999999
W	27.9923180000000009	21.3079929999999997	3.4874689999999999
W	26.2261570000000006	23.4954210000000003	3.5581399999999999
W	24.4081159999999997	27.0973480000000002	3.3879009999999998

W	22.7241530000000012	29.4111280000000015	3.4428150000000000
W	21.3853240000000007	32.0518870000000007	3.4774370000000001
W	42.4961699999999993	1.0642160000000001	3.5753879999999998
W	41.2062639999999973	3.2889360000000001	3.6512560000000001
W	39.5149959999999965	6.7976450000000002	3.4910679999999998
W	37.9311429999999987	9.0716909999999995	3.5873409999999999
W	36.1859170000000034	12.6260670000000008	3.4816110000000000
W	34.6638820000000010	14.8969190000000005	3.5769880000000001
W	32.6684669999999997	18.2542130000000000	3.5848480000000000
W	31.3798740000000009	20.5894359999999992	3.5400740000000002
W	29.2978850000000008	23.9122950000000003	3.6189230000000001
W	28.2494090000000000	26.8856380000000001	3.5888749999999998
W	26.6192379999999993	29.4676180000000016	3.5028370000000000
W	24.6302459999999996	32.8546440000000004	3.5075889999999998
W	44.5044639999999987	3.2695599999999998	4.1169710000000004
W	42.5500520000000009	6.5325610000000003	3.7040430000000000
W	41.0195050000000023	9.0932160000000000	3.6370990000000001
W	39.4929079999999999	11.9603699999999993	3.6725159999999999
W	37.6479450000000000	15.0052590000000006	3.6539670000000002
W	36.1347200000000015	17.6757349999999995	3.7626170000000001
W	34.2617789999999971	20.9477089999999997	3.8391929999999999
W	32.8372120000000010	23.4412839999999996	3.8546770000000001
W	30.9682920000000017	26.8340770000000006	3.7650440000000001
W	29.3316669999999995	29.5287679999999995	3.4914649999999998
W	27.7223089999999992	32.3536140000000003	3.4526590000000001
Se	34.2719730000000027	-0.7407940000000000	4.1767519999999996
Se	32.7542929999999970	2.6984870000000001	5.1038519999999998
Se	31.1421029999999988	5.5128459999999997	5.1940299999999997
Se	29.3676640000000013	8.3157759999999996	5.2094279999999999
Se	27.7132150000000017	11.1500920000000008	5.1213129999999998
Se	26.0046730000000004	14.0514060000000001	4.7961119999999999
Se	24.2943099999999994	16.9795480000000012	5.1424240000000001
Se	22.6915869999999984	19.8146340000000016	5.1111899999999997

Se	21.086165999999986	22.722211999999990	5.014875000000000
Se	19.434570999999983	25.647497999999988	4.737573000000003
Se	17.945074000000017	28.583881000000016	5.035264999999999
Se	15.979988999999998	31.224457999999985	5.198668999999998
Se	37.780980999999970	-0.797351999999999	4.346848999999997
Se	36.158011000000019	2.443725000000001	5.293156999999999
Se	34.585019000000026	5.456312999999997	4.773971000000004
Se	32.783028999999991	8.326268999999999	5.333050000000001
Se	31.149498999999987	11.269002999999997	4.729306000000002
Se	29.373139999999994	14.033625000000007	5.241587000000000
Se	27.744492000000010	16.987155000000013	4.716371999999998
Se	26.150645999999983	19.936592000000010	4.897050000000001
Se	24.490331999999987	22.699667999999991	5.231145999999999
Se	22.860089999999996	25.645492000000008	4.777590000000000
Se	21.237096000000011	28.543355999999993	5.271094999999999
Se	19.447146000000000	31.398710999999987	4.888531999999997
Se	41.221023000000024	-0.708969000000000	4.538678000000000
Se	39.473936000000019	2.497322000000000	5.358064999999999
Se	37.847358999999973	5.412116000000001	4.969998999999996
Se	36.199303000000005	8.370860000000004	5.345152999999998
Se	34.505386000000014	11.226043999999999	4.940764999999999
Se	32.786344999999972	14.209255000000006	5.205547000000001
Se	31.173801000000010	16.933225000000002	5.220328000000003
Se	29.453426000000003	19.797868999999986	5.016821000000002
Se	27.836434000000006	22.915510999999986	5.433277999999996
Se	26.196176999999987	25.798479000000004	4.830804999999998
Se	24.613215000000003	28.730782000000014	5.158826000000004
Se	23.002169999999996	31.449414000000009	5.167700000000000
Se	42.775354000000001	2.507064999999999	5.642877999999996
Se	41.053731999999966	5.479559000000001	5.236530000000001
Se	39.525182000000009	8.460604000000000	5.473055999999997
Se	37.782628000000025	11.241377000000000	5.168441999999998
Se	36.224156999999982	14.206210000000004	5.499672000000003

Se	34.436698999999973	16.988340999999984	5.258335999999999
Se	32.876941000000022	19.914259000000013	5.537871000000000
Se	31.106738000000000	22.657686000000018	5.264829999999999
Se	29.569483999999992	25.712669000000018	5.442173000000004
Se	28.021383000000002	28.642423999999983	5.433233999999997
Se	26.243410000000008	31.518333999999994	5.131901000000000
Se	46.541575999999992	2.789178000000002	5.022001999999996
Se	44.798065000000011	5.694618000000002	4.592158000000004
Se	43.246920000000029	8.605413000000004	4.741188000000002
Se	41.678182999999971	11.443626999999993	4.545137000000004
Se	40.005634000000006	14.339059000000007	4.304803999999999
Se	38.311143999999988	17.204277999999986	4.712418999999997
Se	36.581462000000019	20.073214000000001	4.456068000000001
Se	35.058075000000023	23.051482000000000	4.822569999999998
Se	33.073165000000030	25.739125000000014	4.811974000000002
Se	31.701938999999994	28.949781000000015	4.552889000000004
Se	29.999468000000002	31.804054000000007	4.330681000000002
Se	30.916156000000009	1.402174000000000	2.328415000000001
Se	29.113438999999996	4.264262999999997	2.457681000000000
Se	27.403507999999986	7.104309999999999	2.622949999999999
Se	25.719954000000013	9.923054000000005	2.501090000000000
Se	24.294771000000008	13.122237000000002	2.161017000000002
Se	22.282509000000010	15.866516000000007	2.417263000000002
Se	20.726873000000012	18.763142999999995	2.274265999999999
Se	19.089372999999984	21.573070999999988	2.301423000000002
Se	17.557991000000012	24.586656999999989	2.387496000000001
Se	15.689054000000005	27.410087999999982	2.271602000000001
Se	14.073171999999996	30.311441999999996	2.349384000000001
Se	34.641503999999976	1.531760999999999	1.424612000000000
Se	33.002583999999988	4.562738000000004	1.741965999999999
Se	31.157588000000005	7.317447999999997	1.471805000000000
Se	29.614944000000013	10.276450999999998	1.783606999999999
Se	27.748927999999994	13.174960000000004	1.372009000000000

Se	26.225557999999995	16.145824000000011	1.602584999999999
Se	24.415217999999994	19.060327000000009	1.475314999999999
Se	22.849923000000004	21.847995000000009	1.389545999999999
Se	21.361336000000014	24.767233000000009	1.638884000000000
Se	19.518992999999983	27.598243000000001	1.389411000000000
Se	17.982327999999990	30.555897999999991	1.715931000000001
Se	16.163209999999994	33.521940999999982	1.476838000000001
Se	37.868085999999981	1.506936000000001	1.498122000000000
Se	36.292116000000000	4.556265999999999	1.954140999999999
Se	34.561109999999993	7.345049999999996	1.673932000000000
Se	32.915512999999971	10.291892000000007	2.023229000000002
Se	31.155021999999989	13.158474999999993	1.767582000000000
Se	29.531441000000009	16.065180999999990	1.506195000000000
Se	27.880036000000005	19.068833999999990	2.040217999999999
Se	26.213726999999987	21.794246000000011	1.749468000000000
Se	24.591219999999999	24.808562999999995	1.961988000000001
Se	22.891203000000009	27.714860999999991	1.492339000000001
Se	21.287026000000009	30.457173000000009	1.568052999999999
Se	19.524581000000013	33.436300000000028	2.152632999999998
Se	41.062455999999974	1.587150000000001	1.667683999999999
Se	39.551913999999965	4.557870000000003	2.115826000000002
Se	37.969934999999995	7.467257000000000	1.583232999999999
Se	36.202807999999974	10.347967999999998	2.163447000000001
Se	34.647013000000012	13.264613000000007	1.587698000000001
Se	32.859251999999979	16.095264000000002	2.147711999999998
Se	31.254349000000013	18.979050000000009	1.595085000000001
Se	29.721280000000001	22.005984000000015	1.914382999999999
Se	27.840512000000004	24.864840000000009	1.925275000000001
Se	26.363015999999982	27.649557999999990	1.825668000000001
Se	24.662623000000000	30.597418999999986	2.180429999999999
Se	22.870499999999998	33.481147999999975	1.876541000000000
Se	44.615546999999994	1.313814000000000	2.463544000000002
Se	43.094737999999995	4.497099999999997	2.219113000000001

Se	41.309626999999990	7.397262999999997	1.7449150000000000
Se	39.6075209999999984	10.2603890000000000	1.8474330000000001
Se	38.1443650000000005	13.2249160000000003	1.8758670000000000
Se	36.2697659999999971	16.0774429999999988	1.8398960000000000
Se	34.6876660000000001	19.0458609999999986	2.1022979999999998
Se	32.9540399999999991	21.8656509999999997	1.9035230000000001
Se	31.4157790000000006	24.8574680000000008	2.1883260000000000
Se	29.8304660000000013	27.7983179999999983	1.7230639999999999
Se	28.0098389999999995	30.6200249999999983	1.6515150000000001
Se	26.3283659999999990	33.4557509999999994	1.6530480000000001
W	16.5451410000000010	35.1852129999999974	3.3547449999999999
W	19.4424279999999996	35.6445470000000029	3.5962900000000002
W	17.9252800000000008	38.0399329999999978	3.8914260000000001
W	23.1561710000000005	35.4829999999999970	3.6022170000000000
W	20.9696330000000017	37.8648159999999976	3.7091740000000000
W	26.0271700000000017	35.1441980000000029	3.4884860000000000
W	24.3024619999999985	37.8339530000000011	3.6262870000000000
Se	13.9919720000000005	34.3150699999999986	4.2062510000000000
Se	17.8468310000000017	34.2604809999999986	5.2080270000000004
Se	15.4514709999999997	37.1852110000000025	4.1134779999999997
Se	21.2382199999999983	34.2745620000000031	4.9237940000000000
Se	19.4215000000000018	37.2351019999999977	5.6295089999999997
Se	16.8793299999999995	39.7553279999999987	5.0652379999999999
Se	24.6183729999999983	34.4702950000000001	5.4368220000000003
Se	22.7246670000000002	37.2768889999999971	5.4716399999999998
Se	28.3157989999999984	34.6887049999999988	4.3064190000000000
Se	26.4630229999999997	37.6555579999999992	4.5437649999999996
Se	17.8634459999999997	36.5160440000000008	1.7252030000000000
Se	21.2535540000000012	36.2503669999999971	1.9190790000000000
Se	19.5317860000000003	39.5282190000000000	2.6547510000000001
Se	24.7333710000000018	36.3667960000000008	1.6791760000000000
Se	22.9384839999999990	39.5512439999999970	2.7340819999999999

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,258.687\,202\,18$ eV; $E_{rel} = 67.491\,419\,863\,6$ meV/f.u.

W	-0.3684040000000000	56.6934860000000000	10.4667510000000004
W	0.7561860000000000	59.1307070000000010	10.4733339999999995
W	-2.1124480000000001	59.4020340000000004	10.3879959999999993
W	-3.7810920000000001	62.1585189999999983	10.3283629999999995
W	-5.4134690000000001	64.9557010000000048	10.3181270000000005
W	-7.0398980000000000	67.7474859999999950	10.3244790000000002
W	-8.6631909999999994	70.5370510000000053	10.3337389999999996
W	-10.2816259999999993	73.3292069999999967	10.3421249999999993
W	-11.8961089999999992	76.1222949999999940	10.3452529999999996
W	-13.5093829999999997	78.9171500000000066	10.3405509999999996
W	-15.1197189999999999	81.7156930000000017	10.3314059999999994
W	-16.7256819999999991	84.5182340000000067	10.3236329999999992
W	-18.3307870000000008	87.3250419999999963	10.3188010000000006
W	2.8808389999999999	56.5585909999999998	10.6692780000000003
W	-0.8969660000000000	61.8062150000000017	10.3871640000000003
W	-2.5518220000000000	64.5864140000000049	10.3744189999999996
W	-4.2037009999999997	67.4049380000000014	10.3759730000000001
W	-5.8484100000000003	70.2188699999999955	10.3843929999999993
W	-7.4856980000000002	73.0316459999999950	10.3940900000000003
W	-9.1183390000000006	75.8490939999999938	10.3994999999999997
W	-10.7476009999999995	78.6702229999999929	10.3986909999999995
W	-12.3714279999999999	81.4926999999999992	10.3925129999999992
W	-13.9891150000000000	84.3162880000000001	10.3832380000000004
W	-15.6034629999999996	87.1476519999999937	10.3760279999999998
W	5.8230350000000000	56.4654340000000019	10.9346300000000003
W	4.6484360000000002	59.0162169999999975	10.7791890000000006
W	2.9798520000000002	62.4229320000000030	10.7354330000000004
W	1.4052670000000000	65.1384500000000060	10.7028639999999999
W	-0.2183790000000000	67.8919329999999945	10.6717689999999994
W	-1.8537999999999999	70.6848420000000033	10.6735199999999999
W	-3.4863990000000000	73.4855490000000060	10.6877759999999995

W	-5.1130129999999996	76.2929239999999993	10.6999230000000001
W	-6.7396839999999996	79.1006469999999950	10.7044610000000002
W	-8.3586869999999998	81.9128259999999955	10.6998040000000003
W	-9.9774390000000004	84.7250339999999937	10.6878399999999996
W	-11.5871169999999992	87.5392269999999968	10.6738830000000000
W	8.8497749999999993	56.3419949999999972	11.1530120000000004
W	7.2834969999999997	59.0590850000000032	11.0780419999999999
W	5.7597690000000004	62.0541320000000027	10.8257410000000007
W	4.1936749999999998	64.8892100000000056	10.7275690000000008
W	2.5801280000000002	67.6509920000000022	10.7502969999999998
W	0.9433490000000000	70.4283879999999982	10.7560219999999997
W	-0.6938900000000000	73.2172079999999994	10.7645959999999992
W	-2.3220950000000000	76.0193050000000028	10.7803380000000004
W	-3.9523299999999999	78.8345470000000006	10.7931729999999995
W	-5.5794280000000001	81.6514949999999970	10.7931290000000004
W	-7.2030269999999996	84.4700950000000006	10.7804760000000002
W	-8.8158750000000001	87.2800280000000015	10.7645250000000008
Se	0.8687910000000000	54.9482179999999971	11.4912469999999995
Se	-0.8851740000000000	58.2438799999999972	12.3103920000000002
Se	-2.5663360000000002	61.0086609999999965	12.2326899999999998
Se	-4.2203650000000001	63.7610790000000023	12.1999440000000003
Se	-5.8549400000000000	66.5447640000000007	12.2039559999999998
Se	-7.4909090000000003	69.3325190000000049	12.2135320000000007
Se	-9.1196479999999998	72.1247149999999948	12.2231769999999997
Se	-10.7419060000000002	74.9223669999999942	12.2288720000000009
Se	-12.3593820000000001	77.7241640000000018	12.2280689999999996
Se	-13.9723910000000000	80.5276219999999938	12.2206960000000002
Se	-15.5767439999999997	83.3348040000000054	12.2115440000000000
Se	-17.1737819999999992	86.1468679999999978	12.2032840000000000
Se	4.1631229999999997	54.7396049999999974	11.6622199999999996
Se	2.5932270000000002	58.2937259999999995	12.2681710000000006
Se	1.0111889999999999	61.1693229999999986	12.0286019999999994
Se	-0.5985290000000000	63.9105830000000026	11.9351050000000001

Se	-2.2371660000000002	66.6908080000000041	11.9084430000000001
Se	-3.8796879999999998	69.4897169999999988	11.9145400000000006
Se	-5.5170820000000003	72.2953219999999988	11.9265080000000001
Se	-7.1492199999999997	75.1080699999999979	11.9345610000000004
Se	-8.7789859999999997	77.9249769999999984	11.9377940000000002
Se	-10.4045179999999995	80.7441129999999987	11.9339040000000001
Se	-12.0248279999999994	83.5631539999999973	11.9259339999999998
Se	-13.6360069999999993	86.3837900000000047	11.9145850000000006
Se	7.3655059999999999	54.7822450000000032	12.1563079999999992
Se	5.8414460000000004	58.0356730000000027	12.8307839999999995
Se	4.2855639999999999	61.0458610000000022	12.4635599999999993
Se	2.7448549999999998	64.0545510000000036	12.6145119999999995
Se	1.0684890000000000	66.7951029999999975	12.5680230000000002
Se	-0.5813400000000000	69.5499310000000008	12.5485589999999991
Se	-2.2189209999999999	72.3366520000000008	12.5570670000000000
Se	-3.8508360000000001	75.1394520000000057	12.5702689999999997
Se	-5.4821689999999998	77.9505979999999994	12.5795239999999993
Se	-7.1077649999999997	80.7651010000000014	12.5794979999999992
Se	-8.7275039999999997	83.5828549999999950	12.5702569999999998
Se	-10.3392990000000005	86.3972689999999943	12.5572309999999998
Se	10.7358750000000001	55.2984429999999989	10.4410039999999995
Se	9.3535670000000000	58.1863770000000002	12.5223200000000007
Se	7.9400500000000003	61.2072760000000002	12.0525520000000004
Se	6.5144279999999997	64.2149749999999955	11.6665919999999996
Se	4.8089430000000002	67.0782010000000071	11.8131269999999997
Se	3.1726730000000001	69.8974319999999949	11.7860090000000000
Se	1.5402670000000001	72.6820220000000035	11.7783999999999995
Se	-0.1072660000000000	75.4550090000000040	11.8251469999999994
Se	-1.7143830000000000	78.2612479999999948	11.8019259999999999
Se	-3.3632279999999999	81.0494810000000001	11.8569150000000008
Se	-4.9538919999999997	83.8710990000000010	11.8014119999999991
Se	-6.5815549999999998	86.6655930000000012	11.8251950000000008
Se	-2.4479329999999999	56.7833010000000016	9.4092330000000004

Se	-4.2708680000000001	59.7090079999999972	9.3581029999999998
Se	-5.9481909999999996	62.5751980000000003	9.3066960000000005
Se	-7.5948289999999998	65.4134990000000016	9.2964059999999993
Se	-9.2287920000000003	68.2441910000000007	9.2862069999999992
Se	-10.8664520000000007	71.0692540000000008	9.2931819999999998
Se	-12.4941899999999997	73.8973610000000036	9.2878720000000001
Se	-14.1285209999999992	76.7209440000000029	9.2920999999999996
Se	-15.7617729999999998	79.5468390000000056	9.2904640000000001
Se	-17.3943049999999992	82.3764780000000059	9.2907130000000002
Se	-19.0289810000000017	85.2083310000000012	9.3018310000000000
Se	-20.6632910000000010	88.0544680000000000	9.3141770000000008
Se	1.3097920000000001	57.2658419999999992	8.7506290000000000
Se	-0.5501120000000000	60.0802189999999996	8.5497099999999993
Se	-2.2170410000000000	62.9008949999999984	8.5124800000000000
Se	-3.8492449999999998	65.7252210000000048	8.5118679999999998
Se	-5.4921650000000000	68.5461169999999953	8.5143599999999994
Se	-7.1296819999999999	71.3631259999999941	8.5221020000000003
Se	-8.7600750000000005	74.1794069999999977	8.5304529999999996
Se	-10.3879040000000007	76.9961160000000007	8.5334389999999996
Se	-12.0146210000000000	79.8139520000000005	8.5292230000000000
Se	-13.6391600000000004	82.6341249999999974	8.5205870000000008
Se	-15.2610949999999992	85.4607490000000070	8.5139510000000005
Se	-16.8819750000000006	88.2944540000000018	8.5126810000000006
Se	4.4995719999999997	57.2730990000000020	8.9126600000000007
Se	2.8363380000000000	60.2254000000000005	9.3078420000000008
Se	1.1234900000000001	63.0367710000000017	9.1139600000000005
Se	-0.5237130000000000	65.8007520000000028	9.1269460000000002
Se	-2.1758890000000002	68.6063180000000017	9.1275739999999992
Se	-3.8182820000000000	71.4159760000000006	9.1379439999999992
Se	-5.4497299999999997	74.2244180000000000	9.1512709999999995
Se	-7.0757770000000004	77.0337470000000053	9.1586040000000004
Se	-8.6988990000000008	79.8442679999999996	9.1583570000000005
Se	-10.3194809999999997	82.6569080000000014	9.1506609999999995

Se	-11.936733999999995	85.473733999999932	9.137774000000003
Se	-13.548992000000001	88.301064999999941	9.128087000000007
Se	7.710486000000004	57.297227999999969	9.239867999999995
Se	6.233113000000003	60.285715000000033	9.111852000000007
Se	4.620867999999998	63.209387999999970	8.894704000000008
Se	3.027124999999998	66.053460000000012	8.855017999999994
Se	1.426345999999999	68.849857000000001	8.861387000000006
Se	-0.208228000000000	71.637994000000062	8.868474000000009
Se	-1.840104000000000	74.439296999999963	8.883922000000001
Se	-3.468623000000000	77.244680999999999	8.898725000000007
Se	-5.089183000000002	80.055847999999975	8.907133999999992
Se	-6.714356999999997	82.864142000000011	8.898687000000007
Se	-8.330130000000005	85.676244999999944	8.883893000000005
Se	-9.940628999999995	88.489002999999967	8.868223999999997
W	-19.935790999999983	90.139990999999949	10.329506999999996
W	-18.795859000000001	92.813039000000034	10.387081999999995
W	-21.485392999999984	92.965577999999936	10.384855999999992
W	-22.956935000000014	95.831929999999998	10.455650999999996
W	-17.217347000000002	89.988168000000017	10.375315000000005
W	-20.284960000000017	95.585262000000002	10.469383000000005
W	-21.446504000000009	98.714302000000035	10.661495000000004
W	-13.187822999999999	90.352733999999981	10.672413000000006
W	-14.758798000000005	93.137141999999972	10.703671999999992
W	-16.321975999999994	95.861018999999989	10.735212999999999
W	-18.435043000000003	99.011268000000012	10.780585999999996
W	-20.053435000000003	101.306324000000036	10.935878000000007
W	-10.411721999999993	90.091409999999962	10.755720000000002
W	-11.997078999999994	92.897154000000005	10.749993999999992
W	-13.579491000000009	95.675933999999980	10.728478000000008
W	-15.248843000000008	98.450939000000053	10.830000000000001
W	-17.077642000000009	101.269172999999950	11.088312999999994
W	-18.644321999999990	103.985855999999983	11.167543000000002
Se	-18.767620000000009	88.956768999999942	12.200506000000007

Se	-20.324163999999997	91.768727999999959	12.231887000000004
Se	-21.878650000000004	94.609626000000058	12.303542000000002
Se	-23.851739999999995	97.778816000000062	11.473575000000003
Se	-15.238070999999997	89.206474999999975	11.909361000000005
Se	-16.825404999999999	92.017527000000012	11.936082000000007
Se	-18.394127000000010	94.784931999999977	12.027858999999994
Se	-20.093966999999992	97.594488999999958	12.264212999999998
Se	-22.382293000000007	100.733553999999980	11.654268000000001
Se	-11.933614000000004	89.209130999999993	12.548856000000007
Se	-13.493394999999996	92.016180000000056	12.568500999999995
Se	-15.028007999999998	94.839460000000025	12.614848000000003
Se	-16.862214000000016	97.678201000000014	12.465102999999992
Se	-18.691265999999988	100.530882000000054	12.834390000000009
Se	-20.740899999999999	103.480532999999941	12.163531000000008
Se	-8.158913999999993	89.478768999999998	11.777340000000006
Se	-9.754004000000001	92.284356000000025	11.785830000000007
Se	-11.376144000000000	95.111356000000007	11.814503000000002
Se	-12.998694000000004	98.022136000000033	11.665606999999996
Se	-14.893252999999996	100.756652000000025	12.068986000000007
Se	-16.798646000000015	103.493351000000041	12.539265000000003
Se	-18.601071999999985	106.143366999999978	10.462763000000007
Se	-22.302959000000013	90.941689999999941	9.361271999999996
Se	-23.916962999999991	93.985449000000027	9.398735000000003
Se	-18.509294000000006	91.121162999999957	8.513458000000000
Se	-20.113558999999986	93.977339999999981	8.547520999999997
Se	-21.616219000000010	96.999522999999964	8.743254000000003
Se	-15.151579999999992	91.135706999999965	9.128102000000002
Se	-16.719160999999997	93.945899999999946	9.114395999999993
Se	-18.293890000000011	96.838639000000006	9.307251000000008
Se	-20.012246999999986	99.759787000000029	8.910935000000003
Se	-11.537088999999999	91.298276999999988	8.861102000000007
Se	-13.156501000000004	94.083675999999970	8.855389000000006
Se	-14.818669999999991	96.888823999999996	8.896909000000008

Se	-16.5390890000000006	99.7505890000000051	9.1181649999999994
Se	-18.3837229999999998	102.5277870000000036	9.2504950000000008

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,260.821\,285\,15$ eV; $E_{rel} = 35.156\,829\,409\,0$ meV/f.u.

W	19.8966950000000011	1.9305330000000001	4.0731560000000000
W	17.9541080000000015	3.9589580000000000	2.8899100000000000
W	16.3821699999999986	6.6962270000000004	3.0342530000000001
W	14.7756930000000004	9.5127559999999995	3.2490839999999999
W	13.1944260000000000	12.2947489999999995	3.3888630000000002
W	11.6333509999999993	15.0568530000000003	3.4518960000000001
W	10.0434809999999999	17.8345880000000001	3.2906659999999999
W	8.1422220000000003	21.2275680000000015	3.0483669999999998
W	6.6628179999999997	23.9916170000000015	3.1497069999999998
W	5.1693210000000001	26.6893719999999988	3.0663499999999999
W	3.5395740000000000	29.3006489999999999	3.0167639999999998
W	21.0000409999999995	3.8715549999999999	2.8923869999999998
W	19.3649929999999983	6.3224739999999997	3.0182560000000000
W	17.6807780000000001	9.0488660000000003	3.1375160000000002
W	16.0098969999999987	11.9331189999999996	3.2890760000000001
W	14.3794620000000002	14.7530889999999992	3.3583530000000001
W	12.8177439999999994	17.5647370000000009	3.3648840000000000
W	11.4201090000000001	21.1528680000000016	3.2772880000000000
W	9.9408309999999993	23.4520569999999999	3.3402080000000001
W	7.9124020000000002	26.8462439999999987	3.2006700000000001
W	6.6670850000000002	29.2017260000000007	3.0462319999999998
W	22.5939060000000005	6.3115769999999998	2.9811860000000001
W	21.5794829999999997	9.5438949999999991	3.2901440000000002
W	20.0728989999999996	12.3041359999999997	3.5105840000000001
W	18.4133400000000016	15.1316050000000004	3.5382840000000000
W	16.8280659999999997	17.8982619999999990	3.4959739999999999
W	14.6723099999999995	21.1665990000000015	3.3909460000000000
W	13.1299069999999993	23.4166589999999992	3.4851480000000001

W	11.6881900000000005	27.0831769999999992	3.2557320000000001
W	10.0314189999999996	29.3145360000000004	3.2678820000000002
W	24.6546990000000008	9.4258930000000003	3.0285000000000002
W	23.0117709999999995	11.8005490000000002	3.3681369999999999
W	21.1509849999999998	15.1546629999999993	3.5101610000000001
W	19.7194530000000015	17.6501580000000011	3.4923579999999999
W	17.8205799999999996	21.0687069999999999	3.4864229999999998
W	16.3637739999999994	23.3965570000000014	3.5587860000000000
W	14.8600589999999997	27.0858319999999999	3.3205920000000000
W	13.2731530000000006	29.3615010000000005	3.3606799999999999
W	26.3338859999999997	12.4053269999999998	3.4083429999999999
W	25.1872480000000003	14.8921869999999998	3.4223759999999999
W	22.7242080000000009	18.0325960000000016	3.6005120000000002
W	21.6443800000000017	20.9672179999999990	3.5247760000000001
W	19.6855989999999998	23.3390909999999998	3.6124869999999998
W	18.0827379999999991	27.0584840000000000	3.3777800000000000
W	16.4870130000000010	29.3548989999999996	3.3541870000000000
W	27.9134360000000008	15.1448380000000000	3.5415420000000002
W	26.7268070000000009	17.6263299999999994	3.4037190000000002
W	24.4061640000000004	20.9452950000000016	3.4986700000000002
W	23.0591159999999995	23.3749450000000003	3.5117140000000000
W	21.3364300000000000	27.0378380000000007	3.3828330000000002
W	19.7173769999999990	29.3360750000000010	3.3616690000000000
W	29.4744069999999994	17.8960059999999999	3.3578679999999999
W	28.1767250000000011	21.1676399999999987	3.3457759999999999
W	26.3960380000000008	23.3785179999999997	3.5203110000000000
W	24.5748889999999989	27.0616130000000013	3.3232610000000000
W	22.9407689999999995	29.3305439999999997	3.3539610000000000
W	31.3361529999999995	21.2856090000000009	3.0584820000000001
W	29.5387729999999991	23.5156279999999995	3.3569390000000001
W	27.7406299999999995	27.1020879999999984	3.2563770000000001
W	26.1395669999999996	29.3598759999999999	3.3569900000000001
W	32.7666979999999981	24.0684080000000016	3.1428280000000002

W	31.5084090000000003	26.9175930000000001	3.2010160000000001
W	29.3742710000000002	29.3548119999999990	3.2607879999999998
W	34.2538539999999969	26.7669740000000012	3.0607530000000001
W	32.7349809999999977	29.2797990000000006	3.0424709999999999
W	35.8643310000000000	29.3955769999999994	3.0180020000000001
Se	20.4000449999999987	2.0173580000000002	6.2923970000000002
Se	17.6934569999999987	5.4420690000000000	4.8242820000000002
Se	16.0826649999999987	8.2369719999999997	5.0102719999999996
Se	14.4523480000000006	11.0621799999999997	5.1879710000000001
Se	12.8388240000000007	13.8974689999999992	5.2963120000000004
Se	11.2232810000000001	16.7999469999999995	5.2623749999999996
Se	9.5602780000000003	19.8986289999999997	4.7784620000000002
Se	8.0340889999999998	22.8688439999999993	4.9803949999999997
Se	6.4727810000000003	25.6926519999999989	4.9990059999999996
Se	4.9197259999999998	28.6031540000000000	4.8852820000000001
Se	21.0810069999999996	5.4367340000000004	4.7815190000000003
Se	19.6573460000000004	8.3422090000000004	4.6274569999999997
Se	18.0255919999999996	11.1370400000000007	4.7072909999999997
Se	16.3875230000000016	14.0086429999999993	4.8451480000000000
Se	14.7432239999999997	16.8667259999999999	4.8865170000000004
Se	12.9674619999999994	19.7830650000000006	4.8109520000000003
Se	11.4150170000000006	22.8003539999999987	5.2429839999999999
Se	9.8582190000000001	25.7701379999999993	4.6137750000000004
Se	8.2583479999999998	28.7371550000000013	4.9708019999999999
Se	23.1705299999999994	8.0966600000000000	4.7557710000000002
Se	21.4573070000000001	11.1015499999999996	5.2529599999999999
Se	19.7862779999999994	13.9904960000000003	5.3507009999999999
Se	18.1123590000000014	16.8958049999999993	5.3758010000000001
Se	16.2815709999999996	19.8430970000000002	5.0767119999999997
Se	14.6984440000000003	22.8150529999999989	5.3622470000000000
Se	13.1579540000000001	25.7380369999999985	4.8288029999999997
Se	11.5967289999999998	28.8158420000000000	5.1747610000000002
Se	24.8892880000000005	11.0251730000000006	5.0197050000000001

Se	23.153908999999987	14.003954000000002	4.8028579999999996
Se	21.364466000000002	16.907350000000010	5.3645980000000000
Se	19.705407000000010	19.869689999999985	4.855826999999997
Se	18.011158999999993	22.754668999999998	5.391855999999998
Se	16.406258999999986	25.718265999999998	4.8730370000000001
Se	14.861245000000003	28.898783000000017	5.2253740000000004
Se	26.636555999999988	13.963775000000000	5.359714999999996
Se	24.785620999999990	16.932732999999989	4.956110999999999
Se	23.068795000000015	19.833096000000012	5.3448460000000004
Se	21.402560999999986	22.766023000000006	5.3633670000000002
Se	19.701847999999983	25.695962999999990	4.8865590000000001
Se	18.094028000000016	28.914279000000005	5.2372100000000001
Se	28.271381000000016	16.892237000000015	5.3345200000000004
Se	26.460990999999999	19.842535999999991	4.7931130000000000
Se	24.757446999999991	22.731213000000003	5.3188700000000004
Se	23.027497000000003	25.685582000000001	4.858546999999997
Se	21.334582000000010	28.899239000000015	5.239054999999996
Se	29.951133999999997	19.934446999999987	4.8674410000000004
Se	28.098534999999983	22.800699000000016	5.2835710000000002
Se	26.293559999999994	25.729251999999989	4.826509999999999
Se	24.562729999999984	28.879402999999999	5.225724999999997
Se	31.449846999999983	22.921734000000007	4.990096999999996
Se	29.584955000000008	25.820284000000009	4.628403999999997
Se	27.822146000000000	28.842446999999999	5.1726890000000001
Se	32.953560000000031	25.769719999999995	4.9943770000000001
Se	31.151586000000018	28.806582999999998	4.969700999999997
Se	17.496905000000017	1.676031000000000	3.658034999999999
Se	16.015204000000007	4.392231999999999	1.613505000000000
Se	14.113251000000000	7.089364999999999	2.330667000000000
Se	12.573817999999993	10.010313999999993	2.301816000000000
Se	10.953153000000004	12.883644000000003	2.378663000000000
Se	9.262527999999997	15.713972000000001	2.519820000000002
Se	7.915181999999997	18.866783000000016	2.224450000000000

Se	5.9113360000000004	21.6797709999999988	2.2979330000000000
Se	4.4255149999999999	24.4958209999999994	2.1866420000000000
Se	2.9320529999999998	27.3349200000000003	1.8557910000000000
Se	1.7009179999999999	30.3875309999999992	3.7864599999999999
Se	21.6379829999999984	1.3569760000000000	2.5524870000000002
Se	19.5428050000000013	4.5739799999999997	1.0672180000000000
Se	17.8912799999999983	7.4308170000000002	1.2181219999999999
Se	16.2812820000000009	10.2776669999999992	1.3948240000000001
Se	14.6443130000000004	13.0817540000000001	1.4870209999999999
Se	13.0203059999999997	15.8971269999999993	1.5103070000000001
Se	11.4533810000000003	18.9122169999999983	1.6527609999999999
Se	9.7844960000000007	21.8058440000000004	1.3661500000000000
Se	8.2954690000000006	24.7600020000000001	1.6118900000000000
Se	6.5071139999999996	27.5660449999999990	1.1827810000000001
Se	4.9049750000000003	30.7182749999999984	1.7337350000000000
Se	23.2755219999999987	4.2819190000000003	1.8487009999999999
Se	21.2104309999999998	7.5273490000000001	1.4866230000000000
Se	19.6573579999999986	10.3307359999999999	1.8283229999999999
Se	18.0351539999999986	13.0960809999999999	2.0001380000000002
Se	16.3679869999999994	15.9141790000000007	2.0303990000000001
Se	14.7778559999999999	18.8335140000000010	2.0921599999999998
Se	13.0912590000000009	21.7687700000000000	1.5121659999999999
Se	11.5755940000000006	24.7943409999999993	1.8769480000000001
Se	9.8586569999999991	27.6170720000000003	1.5427329999999999
Se	8.1970740000000006	30.8971130000000009	2.1869380000000000
Se	24.9649700000000010	7.0476340000000004	2.3573520000000001
Se	23.1203579999999995	10.2245030000000003	1.3280559999999999
Se	21.5395040000000009	13.2178760000000004	1.7507820000000001
Se	19.7758579999999995	16.0000299999999989	1.5641540000000000
Se	18.1749149999999986	18.9310140000000011	1.7931310000000000
Se	16.3522950000000016	21.7565999999999988	1.5786169999999999
Se	14.8073820000000005	24.7921380000000013	2.0048400000000002
Se	13.2559810000000002	27.7487490000000001	1.4210039999999999

Se	11.512506000000001	31.077649999999984	2.4956170000000002
Se	26.8452790000000014	9.994809999999993	2.3131460000000001
Se	24.772073999999999	13.079717999999997	1.6926460000000001
Se	23.197238999999997	16.014556999999999	2.0789840000000002
Se	21.341532999999983	18.939278000000016	1.8343970000000001
Se	19.7347110000000008	21.691942999999984	1.8194330000000001
Se	18.0917800000000000	24.741807999999989	2.0931419999999998
Se	16.490684999999991	27.667871000000017	1.489789999999999
Se	14.8394750000000002	31.0190710000000003	2.3254410000000001
Se	28.5746900000000004	12.8434200000000001	2.5795979999999998
Se	26.5609810000000017	15.927319999999999	1.5424199999999999
Se	24.774696999999997	18.826091999999992	2.0651739999999998
Se	23.0326290000000000	21.801507999999983	1.5571880000000000
Se	21.3405650000000016	24.735278999999985	2.0761980000000002
Se	19.715312999999983	27.6277110000000015	1.5241279999999999
Se	18.105640999999985	31.025536999999999	2.3732270000000000
Se	30.2452170000000002	15.750920999999999	2.5763010000000000
Se	28.104334999999990	18.957550000000012	1.6845209999999999
Se	26.2974180000000004	21.709140999999989	1.7138679999999999
Se	24.643436999999987	24.7620970000000007	2.0148020000000000
Se	22.9367640000000002	27.633051999999993	1.4970770000000000
Se	21.3311180000000000	31.0152530000000013	2.3731979999999999
Se	31.619652999999996	18.918438999999993	2.2997600000000000
Se	29.6962620000000008	21.876872999999998	1.3676429999999999
Se	27.8370320000000007	24.808721999999995	1.8969090000000000
Se	26.166527999999996	27.743670000000016	1.4207580000000000
Se	24.5686350000000004	30.999476999999988	2.3055539999999999
Se	33.5293720000000022	21.7750410000000016	2.2276189999999998
Se	31.1272300000000008	24.831503999999989	1.6078859999999999
Se	29.558288999999985	27.6547230000000006	1.5389230000000000
Se	27.876623999999996	31.096713999999986	2.4788239999999999
Se	31.1905010000000011	30.954032999999990	2.1716780000000000
Se	34.485785999999974	28.686057999999992	4.8814669999999998

Se	32.9116270000000029	27.6416870000000010	1.1818470000000001
Se	35.0134290000000021	24.5834040000000016	2.1870080000000001
Se	36.4873550000000009	27.4350759999999987	1.8561160000000001
Se	34.4905339999999967	30.8062439999999995	1.7348110000000001
Se	37.6930419999999984	30.4955239999999996	3.7909679999999999

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,261.457\,186\,48$ eV; $E_{rel} = 25.521\,960\,772\,7$ meV/f.u.

W	22.8944019999999995	1.1193730000000000	3.1502610000000000
W	21.2459769999999999	3.9358670000000000	3.1942100000000000
W	17.6593760000000017	14.8005279999999999	3.3661340000000002
W	19.7335080000000005	6.7650090000000001	3.3322699999999998
W	18.1393179999999994	9.5327710000000003	3.3865319999999999
W	16.5108829999999998	12.2846209999999996	3.4298760000000001
W	14.8971610000000005	15.0446209999999994	3.5032500000000000
W	13.3025140000000004	17.8358220000000003	3.4933670000000001
W	11.7418019999999999	20.8194890000000008	3.4006419999999999
W	26.0978640000000013	0.8599790000000000	3.7086440000000001
W	24.2961430000000007	3.4350589999999999	3.3101360000000000
W	22.7015749999999983	6.2010249999999996	3.2592780000000001
W	20.9729230000000015	9.1802960000000002	3.3076390000000000
W	19.3233330000000016	12.0061950000000000	3.3451080000000002
W	16.0349649999999997	17.5992390000000007	3.4024760000000001
W	14.3932050000000000	21.0343480000000014	3.4784869999999999
W	13.2123779999999993	23.6913379999999982	3.3829300000000000
W	27.1664080000000006	3.5063730000000000	3.6803889999999999
W	26.4965679999999999	6.8117310000000000	3.3141099999999999
W	24.9778430000000000	9.5651829999999993	3.4392790000000000
W	23.3737199999999987	12.3841549999999998	3.4847850000000000
W	21.7000530000000005	15.2473489999999998	3.5105749999999998
W	20.0185180000000003	18.0481119999999997	3.5096720000000001
W	18.3726289999999999	20.8013310000000011	3.4233110000000000
W	15.8803990000000006	23.8511309999999987	3.5006279999999999

W	14.7584750000000007	26.4537060000000004	3.3823949999999998
W	27.7699159999999985	9.2934990000000006	3.2025039999999998
W	26.1610799999999983	12.0924239999999994	3.3320580000000000
W	24.4810760000000016	14.9338169999999995	3.3494760000000001
W	22.8152410000000003	17.8278110000000005	3.3567469999999999
W	21.0814850000000007	20.6327759999999998	3.3431400000000000
W	19.9587560000000011	23.5586839999999995	3.3023400000000001
W	17.4835959999999986	26.6433649999999993	3.5197500000000002
W	16.3618610000000011	29.1744489999999992	3.5547520000000001
W	29.7231990000000010	12.5915739999999996	3.4019610000000000
W	28.5734250000000003	15.1767909999999997	3.3941720000000002
W	26.1848109999999998	18.3564639999999990	3.4742570000000002
W	25.0208520000000014	20.8871840000000013	3.3942190000000001
W	22.9140030000000010	24.0024760000000015	3.4174240000000000
W	21.5280559999999994	26.4039639999999984	3.4111560000000001
W	19.6921830000000000	29.7890709999999999	3.5932050000000002
W	18.0106910000000013	32.1190750000000023	3.9734180000000001
W	31.2998569999999994	15.3683309999999995	3.5797129999999999
W	30.1831490000000002	17.9568660000000015	3.4132669999999998
W	27.7041520000000006	21.0335250000000009	3.4455510000000000
W	25.9972199999999987	23.6780130000000000	3.3394469999999998
W	24.3102899999999984	26.5269399999999997	3.4246610000000000
W	22.6388029999999993	29.3132920000000006	3.4268000000000001
W	21.1316300000000012	32.0678709999999967	3.6471010000000001
W	19.9655549999999984	35.3645410000000027	3.9133010000000001
W	32.8443389999999980	18.1148510000000016	3.5579719999999999
W	31.6661220000000014	20.7777749999999983	3.4144350000000001
W	30.0065179999999998	24.1646460000000012	3.4972930000000000
W	28.3577949999999994	26.9514069999999997	3.5342080000000000
W	26.7050389999999993	29.7166260000000015	3.6068840000000000
W	25.0729380000000006	32.4589349999999968	3.6980490000000001
W	23.0417500000000004	35.5479089999999971	3.7781389999999999
W	21.4426039999999993	37.8875570000000010	3.9403779999999999

W	34.315224999999981	20.985845000000012	3.5127169999999999
W	32.741202999999987	23.964332999999999	3.4258980000000001
W	31.1211260000000003	26.7430480000000017	3.4228719999999999
W	29.483388999999990	29.4947760000000017	3.5095670000000001
W	27.844377999999990	32.232979999999977	3.5500330000000000
W	26.1771110000000000	34.9991380000000021	3.6753390000000001
W	24.3952220000000004	37.824585999999965	3.8834110000000002
W	22.8612070000000003	40.561484999999976	3.9325580000000002
Se	23.841242999999986	-0.8308280000000000	3.9789059999999998
Se	22.439302999999989	2.6710440000000002	5.0235510000000003
Se	21.0335000000000001	5.5351850000000002	5.1284910000000004
Se	19.421527999999986	8.3671380000000006	5.2245920000000003
Se	17.7732640000000011	11.1397180000000002	5.2714639999999999
Se	16.159649999999992	13.9130470000000006	5.3230919999999999
Se	14.5505540000000000	16.7378900000000002	5.3592579999999996
Se	12.984603999999991	19.693844999999996	5.2357170000000002
Se	10.7817640000000008	22.7459370000000014	4.3332600000000001
Se	27.0843950000000007	-0.8331050000000000	4.9095089999999999
Se	25.6537010000000016	2.5796820000000000	5.3828709999999997
Se	24.613576999999994	5.5818399999999997	4.8115949999999996
Se	22.9756670000000014	8.4015590000000007	4.7279939999999998
Se	21.340341999999997	11.2691130000000008	4.8096399999999999
Se	19.681291999999991	14.108995999999994	4.8397639999999997
Se	18.014825999999993	16.926310999999983	4.8707330000000004
Se	16.3191300000000012	19.8195230000000002	4.7890569999999997
Se	14.5054820000000007	22.7344690000000007	5.3166219999999997
Se	12.457335999999997	25.794474999999985	4.3961660000000000
Se	28.382274999999999	5.2327579999999996	4.7376009999999997
Se	26.4562330000000010	8.406219999999994	5.2010490000000003
Se	24.7390720000000002	11.2641880000000008	5.2869830000000002
Se	23.052500999999995	14.106645999999996	5.3100759999999996
Se	21.376478999999998	16.998312999999996	5.3181360000000000
Se	19.655598999999987	19.8276550000000000	5.3178060000000000

Se	17.9053350000000009	22.7954660000000011	4.8701119999999998
Se	16.0932420000000000	25.6044330000000002	5.3500750000000004
Se	14.0937149999999995	28.7308430000000001	4.3450470000000001
Se	28.1776090000000003	11.2122019999999996	4.9126589999999997
Se	26.5354090000000014	14.1796100000000003	4.7842310000000001
Se	24.7233640000000001	16.9989969999999992	4.9890819999999998
Se	23.0645600000000002	19.9088729999999998	4.8622790000000000
Se	21.3901649999999997	22.6582760000000007	5.0637460000000001
Se	19.5177359999999993	25.5624879999999983	4.8736980000000001
Se	17.9391759999999998	28.4699610000000014	5.2450609999999998
Se	15.8212130000000002	31.5345300000000002	4.6943549999999998
Se	29.9454829999999994	14.1654140000000002	5.3498469999999996
Se	28.1488380000000014	17.1600199999999994	4.9145799999999999
Se	26.4126869999999982	20.0326179999999994	5.3615399999999998
Se	24.6072080000000000	22.8013159999999999	5.1398229999999998
Se	22.9657119999999999	25.6379650000000012	5.3675689999999996
Se	21.2020009999999992	28.3840229999999991	5.1902999999999997
Se	19.6130589999999998	31.3719579999999993	5.6341570000000001
Se	31.5841309999999993	17.0234640000000006	5.4210320000000003
Se	29.7145060000000001	20.0237340000000010	4.9119299999999999
Se	28.0727989999999998	23.0171750000000017	4.9295249999999999
Se	26.3864240000000017	25.7380150000000008	4.8623770000000004
Se	24.6960419999999985	28.5740480000000012	4.9333929999999997
Se	23.0672050000000013	31.3069389999999999	5.0904350000000003
Se	33.1452609999999979	19.8724060000000016	5.3797470000000001
Se	31.4373150000000017	22.8604300000000009	5.1474510000000002
Se	29.7763430000000007	25.8513739999999999	5.3540109999999999
Se	28.0802179999999986	28.6170130000000000	5.4156589999999998
Se	26.4708970000000008	31.4253229999999988	5.5052120000000002
Se	35.1531909999999996	22.9869160000000008	4.4337720000000003
Se	33.5499620000000007	26.0526499999999999	4.2560799999999999
Se	31.8075660000000013	28.8900900000000007	4.4547660000000002
Se	30.0938429999999997	31.7082599999999992	4.5688170000000001

Se	20.907554999999986	1.4349909999999999	1.9632449999999999
Se	19.017580999999998	4.2986079999999998	2.4739949999999999
Se	17.5098200000000013	7.1898330000000001	2.4286310000000002
Se	15.8913980000000006	10.0379719999999999	2.4067430000000001
Se	14.2008089999999996	12.8775619999999993	2.4916890000000000
Se	12.4771889999999992	15.7447700000000008	2.6761290000000000
Se	10.8953059999999997	18.8146990000000010	2.4943879999999998
Se	24.7602359999999990	1.5314369999999999	1.5643810000000000
Se	22.8444119999999984	4.4786089999999996	1.4068110000000000
Se	21.2741059999999997	7.4238020000000002	1.4886150000000000
Se	19.6049819999999997	10.2952860000000008	1.4875270000000000
Se	17.9360169999999997	13.1001460000000005	1.5193530000000000
Se	16.2351810000000008	15.9027960000000004	1.5473370000000000
Se	14.6039870000000001	18.9298000000000002	1.7624130000000000
Se	12.8931439999999995	21.9532530000000001	1.5372170000000001
Se	28.1615539999999989	1.6655210000000000	2.5424820000000001
Se	26.1651670000000003	4.6069699999999996	1.8088620000000000
Se	24.6286859999999983	7.4701779999999998	1.8508370000000001
Se	22.9715759999999989	10.3020949999999996	1.9477670000000000
Se	21.3141339999999992	13.1497630000000001	2.0114060000000000
Se	19.6368180000000017	15.9764920000000004	2.0093800000000002
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Se	16.3446700000000007	21.7965349999999987	1.9733590000000001
Se	14.4517199999999999	24.8030359999999988	1.5248050000000000
Se	28.4353400000000001	7.3249290000000000	1.9134690000000001
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Se	24.7977099999999986	13.2097979999999993	1.5278760000000000
Se	23.1195410000000017	16.0547919999999991	1.5521090000000000
Se	21.3706910000000008	18.8870450000000005	1.5390260000000000
Se	19.6993420000000015	21.7626689999999989	1.5071440000000000
Se	17.9027560000000001	24.6511519999999997	1.9925160000000000
Se	16.0657280000000000	27.6483269999999983	1.5909930000000001
Se	30.0013210000000008	10.2553859999999997	2.4003280000000000

Se	28.119586999999992	13.262238000000000	1.730202999999999
Se	26.494270000000000	16.164740999999994	2.041932000000000
Se	24.677098999999983	19.011444000000009	1.671189000000000
Se	23.007594000000010	21.824953000000007	2.008694999999999
Se	21.300115999999992	24.701046999999991	1.534322000000000
Se	19.530485999999998	27.583666999999984	2.162214000000001
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Se	31.999441000000009	13.032982999999998	2.715329000000001
Se	29.983857000000004	16.160471000000011	1.578384000000000
Se	28.203877999999996	18.983945999999995	1.995366999999999
Se	26.379025999999996	21.917611999999983	1.507382000000000
Se	24.589069999999995	24.746023999999985	1.581194000000000
Se	22.879759000000000	27.602302000000017	1.598222000000000
Se	21.220731000000007	30.502452999999992	1.694564000000000
Se	19.448601000000000	33.472526000000020	2.234576000000001
Se	33.594053999999999	15.989511999999995	2.563435000000001
Se	31.589455000000010	19.043098000000005	1.597039000000001
Se	29.740076999999994	21.967126000000004	2.068225000000000
Se	28.016026000000001	24.843506999999989	2.032278999999999
Se	26.315785000000018	27.660506000000016	2.078726000000001
Se	24.662389000000010	30.472643999999990	2.142421000000001
Se	23.007197000000015	33.334184000000005	2.329587000000001
Se	35.275171000000003	19.047167000000017	2.604931999999998
Se	33.087059000000036	22.120547999999994	1.672661000000000
Se	31.493451000000003	25.061450000000007	1.559469000000000
Se	29.869600999999994	27.888026000000000	1.602570000000001
Se	28.216833999999986	30.640784000000000	1.669049000000000
Se	26.492781999999983	33.394184000000028	1.758129000000001
Se	17.669955000000016	34.477392999999993	4.676651999999998
Se	21.398695000000000	34.187835999999972	5.391760999999998
Se	19.182808999999989	37.403027999999991	4.935268999999999
Se	24.655170999999993	34.279409000000011	5.438818999999996
Se	22.919049999999986	37.156424999999987	5.770226000000001

Se	20.8583619999999996	40.1218969999999970	5.1238330000000003
Se	28.4617879999999985	34.5942009999999982	4.4231280000000002
Se	26.6298369999999984	37.3590999999999980	4.7667590000000004
Se	24.7961139999999993	40.1252939999999967	5.1935209999999996
Se	22.8568089999999984	42.6797070000000005	3.1131410000000002
Se	21.3094110000000008	36.2114339999999970	2.0051779999999999
Se	24.7986480000000000	36.2245419999999996	1.9617920000000000
Se	22.9772210000000001	39.0071650000000005	2.0760160000000001

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,261.656\,231\,80$ eV; $E_{rel} = 22.506\,122\,590\,9$ meV/f.u.

W	27.4276629999999990	-0.9654500000000000	3.1514069999999998
W	25.7772779999999990	1.9002939999999999	3.3074550000000000
W	24.2055620000000005	4.6858009999999997	3.3519549999999998
W	22.6335200000000007	7.4597720000000001	3.3389650000000000
W	21.0455739999999984	10.2603039999999996	3.3454320000000002
W	19.4269700000000007	13.0600030000000000	3.3755350000000002
W	17.7953340000000004	15.8504919999999991	3.4158750000000002
W	16.2220839999999988	18.6718159999999997	3.4039290000000002
W	14.6611349999999998	21.6445690000000006	3.3517570000000001
W	28.9810629999999989	1.2006829999999999	3.3950260000000001
W	30.6010199999999983	-1.2231050000000001	3.6294510000000000
W	26.9864330000000017	4.3502980000000004	3.3051710000000001
W	25.4244920000000008	7.1421989999999997	3.2998970000000001
W	23.8268449999999987	9.9512540000000005	3.3099289999999999
W	22.1998980000000010	12.8290430000000004	3.3308430000000002
W	20.5092749999999988	15.6532970000000002	3.3166989999999998
W	18.9538750000000000	18.4384979999999992	3.3397980000000000
W	17.3165650000000007	21.8919589999999999	3.4599609999999998
W	16.1141199999999998	24.516999999999995	3.4093030000000000
W	31.9889480000000006	1.4088449999999999	3.5164700000000000
W	30.9620840000000008	4.6038670000000002	3.5149979999999998
W	29.5210009999999983	7.4298909999999996	3.5128249999999999

W	27.957364999999994	10.3097060000000003	3.5303700000000000
W	26.2898660000000000	13.0303369999999994	3.3982209999999999
W	24.4235149999999983	16.2501500000000014	3.4047909999999999
W	22.9260580000000012	18.9528880000000015	3.5028480000000002
W	21.3162230000000008	21.6502990000000004	3.3843670000000001
W	18.7936930000000011	24.7200780000000009	3.5349640000000000
W	17.6271750000000011	27.3377920000000003	3.4767990000000002
W	33.6011209999999991	4.1129280000000001	3.5230809999999999
W	32.2730389999999971	7.0911160000000004	3.3741240000000001
W	30.7875799999999984	9.8552090000000003	3.3912550000000001
W	29.0217090000000013	13.1275999999999993	3.4160770000000000
W	27.5599530000000001	15.9359040000000007	3.3750670000000000
W	25.9816460000000014	18.6251360000000012	3.4164260000000000
W	24.0758389999999984	21.9260759999999983	3.4884750000000002
W	22.8475339999999996	24.4526679999999992	3.3931890000000000
W	20.3507810000000013	27.5573909999999991	3.5998090000000000
W	19.2022919999999999	30.1191770000000005	3.5108299999999999
W	34.1696979999999968	10.3387899999999995	3.3735560000000002
W	33.0652729999999977	13.0763069999999999	3.3766069999999999
W	30.4780659999999983	15.9395699999999998	3.4001190000000001
W	28.9116299999999988	18.6351510000000005	3.3239339999999999
W	27.4146609999999988	21.2881880000000017	3.4374189999999998
W	25.6020889999999994	24.7584209999999985	3.5646550000000001
W	24.4273489999999995	27.2601720000000007	3.4803020000000000
W	21.9368949999999998	30.3190500000000007	3.6812870000000002
W	35.7149369999999990	13.1206730000000000	3.5299140000000002
W	34.5290910000000011	15.7729440000000007	3.3803990000000002
W	32.8900250000000014	19.1370180000000012	3.4487030000000001
W	31.3320019999999992	21.9161970000000004	3.5099770000000001
W	29.6675080000000015	24.6344500000000011	3.5744919999999998
W	27.2259069999999994	27.6126719999999999	3.7144990000000000
W	25.9733389999999993	30.0553939999999997	3.6571310000000001
W	37.1604049999999972	15.9416869999999999	3.4745520000000001

W	35.606845999999973	18.885661999999999	3.369669000000000
W	34.049948999999980	21.675052999999983	3.344805000000000
W	32.452564000000024	24.408614000000000	3.440064000000000
W	30.813779000000003	27.168769000000011	3.706560000000001
W	28.787019000000008	30.500063000000008	3.994505999999999
W	20.845797000000010	32.891916000000019	3.638875000000001
W	24.021490000000000	33.494433000000008	3.767342999999999
W	22.595558000000005	35.740954999999996	3.884809999999999
W	27.101773999999989	33.191436000000030	3.875961999999999
W	25.531752999999984	35.803919000000005	3.926502000000002
W	24.063690999999986	38.504817000000027	3.925540999999999
Se	28.340523999999985	-2.973015000000002	3.864020000000000
Se	27.070689000000016	0.576783000000000	5.074347999999996
Se	25.446269000000009	3.494460000000001	5.211548999999998
Se	23.837147000000016	6.298112999999999	5.214578000000004
Se	22.235963000000017	9.086940000000002	5.210731000000000
Se	20.647939000000009	11.892573999999998	5.224103000000004
Se	19.029039999999984	14.697497000000003	5.252726000000000
Se	17.451844000000012	17.553689999999996	5.270992999999998
Se	15.906990000000004	20.508268999999985	5.175552999999998
Se	13.658302000000008	23.537244000000012	4.293629000000001
Se	31.428929000000001	-2.940173000000001	4.933174000000002
Se	30.499862000000003	0.510515000000001	5.339710000000002
Se	28.939122000000011	3.452288999999999	4.761922000000002
Se	27.427088000000012	6.364969000000003	4.823160999999998
Se	25.852830000000009	9.199182999999997	4.792818999999997
Se	24.222979999999997	12.038183000000001	4.783464999999996
Se	22.524354999999999	14.974214999999992	4.780717000000001
Se	20.904196999999999	17.775279999999986	4.825891999999996
Se	19.255925000000013	20.651236999999983	4.741412999999997
Se	17.414941999999999	23.557992999999997	5.330441999999997
Se	15.277528999999995	26.574045999999992	4.403076000000004
Se	32.189884999999968	3.223366000000000	5.337938000000003

Se	30.842638000000009	6.291369999999997	5.3496930000000003
Se	29.271280999999983	9.182344000000005	5.3355020000000000
Se	27.630956000000012	12.077761000000006	5.3048929999999999
Se	25.822939000000016	14.903750000000005	5.057363999999997
Se	24.323214000000001	17.847816000000017	5.301542999999997
Se	22.633756000000018	20.739982999999987	5.2943270000000000
Se	20.805073000000001	23.612185000000002	4.8968290000000003
Se	18.977751000000014	26.437760999999983	5.3977380000000004
Se	16.914094999999997	29.500821999999994	4.4828299999999999
Se	34.621031999999996	5.962303999999996	4.5244470000000003
Se	32.706648000000013	9.081576000000001	5.0280849999999999
Se	31.023156000000002	12.073653999999994	4.735204999999997
Se	29.156114999999998	14.944105999999997	5.2196040000000004
Se	27.571574999999993	17.772663000000014	5.2191280000000004
Se	25.844274999999997	20.653219000000000	5.133747999999998
Se	24.266856000000006	23.607638000000015	5.3603399999999999
Se	22.376974000000006	26.466080000000016	4.942809999999997
Se	20.536802000000016	29.297307000000000	5.487345999999996
Se	34.386432999999967	11.950518999999999	5.317867999999998
Se	32.558883000000016	14.989957999999997	4.9261059999999999
Se	30.954229000000015	17.944424999999990	4.854626999999998
Se	29.374264000000002	20.709523000000008	4.8647770000000001
Se	27.601389000000011	23.530508999999986	4.8407220000000004
Se	25.856946000000007	26.441050000000006	5.4554190000000000
Se	23.971154999999995	29.278980000000007	5.0872460000000004
Se	35.971767999999973	14.852406000000002	5.3576969999999999
Se	34.290478999999977	17.798058000000010	5.1027170000000002
Se	32.738143000000009	20.808699000000007	5.3220660000000004
Se	31.051998000000011	23.612200000000014	5.3963520000000003
Se	29.160776999999995	26.448167999999990	5.3193760000000001
Se	27.445709999999983	29.340219999999986	5.6455679999999999
Se	38.001553000000012	17.932704000000011	4.421224999999997
Se	36.424500000000019	20.975075000000004	4.2371730000000003

Se	34.6940290000000005	23.8621370000000006	4.4448949999999998
Se	33.0465269999999975	26.7748640000000009	4.4432309999999999
Se	30.9310820000000000	29.5027690000000007	4.8331549999999996
Se	25.3697909999999993	-0.5649000000000000	2.0904099999999999
Se	23.5766039999999997	2.2873720000000000	2.4388120000000000
Se	22.0165289999999985	5.2054809999999998	2.2828390000000001
Se	20.3768230000000017	8.0512440000000005	2.3388330000000002
Se	18.7352990000000013	10.8729920000000000	2.4053320000000000
Se	17.0762970000000003	13.7101319999999998	2.4370210000000001
Se	15.3794350000000009	16.6034690000000005	2.5762459999999998
Se	13.8336629999999996	19.6665039999999998	2.3804910000000001
Se	29.2267830000000011	-0.5854150000000000	1.5008940000000000
Se	27.4327019999999990	2.4742150000000001	1.6231420000000001
Se	25.6924220000000005	5.4103630000000003	1.4361660000000001
Se	24.1071109999999997	8.2519060000000000	1.4536290000000001
Se	22.5121180000000010	11.1270930000000003	1.4882830000000000
Se	20.8573559999999993	13.9439480000000007	1.4905740000000001
Se	19.1226340000000015	16.7615869999999987	1.4750589999999999
Se	17.5422370000000001	19.8081269999999989	1.7162890000000000
Se	15.8250370000000000	22.8194249999999990	1.5230079999999999
Se	32.5998310000000018	-0.6628270000000001	2.3352400000000002
Se	30.6576039999999992	2.4824489999999999	1.8591670000000000
Se	29.0548089999999988	5.3745380000000003	1.9530430000000001
Se	27.4855620000000016	8.2564779999999995	2.0122220000000000
Se	25.8541750000000015	11.0450529999999993	1.9545509999999999
Se	24.2374499999999991	14.0054979999999993	2.0265200000000001
Se	22.4754879999999986	16.8683559999999986	1.9520780000000000
Se	20.8965950000000014	19.6282719999999991	1.9397570000000000
Se	19.2699199999999990	22.6661539999999988	1.9840240000000000
Se	17.3318820000000002	25.6897379999999984	1.5864460000000000
Se	34.4275719999999978	2.0426899999999999	2.6901850000000000
Se	32.5999120000000033	5.2825639999999998	1.6049240000000000
Se	30.9971379999999996	8.1672309999999992	1.5254500000000000

Se	29.3796910000000011	11.1685250000000007	1.6949500000000000
Se	27.5931269999999991	14.0130060000000007	1.5383190000000000
Se	25.8868140000000011	16.8819340000000011	1.5448370000000000
Se	24.3423480000000012	19.8938309999999987	1.7752720000000000
Se	22.5990600000000015	22.7033050000000003	1.5414610000000000
Se	20.8131880000000002	25.5387169999999983	2.0646550000000001
Se	18.8866990000000001	28.4937560000000012	1.6437630000000001
Se	34.5259890000000027	8.1812629999999995	2.2793809999999999
Se	32.6081190000000021	11.0956229999999998	1.7349500000000000
Se	31.0455550000000002	14.0197120000000002	1.9061269999999999
Se	29.1732750000000003	16.8697160000000004	1.5205620000000000
Se	27.4994979999999991	19.7032389999999999	1.5304819999999999
Se	25.9764319999999991	22.7780260000000006	1.9136100000000000
Se	24.1825609999999998	25.6054710000000014	1.5979120000000000
Se	22.4023380000000003	28.3790419999999983	2.1231710000000001
Se	20.5442110000000007	31.2834059999999994	1.7282270000000000
Se	36.5346959999999967	10.8969869999999993	2.7587940000000000
Se	34.4912020000000012	13.9995720000000006	1.5321659999999999
Se	32.5666760000000011	16.9292450000000017	2.0684680000000002
Se	30.9076799999999992	19.8255279999999985	1.9788250000000001
Se	29.3008370000000014	22.6418959999999991	2.0202160000000000
Se	27.6680549999999990	25.6253409999999988	2.1680100000000002
Se	25.8229350000000011	28.4629200000000004	1.7449250000000001
Se	24.0124950000000013	31.2714029999999994	2.3620800000000002
Se	38.1259999999999977	13.9826029999999992	2.5984280000000002
Se	35.9607000000000028	17.0591949999999990	1.6064929999999999
Se	34.3717680000000030	19.9855419999999988	1.4915950000000000
Se	32.7807540000000017	22.8374179999999996	1.5306700000000000
Se	31.1122620000000012	25.6834670000000003	1.6900340000000000
Se	29.2526410000000006	28.6364850000000004	2.2425700000000002
Se	27.4526299999999992	31.4360129999999991	2.0529030000000001
Se	18.5485210000000009	32.4490559999999988	4.3773619999999998
Se	22.3646129999999985	32.1785959999999989	5.3915519999999999

Se	20.3521420000000006	35.2395160000000018	4.7269709999999998
Se	25.6157269999999997	32.1288630000000026	5.3875770000000003
Se	24.0677500000000002	35.0832669999999993	5.7785010000000003
Se	22.1299489999999999	38.0262430000000009	5.1754009999999999
Se	29.4766109999999983	32.6602699999999970	4.7637939999999999
Se	27.7780340000000017	35.3559180000000026	4.8727039999999997
Se	26.0548310000000001	38.0734489999999965	5.1264349999999999
Se	24.0352169999999994	40.6332570000000004	3.1343030000000001
Se	22.2454719999999995	34.1303529999999995	1.9545319999999999
Se	25.7561180000000007	34.1721110000000010	1.9956460000000000
Se	24.0129309999999982	36.9513609999999986	2.0683569999999998

$\mathbf{W}_{66}\mathbf{Se}_{132}$; $E_{tot} = -38\,662\,262.737\,404\,66$ eV; $E_{rel} = 6.124\,715\,621\,2$ meV/f.u.

W	28.0058310000000006	4.1222490000000001	3.4420999999999999
W	26.2151810000000012	6.8279790000000000	3.3797229999999998
W	24.5276350000000001	9.6018279999999994	3.3114789999999998
W	22.8938549999999985	12.4191830000000003	3.2756090000000002
W	21.2704139999999988	15.2295949999999998	3.2712880000000002
W	19.6523220000000016	18.0369840000000003	3.2898149999999999
W	18.0563700000000011	20.8507409999999993	3.3278249999999998
W	16.5073960000000000	23.6660980000000016	3.3517589999999999
W	14.9802190000000000	26.5089019999999991	3.2248420000000002
W	13.4038989999999991	29.4519300000000008	2.9156659999999999
W	11.7572639999999993	32.1034369999999996	2.8458049999999999
W	31.3317750000000004	4.0257680000000002	3.5137149999999999
W	29.0974649999999997	6.5496990000000004	3.3529320000000000
W	27.4101420000000005	9.2337769999999999	3.2872309999999998
W	25.7459869999999995	12.0453189999999992	3.2656849999999999
W	24.0983429999999998	14.8874849999999999	3.2606370000000000
W	22.4664399999999986	17.7149970000000003	3.2745769999999998
W	20.8455219999999990	20.5384869999999999	3.2976909999999999
W	19.2511000000000010	23.3578940000000017	3.3102230000000001

W	17.731076999999991	26.171611999999997	3.2719779999999998
W	16.0900350000000003	29.571878999999991	3.1714509999999998
W	14.8529780000000002	31.967117999999993	3.0145940000000002
W	34.4975730000000027	4.0224419999999999	3.5741730000000000
W	33.0291580000000025	6.5624870000000000	3.5010770000000000
W	31.3089210000000016	9.8429359999999999	3.5096550000000000
W	29.7188690000000015	12.5817359999999994	3.5035280000000002
W	28.1015230000000003	15.3562550000000009	3.4863700000000000
W	26.4872039999999984	18.1631500000000017	3.4913919999999998
W	24.8718010000000014	20.9596939999999989	3.4985770000000000
W	23.2539569999999998	23.7515619999999998	3.5152040000000002
W	21.6665670000000006	26.6569879999999984	3.5399140000000000
W	20.0158600000000000	29.5265860000000018	3.3800780000000001
W	18.1086759999999991	32.0560059999999964	3.2131390000000000
W	37.6514840000000035	3.9959050000000000	3.7004510000000002
W	35.7445439999999977	6.5249240000000004	3.5334129999999999
W	34.0936599999999999	9.3948359999999997	3.3735170000000001
W	32.5065659999999994	12.3001240000000003	3.3980969999999999
W	30.8887679999999989	15.0921029999999998	3.4144489999999998
W	29.2733770000000000	17.8887180000000008	3.4214940000000000
W	27.6590880000000006	20.6955479999999987	3.4264380000000001
W	26.0416290000000004	23.4701020000000007	3.4095309999999999
W	24.4516060000000017	26.2087159999999990	3.4037419999999998
W	22.7310979999999994	29.4892189999999985	3.4123999999999999
W	21.2626239999999989	32.0292900000000031	3.3396810000000001
W	40.9073750000000018	4.0845750000000001	3.8983850000000002
W	39.6701490000000021	6.4799199999999999	3.7413820000000002
W	38.0294310000000024	9.8801179999999995	3.6415929999999999
W	36.5094289999999972	12.6939279999999997	3.6032169999999999
W	34.9150440000000017	15.5130490000000005	3.6155070000000000
W	33.2941270000000031	18.3367700000000013	3.6383320000000001
W	31.6621559999999995	21.1643690000000007	3.6522670000000002
W	30.0145179999999989	24.0064430000000009	3.6472680000000000

W	28.3502189999999992	26.8180030000000009	3.6258840000000001
W	26.6631309999999999	29.5019419999999997	3.5602659999999999
W	24.4283989999999989	32.0260450000000034	3.3998539999999999
W	44.0024560000000022	3.9483169999999999	4.0668080000000000
W	42.3564950000000024	6.5994529999999996	3.9971869999999998
W	40.7798149999999993	9.5428599999999992	3.6882799999999998
W	39.2532769999999971	12.3854290000000002	3.5614040000000000
W	37.7043299999999988	15.2007530000000006	3.5853519999999999
W	36.1083569999999980	18.0147650000000006	3.6233930000000001
W	34.4900599999999997	20.8222899999999989	3.6417679999999999
W	32.8666679999999971	23.6325499999999984	3.6371970000000000
W	31.2327389999999987	26.4501090000000012	3.6013050000000000
W	29.5453079999999986	29.2236750000000001	3.5331830000000002
W	27.7544830000000005	31.9294639999999994	3.4709669999999999
Se	29.3532609999999998	2.4062310000000000	4.3936900000000003
Se	27.5243929999999999	5.7037409999999999	5.2722550000000004
Se	25.7937179999999984	8.4764029999999995	5.1983899999999998
Se	24.1242570000000001	11.2489369999999997	5.1501929999999998
Se	22.4874560000000017	14.0434509999999992	5.1386500000000002
Se	20.8595180000000013	16.8397240000000004	5.1499300000000003
Se	19.2489729999999994	19.6440459999999995	5.1796300000000004
Se	17.6741600000000005	22.4802450000000000	5.2120030000000002
Se	16.1391269999999984	25.3929639999999992	5.1609600000000002
Se	14.5705770000000001	28.3633999999999986	4.9029040000000004
Se	13.0140870000000000	31.3004290000000012	4.7608189999999997
Se	32.7489139999999992	2.2652230000000002	4.3290639999999998
Se	31.0441360000000017	5.7854900000000002	5.0775470000000000
Se	29.3699720000000006	8.6165959999999995	4.8711409999999997
Se	27.7273749999999986	11.3764550000000000	4.7862320000000000
Se	26.0917069999999995	14.1777080000000009	4.7624449999999996
Se	24.4671759999999985	16.9900699999999993	4.7708899999999996
Se	22.8464390000000002	19.8046399999999991	4.7890530000000000
Se	21.2217440000000011	22.6308879999999988	4.8226310000000003

Se	19.622357999999984	25.4846730000000008	4.8295480000000000
Se	17.959351999999991	28.411753999999984	4.6219299999999999
Se	16.366192999999991	31.4393120000000010	4.9597110000000004
Se	36.0479010000000031	2.2840460000000000	4.4966600000000003
Se	34.3551980000000015	5.5991920000000004	5.4694940000000001
Se	32.686075999999999	8.5211240000000004	5.2177100000000003
Se	31.0795670000000008	11.486948999999992	5.3714050000000002
Se	29.420284999999998	14.2632420000000000	5.3478669999999999
Se	27.7932580000000016	17.044959999999997	5.3390730000000000
Se	26.1778620000000011	19.8481230000000011	5.3478300000000001
Se	24.570817999999992	22.6558050000000009	5.3542779999999999
Se	22.9720270000000006	25.5009550000000011	5.3527600000000000
Se	21.284870999999990	28.435380999999996	5.2733949999999998
Se	19.573841999999991	31.372659999999998	5.1256389999999996
Se	39.319324999999992	2.3387639999999998	4.6604169999999998
Se	37.616931999999985	5.7802410000000002	5.2802829999999998
Se	36.0604680000000002	8.6478880000000000	4.9812390000000004
Se	34.515366999999977	11.494996999999997	4.8740459999999999
Se	32.9058890000000019	14.3688070000000003	4.9329900000000002
Se	31.2832860000000004	17.1826140000000009	4.9470900000000002
Se	29.657575999999988	19.9932200000000009	4.9525880000000004
Se	28.0186390000000003	22.8136140000000012	4.9516970000000002
Se	26.378748999999991	25.601151999999990	4.9620480000000002
Se	24.6541460000000008	28.416461999999992	4.8292359999999999
Se	22.8693770000000001	31.370332999999987	5.2203520000000001
Se	42.5484000000000009	2.4751949999999998	5.1978410000000004
Se	40.948583999999968	5.6662850000000002	5.8062760000000004
Se	39.349626999999981	8.559015999999997	5.3874529999999998
Se	37.8342140000000029	11.566167999999993	5.4845689999999996
Se	36.2335720000000023	14.378494999999991	5.4595719999999996
Se	34.618550999999965	17.2015600000000006	5.4770640000000004
Se	32.989382999999966	20.0336970000000001	5.4952959999999997
Se	31.3536380000000001	22.8794760000000004	5.4919900000000004

Se	29.726130999999987	25.735941000000004	5.4746319999999997
Se	28.050871000000008	28.577659000000006	5.4399709999999999
Se	26.115293999999987	31.401710999999988	5.251598000000004
Se	45.873784999999980	2.860654999999999	3.3809079999999998
Se	44.524532999999981	5.844574999999999	5.352762000000002
Se	43.077446000000019	8.757771999999992	4.807065999999998
Se	41.593786000000015	11.684241999999994	4.477599999999998
Se	39.961705999999995	14.563219999999994	4.583490000000003
Se	38.345753999999995	17.440857000000012	4.610649999999997
Se	36.710557000000014	20.299931999999983	4.635048000000003
Se	35.066383999999993	23.154018000000007	4.636914000000000
Se	33.424473999999965	26.026371999999985	4.585340999999997
Se	31.736391999999986	28.921203999999995	4.502690000000003
Se	29.869738999999992	31.860513000000010	4.457865000000000
Se	25.890505999999985	4.191009000000002	2.454940999999998
Se	24.023993999999983	7.130465000000001	2.410178000000002
Se	22.335848999999996	10.025311000000003	2.327553000000000
Se	20.694088000000007	12.897755999999993	2.276139000000001
Se	19.049945000000010	15.751901000000002	2.278176000000002
Se	17.414782999999999	18.610766999999992	2.302636999999998
Se	15.798731000000001	21.488248999999997	2.329854999999998
Se	14.166624999999998	24.367374000000016	2.435480000000001
Se	12.683329999999998	27.293537000000006	2.105672000000002
Se	11.236046000000000	30.207119999999997	1.559665000000001
Se	9.886765000000005	33.190618000000006	3.531184999999998
Se	29.645119000000011	4.650006999999996	1.661540999999999
Se	27.709664000000001	7.474058999999996	1.473179000000000
Se	26.034352999999994	10.315799999999994	1.438360000000001
Se	24.406895999999997	13.172257999999994	1.420956000000001
Se	22.771129999999994	16.018135999999984	1.417629999999999
Se	21.141991000000009	18.850197000000014	1.435940999999999
Se	19.526952000000014	21.673234000000008	1.453673000000000
Se	17.926292000000001	24.485410000000017	1.428652000000000

Se	16.410844999999984	27.492487000000006	1.5257970000000001
Se	14.811949000000003	30.385146999999999	1.1067330000000000
Se	13.211809999999998	33.576233000000020	1.7148939999999999
Se	32.890934999999989	4.681331000000001	1.6930339999999999
Se	31.106351000000001	7.635324999999999	2.083956999999998
Se	29.382006000000005	10.450582000000007	1.9509730000000001
Se	27.741993999999983	13.238160999999998	1.9612480000000001
Se	26.102942999999998	16.058567000000000	1.9603200000000001
Se	24.477109999999997	18.869136999999985	1.9658599999999999
Se	22.854531999999990	21.682974000000015	1.9801650000000000
Se	21.245414000000002	24.556893999999998	2.0390250000000001
Se	19.700213000000015	27.403867000000018	1.9318949999999999
Se	18.143446000000009	30.271426000000017	1.6331410000000000
Se	16.441216000000007	33.712645000000020	2.2532429999999999
Se	36.186146000000008	4.678835000000003	1.7879550000000000
Se	34.475557999999995	7.616209999999997	1.6400840000000001
Se	32.788485000000014	10.550781999999999	1.5603370000000001
Se	31.189748000000016	13.395886000000008	1.5588409999999999
Se	29.582699000000016	16.203611999999997	1.5651219999999999
Se	27.967212000000000	19.006865999999987	1.5738319999999999
Se	26.340196999999999	21.788609000000010	1.5650729999999999
Se	24.680910000000008	24.564852999999994	1.5416209999999999
Se	23.074184999999999	27.530698000000010	1.6956389999999999
Se	21.405122999999997	30.452628000000007	1.4440759999999999
Se	19.712184000000006	33.767786999999984	2.4170129999999999
Se	39.393686999999999	4.612238999999998	1.9536230000000001
Se	37.800845999999999	7.640204999999999	2.2915540000000001
Se	36.138125000000023	10.567047000000005	2.083956999999998
Se	34.538894999999966	13.420690000000005	2.0905640000000001
Se	32.914214000000012	16.247036000000014	2.1239870000000001
Se	31.293348999999992	19.061679000000016	2.141995999999998
Se	29.668762999999984	21.874068999999987	2.1505350000000001
Se	28.033028999999991	24.675357999999992	2.1268490000000000

Se	26.390350999999990	27.435100999999995	2.041948999999998
Se	24.716090000000012	30.266284999999999	1.835723999999999
Se	23.011285999999984	33.786420999999972	2.584652000000002
Se	42.746256000000025	4.750848000000004	2.151332000000000
Se	41.189402999999987	7.688170000000004	2.010002000000001
Se	39.621586000000006	10.658687000000005	1.752162999999999
Se	38.086505000000025	13.571453999999992	1.701095999999999
Se	36.511690999999990	16.407578000000009	1.733617000000000
Se	34.901097000000000	19.212019000000015	1.763142999999999
Se	33.273119999999987	22.008303000000015	1.774215000000001
Se	31.636215000000000	24.802825999999996	1.762632999999999
Se	29.966658999999999	27.575302000000006	1.714356999999999
Se	28.235834000000005	30.348037999999990	1.640679000000000
Se	26.406952000000004	33.645363000000032	2.519725000000002

W₆₆Se₁₃₂; $E_{tot} = -38\,662\,263.141\,635\,89$ eV; $E_{rel} = 0$ meV/f.u.

W	19.809145999999984	1.137761000000000	3.421914000000001
W	18.011639999999999	3.962508000000001	3.578501999999998
W	16.408463000000011	6.690396999999999	3.690869000000002
W	14.842736000000004	9.443554999999999	3.618471000000000
W	13.285821999999996	12.424398999999993	3.493113000000001
W	23.009301000000007	1.003946999999999	3.290452999999999
W	21.244855999999986	3.344438999999999	3.474232000000002
W	19.156023999999986	6.422799000000004	3.483639999999998
W	17.560175000000010	9.198389000000006	3.502057000000002
W	15.930203999999998	12.647792000000008	3.553828999999999
W	14.755877999999992	15.303699999999992	3.420097000000002
W	26.246448999999984	1.024850000000000	3.208224000000000
W	24.294314000000000	3.314347999999998	3.429275000000001
W	23.160077000000011	6.844720999999998	3.438253000000000
W	21.578638000000015	9.634392000000001	3.590695000000002
W	19.917405999999997	12.411865999999998	3.442057000000001

W	17.4242670000000004	15.4325250000000000	3.5190139999999999
W	16.3337490000000010	18.0914830000000002	3.3361000000000001
W	29.4937630000000013	1.0099030000000000	3.3133859999999999
W	28.1966350000000006	3.3125710000000002	3.4387919999999998
W	26.2544350000000009	6.8711630000000001	3.3395950000000001
W	24.4245759999999983	9.2499179999999992	3.4310510000000001
W	22.6924370000000017	12.5324559999999998	3.4480590000000002
W	21.4627659999999985	15.1483170000000005	3.3451890000000000
W	19.0413220000000010	18.1954290000000007	3.4821700000000000
W	18.0327839999999995	20.8498729999999988	3.3270179999999998
W	32.6896589999999989	1.1394299999999999	3.4562029999999999
W	31.2583559999999991	3.3446899999999999	3.4927139999999999
W	29.3663200000000018	6.8678390000000000	3.4709850000000002
W	28.2694159999999997	9.3752230000000001	3.3537089999999998
W	25.7100159999999995	12.3472399999999993	3.4221949999999999
W	24.2296340000000008	15.0972729999999995	3.3858750000000000
W	23.1143590000000003	17.8949500000000015	3.3489990000000001
W	21.1238980000000005	21.4169650000000011	3.5091489999999999
W	19.7455019999999983	23.6851969999999987	3.4722840000000001
W	34.4834620000000029	3.9581209999999998	3.6040920000000001
W	33.3745770000000022	6.4576630000000002	3.4893960000000002
W	30.9862940000000009	9.6394690000000001	3.5721370000000001
W	29.8012149999999991	12.2674240000000001	3.4205880000000000
W	28.2732859999999988	15.2473060000000000	3.4640409999999999
W	26.2127109999999988	18.4101709999999983	3.4218690000000000
W	24.6176950000000012	20.6397879999999994	3.5044460000000002
W	22.6240340000000018	24.0768939999999994	3.5494479999999999
W	21.4732720000000015	26.5127200000000016	3.4693360000000002
W	36.1197179999999989	6.6809560000000001	3.6618629999999999
W	35.0126100000000022	9.2533499999999993	3.4545129999999999
W	32.5455460000000016	12.3786149999999999	3.5021100000000001
W	30.9997399999999992	15.1343560000000004	3.3708680000000002
W	29.3931649999999998	17.8484830000000017	3.3280110000000001

W	27.8078210000000006	20.6582650000000001	3.5351309999999998
W	26.3728699999999989	24.2960889999999985	3.4977680000000002
W	24.7851640000000017	26.5180250000000015	3.6118899999999998
W	37.6861969999999999	9.4094080000000009	3.6070570000000002
W	36.5409140000000008	12.0546659999999992	3.4486110000000001
W	34.9503180000000029	15.5273889999999994	3.4990410000000001
W	33.4055359999999979	18.3444550000000000	3.5027110000000001
W	31.7796319999999994	21.1247499999999988	3.4959050000000000
W	29.5725429999999996	24.3033460000000012	3.4762870000000001
W	27.9335500000000003	26.5495120000000000	3.6356090000000001
W	39.1963459999999984	12.2496340000000004	3.5447419999999998
W	37.6858209999999971	15.2500110000000006	3.4322339999999998
W	36.1459230000000034	18.0660230000000013	3.3831859999999998
W	34.5527689999999978	20.8298950000000005	3.3965800000000002
W	33.0555930000000018	23.6485920000000007	3.4312920000000000
W	31.0223149999999990	26.6101269999999985	3.4124669999999999
W	34.2105540000000019	26.7098149999999990	3.1175489999999999
Se	21.0687269999999991	-0.6583720000000000	4.2789409999999997
Se	19.4651320000000005	2.7352710000000000	5.2953049999999999
Se	17.7567969999999988	5.5709559999999998	5.4862109999999999
Se	16.1253400000000013	8.4059489999999997	5.5035369999999997
Se	14.5439670000000003	11.3314330000000005	5.3387070000000003
Se	12.3201839999999994	14.3678550000000005	4.3804740000000004
Se	24.5920220000000000	-0.7299780000000000	4.0709920000000004
Se	22.8377219999999994	2.4999500000000001	5.2873409999999996
Se	21.2494459999999989	5.5943949999999996	4.8230760000000004
Se	19.5709640000000000	8.5089500000000005	4.9683940000000000
Se	17.8778560000000013	11.4339969999999997	4.8478930000000000
Se	16.0434850000000004	14.3864900000000002	5.3664170000000002
Se	14.0030750000000008	17.4386119999999991	4.3468689999999999
Se	27.9082270000000001	-0.7275779999999999	4.0778960000000000
Se	26.2427729999999997	2.6161070000000000	5.0386480000000002
Se	24.6092380000000013	5.5089370000000004	4.9519390000000003

Se	22.9313210000000005	8.4316680000000002	5.3613689999999998
Se	21.2029339999999991	11.4380260000000007	5.3259650000000001
Se	19.4334840000000000	14.3864269999999994	4.9139070000000000
Se	17.6291809999999991	17.2630000000000017	5.3255840000000001
Se	15.7067650000000008	20.3978649999999995	4.1464059999999998
Se	31.4266809999999985	-0.6465490000000000	4.3272990000000000
Se	29.6515869999999993	2.5190329999999999	5.3058829999999997
Se	27.8969400000000007	5.5162839999999997	4.9464940000000004
Se	26.2972420000000007	8.5823260000000001	5.1084690000000004
Se	24.3643420000000006	11.3383289999999999	5.1425549999999998
Se	22.8264670000000010	14.2815700000000003	5.3120940000000001
Se	21.0971800000000016	17.1831700000000005	4.8708340000000003
Se	19.4869449999999986	20.1224249999999998	5.1369829999999999
Se	17.4610869999999991	23.2152969999999996	4.2554360000000004
Se	33.0307889999999986	2.7455650000000000	5.3252720000000000
Se	31.2701099999999990	5.6096370000000002	4.8275249999999996
Se	29.6088629999999995	8.4879300000000004	5.3565160000000001
Se	27.7673920000000010	11.4183450000000004	4.8542639999999997
Se	26.2460659999999990	14.2856529999999999	4.8932349999999998
Se	24.6331379999999989	17.0704250000000002	5.0918109999999999
Se	22.8165230000000001	19.9922250000000012	5.0469600000000003
Se	21.2157470000000004	23.0520950000000013	5.4125819999999996
Se	34.7822019999999981	5.5737209999999999	5.4860860000000002
Se	32.9645319999999984	8.5217919999999996	4.9584320000000002
Se	31.2231220000000000	11.3877109999999995	5.3827449999999999
Se	29.6348069999999986	14.1984290000000009	5.2686279999999996
Se	27.8905299999999983	17.1467959999999984	5.1469240000000003
Se	26.2445680000000010	20.0675980000000003	5.3795900000000003
Se	24.5976199999999992	22.9300210000000000	4.8531129999999996
Se	36.4201869999999985	8.3660309999999996	5.4776590000000001
Se	34.5640819999999991	11.3547419999999999	4.9435159999999998
Se	33.0088009999999983	14.3920270000000006	4.9430660000000000
Se	31.3924440000000011	17.2174739999999993	4.8518829999999999

Se	29.7951240000000013	20.0021139999999988	4.9038000000000004
Se	27.9766109999999983	22.9175220000000017	4.9862719999999996
Se	38.0160490000000024	11.1726019999999995	5.4211749999999999
Se	36.3497180000000029	14.1817100000000007	5.1498189999999999
Se	34.7883640000000014	17.2380749999999985	5.3439329999999998
Se	33.1390540000000016	20.0901400000000017	5.3462350000000001
Se	31.3362049999999996	23.0080880000000008	5.1097219999999997
Se	40.0718900000000033	14.2456169999999993	4.4407300000000003
Se	38.5379709999999989	17.3314599999999999	4.2465159999999997
Se	36.8517429999999990	20.2330240000000003	4.3807890000000000
Se	35.1011260000000007	23.0267799999999987	4.6032620000000000
Se	17.6321559999999984	1.4188769999999999	2.5413160000000001
Se	15.7552090000000007	4.3462519999999998	2.7791120000000000
Se	14.0408700000000000	7.3095270000000001	2.8121939999999999
Se	12.4510780000000008	10.3961679999999994	2.6134800000000000
Se	21.3050950000000014	1.6126450000000001	1.5050559999999999
Se	19.5564250000000008	4.5698030000000003	1.7943460000000000
Se	17.7092820000000017	7.4532559999999997	1.6627760000000000
Se	16.1312749999999987	10.5129020000000004	1.8642490000000000
Se	14.4229160000000007	13.5345119999999994	1.6048680000000000
Se	24.5936659999999989	1.6555460000000000	1.4438650000000000
Se	22.8669189999999993	4.6639739999999996	1.8807990000000001
Se	21.1009110000000000	7.5608849999999999	2.0608499999999998
Se	19.5007190000000001	10.3412400000000009	2.0525060000000002
Se	17.8633430000000004	13.3739539999999995	2.0145200000000001
Se	15.9980910000000005	16.3772710000000004	1.5366599999999999
Se	27.9180039999999998	1.6468050000000001	1.4555709999999999
Se	26.2476090000000006	4.5553540000000003	2.1454029999999999
Se	24.5707479999999983	7.5680829999999997	1.5184260000000001
Se	22.9383669999999995	10.4885549999999999	1.7373120000000000
Se	21.1586290000000012	13.3512909999999998	1.5301659999999999
Se	19.4487249999999996	16.2207149999999984	1.9682990000000000
Se	17.6798870000000008	19.1692730000000005	1.5042120000000001

Se	31.202600000000003	1.6072190000000000	1.5305780000000000
Se	29.628040999999996	4.6736149999999999	1.9073570000000000
Se	27.924269999999999	7.5977660000000000	1.5435490000000001
Se	26.2896779999999985	10.3843920000000001	1.9346840000000001
Se	24.4061610000000009	13.3339719999999993	1.5709050000000000
Se	22.8632470000000012	16.2090350000000001	1.5173049999999999
Se	21.1229849999999999	19.1471049999999998	2.1713600000000000
Se	19.4559280000000001	21.991749999999997	1.5969949999999999
Se	34.8727269999999976	1.4083270000000001	2.5868630000000001
Se	32.9412170000000017	4.5747229999999997	1.8242620000000001
Se	31.4175100000000000	7.5475190000000003	2.0506709999999999
Se	29.6512519999999995	10.4800789999999999	1.5852530000000000
Se	27.8018800000000006	13.2527059999999999	1.9774529999999999
Se	26.2346320000000013	16.1688229999999997	2.0743190000000000
Se	24.5533530000000013	19.0407919999999997	1.5776859999999999
Se	22.9494800000000012	22.0142060000000015	1.9312270000000000
Se	21.0202460000000002	24.9034820000000003	1.6547069999999999
Se	36.7375129999999999	4.3081800000000001	2.7874310000000002
Se	34.7918000000000021	7.4556860000000000	1.6571860000000000
Se	33.0302470000000028	10.3642380000000003	2.0383369999999998
Se	31.2465219999999988	13.3232119999999998	1.5841149999999999
Se	29.6068779999999983	16.1382159999999999	1.4992920000000001
Se	27.9241039999999998	19.0526939999999989	1.6085220000000000
Se	26.3181720000000006	22.0680830000000014	2.0614949999999999
Se	24.5141090000000013	24.8765210000000003	1.8376500000000000
Se	38.4026330000000016	7.2635009999999998	2.6179600000000001
Se	36.4178659999999965	10.3290880000000005	1.6359790000000001
Se	34.6286569999999969	13.3049750000000007	2.1324160000000001
Se	33.0082540000000009	16.2394570000000016	1.9973920000000001
Se	31.3874980000000008	19.0627390000000005	2.0006240000000002
Se	29.6884200000000007	21.9868859999999984	2.1578580000000001
Se	27.9573159999999987	24.9766830000000013	1.6459600000000001
Se	40.1284109999999998	10.2885050000000007	2.6507489999999998

Se	37.968533999999982	13.3699320000000004	1.6982770000000000
Se	36.4665570000000017	16.3445770000000010	1.5496570000000001
Se	34.9197330000000008	19.1907309999999995	1.5282199999999999
Se	33.2519920000000013	21.9630089999999996	1.5653390000000000
Se	31.3577049999999993	24.8405510000000014	1.7420420000000001
Se	19.4949450000000013	25.8868240000000007	4.9705560000000002
Se	23.0239310000000010	25.9275820000000010	5.3515980000000001
Se	22.8774450000000016	28.1672030000000007	2.5395569999999998
Se	26.3441469999999995	25.9541080000000015	5.4920030000000004
Se	26.2119460000000011	28.2825969999999991	2.7628270000000001
Se	29.6154539999999997	26.0600050000000003	5.4192039999999997
Se	32.9583060000000003	25.8597919999999988	5.0110869999999998
Se	32.6873300000000029	28.2101900000000008	2.1172740000000001
Se	34.7973270000000028	24.9671389999999995	1.6685470000000000
Se	29.4861269999999998	28.2759730000000005	2.5542400000000001
Se	36.0260450000000034	27.8667909999999992	3.8123010000000002
Se	19.1613830000000007	27.5240259999999992	3.2586260000000000

$W_{105}Se_{210}$; $E_{tot} = -61\,508\,146.516\,497\,63$ eV; $E_{rel} = 41.505\,328\,485\,7$ meV/f.u.

W	21.3106919999999995	-1.1064980000000000	3.3699330000000001
W	19.4448380000000007	1.7124820000000001	3.4306299999999998
W	17.7876800000000017	4.4993119999999998	3.4466640000000002
W	16.1358619999999995	7.2587590000000004	3.3906969999999998
W	14.4590519999999998	10.0176920000000003	3.3454410000000001
W	12.8326630000000002	12.7964230000000008	3.3029620000000000
W	11.1786949999999994	15.5890299999999993	3.1460129999999999
W	9.2037479999999992	18.9401609999999998	3.0735749999999999
W	7.6332769999999996	21.9101670000000013	3.3830909999999998
W	6.1352219999999997	24.7211369999999988	3.5319880000000001
W	4.5862449999999999	27.4966860000000004	3.5136949999999998
W	3.0253030000000001	30.4410789999999984	3.4616609999999999
W	24.5360399999999998	-1.2264320000000000	3.4423550000000001

W	22.829156999999986	1.0808240000000000	3.4778970000000000
W	20.5809390000000000	4.2000609999999998	3.3331330000000001
W	18.9392819999999986	7.0024009999999999	3.3516629999999998
W	17.2129699999999985	9.8109160000000006	3.3017249999999998
W	15.5570450000000005	12.5903360000000006	3.2475200000000002
W	13.9706279999999996	15.3590280000000003	3.2089590000000001
W	12.4340550000000007	18.9221590000000006	3.1886880000000000
W	10.8547390000000004	21.1986729999999994	3.3406110000000000
W	8.8981499999999993	24.6025230000000015	3.4002379999999999
W	7.4614770000000004	27.1828250000000011	3.4397470000000001
W	5.6457030000000001	30.5813519999999990	3.4870220000000001
W	4.5251500000000000	33.2727059999999994	3.3626239999999998
W	27.7565249999999999	-1.2813760000000001	3.5469550000000001
W	29.2294429999999998	1.0319300000000000	3.6096910000000002
W	26.0299849999999999	1.0216920000000000	3.5454810000000001
W	24.5406189999999995	4.6939390000000003	3.3696500000000000
W	23.0748549999999994	7.1643179999999997	3.4453350000000000
W	21.1508530000000015	10.4741999999999997	3.4511250000000002
W	19.5981130000000014	13.1153809999999993	3.4823710000000001
W	18.0115380000000016	15.7820350000000005	3.3246929999999999
W	15.6518020000000000	19.0174750000000010	3.2620830000000001
W	13.9647070000000006	21.2097979999999993	3.3787660000000002
W	12.7412650000000003	24.8323059999999991	3.3249190000000000
W	10.5650689999999994	27.2434699999999985	3.4049820000000000
W	9.6364950000000000	30.3787519999999986	3.3808790000000002
W	7.1845400000000001	33.1902929999999969	3.4452919999999998
W	6.1381589999999999	36.0519419999999968	3.3616860000000002
W	30.9843809999999991	-1.2677410000000000	3.5654119999999998
W	27.7391560000000013	4.7013809999999996	3.3592580000000001
W	26.1593599999999995	6.9785089999999999	3.4722240000000002
W	24.2634919999999994	10.3008900000000008	3.4294840000000000
W	22.5469979999999985	13.0713190000000008	3.4721050000000000
W	21.0696310000000011	15.7174490000000002	3.4225870000000000

W	19.382266999999988	18.9376040000000003	3.3922110000000001
W	17.821913999999996	21.538171999999994	3.4037590000000000
W	15.8927390000000006	24.7793370000000017	3.3696419999999998
W	14.339465999999998	27.074998999999983	3.4913319999999999
W	12.3632340000000003	30.5701280000000004	3.4721540000000002
W	9.1923490000000001	36.5439190000000025	3.5057079999999998
W	11.2355400000000005	33.0681810000000027	3.3805740000000002
W	7.7881210000000003	38.9017440000000008	3.5054660000000002
W	34.376775999999996	-1.2737120000000000	3.7001260000000000
W	36.178159999999983	1.4170689999999999	3.7363189999999999
W	32.3375830000000022	1.0717200000000000	3.6422070000000000
W	30.972640999999994	4.7237349999999996	3.4446970000000001
W	29.3617990000000013	6.9556889999999996	3.5464519999999999
W	27.2158820000000006	10.1832419999999999	3.4589059999999998
W	25.7375860000000003	12.6957760000000004	3.4707270000000001
W	23.8636130000000009	15.8394440000000003	3.4579490000000002
W	22.212976999999986	18.5833620000000010	3.3344740000000002
W	20.5996670000000002	21.4119230000000016	3.3414860000000002
W	18.953307999999998	24.1772740000000006	3.3467539999999998
W	17.4691180000000017	27.0095080000000003	3.5048789999999999
W	16.2101970000000009	30.696729999999987	3.4566759999999999
W	13.999072999999992	33.182468999999975	3.5371579999999998
W	12.9978660000000001	35.867959999999965	3.3637100000000002
W	10.600602999999996	38.9428100000000015	3.6004320000000001
W	9.507564999999996	41.6170090000000030	3.6611669999999998
W	37.434480999999981	-1.2740270000000000	3.9150689999999999
W	34.174098999999982	4.7194019999999997	3.6318429999999999
W	32.646287999999984	6.9963949999999997	3.6989160000000001
W	31.2080410000000015	10.5826080000000005	3.6273200000000001
W	29.661709999999994	13.3650640000000003	3.6192240000000000
W	27.949813999999999	16.147120999999985	3.5829249999999999
W	26.285288999999988	19.0138980000000011	3.5815750000000000
W	24.6335790000000010	21.830595999999999	3.5619350000000001

W	23.002787999999989	24.638642999999983	3.577554999999998
W	21.380845000000008	27.422157999999996	3.582622000000002
W	19.347263000000017	30.649056999999991	3.537970000000001
W	15.871045999999998	36.364966000000026	3.639600999999999
W	17.845418999999997	32.940089999999979	3.622431000000002
W	14.615605999999997	38.741176000000029	3.592979000000001
W	12.702906000000005	42.136812999999965	3.771633000000000
W	11.251699999999996	44.412399000000006	3.966562999999998
W	40.393760999999978	-1.451575000000001	3.865777000000000
W	38.835630999999993	1.258370000000000	3.758054000000000
W	37.414354000000030	4.008487999999998	3.738379999999998
W	35.891818999999981	6.966340999999999	3.977392000000000
W	33.981696999999969	10.345257000000001	3.734726000000002
W	32.368898999999990	13.169173999999999	3.559451999999998
W	30.720382000000007	15.952759000000004	3.553065000000001
W	29.058215000000006	18.736131000000003	3.573064000000000
W	27.430707999999992	21.548489000000000	3.582672000000001
W	25.794940000000004	24.349394000000002	3.575655999999999
W	24.170798000000013	27.133572000000009	3.526694000000000
W	22.546720000000005	29.925961000000009	3.568700000000002
W	20.995065000000003	32.902580999999979	3.808055000000000
W	19.064057999999993	36.237369999999985	3.851707000000002
W	17.391709999999998	38.955810999999971	3.777740000000001
W	15.853752000000001	41.603422000000019	3.784717000000001
W	14.132676999999993	44.416724999999996	3.951992999999999
W	12.694610000000008	47.167547999999965	4.069613999999996
Se	18.085354999999998	41.162771999999968	4.730177000000003
Se	14.484811999999998	42.846764999999978	2.015880999999998
Se	12.695292000000002	45.675097999999984	2.155822000000001
Se	22.470779000000003	-2.882811999999999	4.348245000000004
Se	20.921426000000003	0.541001000000000	5.190455000000000
Se	19.092401999999999	3.343788000000000	5.290813000000000
Se	17.392153000000004	6.144245999999999	5.275807000000004

Se	15.679544999999992	8.896955999999994	5.229080999999999
Se	14.033346999999991	11.693778000000000	5.183968000000001
Se	12.382346000000001	14.549894000000001	5.100168000000000
Se	10.667723999999998	17.592817000000001	4.732699000000002
Se	9.015971000000004	20.567636000000003	5.056972000000000
Se	7.463842999999998	23.500509000000010	5.286918000000000
Se	5.863223999999998	26.427983000000011	5.361799999999997
Se	4.260340000000002	29.307075999999986	5.297348000000004
Se	25.908069999999986	-2.980944000000000	4.402506999999999
Se	24.343724999999992	0.391778000000000	5.352090999999997
Se	22.669872999999991	3.385743999999999	4.729535000000003
Se	20.975860999999983	6.208988999999999	4.822612999999996
Se	19.251936000000006	9.138464000000008	4.783471999999997
Se	17.561455999999997	11.941829999999995	4.763009000000003
Se	15.907412000000008	14.738993000000007	4.734151999999999
Se	14.049079000000008	17.565829000000008	4.653444000000004
Se	12.399544999999998	20.509090000000005	5.210893999999997
Se	10.860359000000008	23.504231000000008	4.680016000000002
Se	9.130950999999996	26.376422000000016	5.247789000000000
Se	7.611691000000004	29.403840999999999	4.785685000000000
Se	19.161135000000016	-0.856479000000000	2.427835000000000
Se	17.228155000000010	2.024458000000001	2.611314999999998
Se	15.564287000000002	4.923767999999999	2.442781999999998
Se	13.885009999999994	7.763242000000000	2.349546000000001
Se	12.181181000000005	10.622495999999999	2.291452000000000
Se	10.446491999999992	13.465524000000003	2.356171999999999
Se	9.013925000000004	16.629232999999993	2.138449000000000
Se	6.946442000000002	19.545714000000003	2.499026999999999
Se	5.394806000000000	22.471773999999999	2.570792000000000
Se	3.771649000000000	25.390812000000004	2.663338000000000
Se	2.175721999999999	28.400275000000006	2.587663000000000
Se	22.918202000000009	-0.686244000000000	1.546750000000001
Se	21.089165000000013	2.278655999999998	1.740701000000001

Se	19.2249990000000004	5.2402680000000004	1.5051040000000000
Se	17.6022069999999999	8.0710390000000007	1.5012010000000000
Se	15.8684849999999997	10.8646200000000004	1.4345200000000000
Se	14.1984589999999997	13.6872450000000008	1.3661140000000001
Se	12.5666580000000003	16.7100159999999995	1.5259640000000001
Se	10.7591160000000006	19.5988679999999995	1.3327640000000001
Se	9.2194439999999993	22.6088729999999991	1.7377870000000000
Se	7.4107799999999999	25.4957309999999993	1.5165569999999999
Se	5.9361319999999997	28.5342370000000010	1.8254960000000000
Se	4.1604429999999999	31.5247050000000009	1.5439900000000000
Se	2.1183000000000001	32.4130480000000034	4.3669669999999998
Se	5.7587440000000001	32.3442920000000029	5.3307729999999998
Se	3.8174389999999998	35.4793980000000033	4.2344039999999996
Se	29.2383629999999997	-2.9237769999999998	4.5932610000000000
Se	27.6148780000000009	0.3630640000000000	5.4300170000000003
Se	26.0313569999999999	3.3231910000000000	4.8964049999999997
Se	24.4718160000000005	6.2860649999999998	5.3200019999999997
Se	22.5701889999999992	9.1124340000000004	5.0622239999999996
Se	20.9711460000000010	12.0785029999999995	5.3319400000000003
Se	19.3032970000000006	14.8987470000000002	5.2450910000000004
Se	17.4159579999999998	17.7834450000000004	4.7849620000000002
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Se	32.5986919999999998	-3.0447970000000000	4.2087399999999997
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Se	29.2696719999999999	3.3159019999999999	4.9173220000000004
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Se	25.8616530000000004	9.1260019999999997	5.1445439999999998
Se	24.2141419999999989	12.0363410000000002	5.2782039999999997
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Se	20.7738860000000010	17.7134649999999993	5.1372470000000003

Se	19.1959739999999996	20.5742919999999998	5.3005529999999998
Se	17.4120990000000013	23.4374490000000009	5.1143799999999997
Se	15.9072410000000009	26.4165780000000012	5.3677169999999998
Se	14.3187750000000005	29.3833449999999985	4.8133660000000003
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Se	15.9135190000000009	16.6805589999999988	1.9501729999999999
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Se	22.6317349999999990	11.1616859999999996	1.6263099999999999
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Se	25.9110200000000006	14.938715999999994	4.869348999999997
Se	24.2524020000000000	17.8647050000000007	4.914996999999996
Se	22.611648999999999	20.6633630000000004	4.8446920000000002
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Se	34.2531040000000004	2.4065620000000001	2.3281480000000001
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Se	19.3727400000000003	28.3419699999999999	2.1954419999999999
Se	17.8160859999999985	31.3491719999999994	1.6433089999999999
Se	15.9993300000000005	32.3036370000000019	5.2743500000000001
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Se	12.5687040000000003	37.9269450000000035	4.9868300000000003
Se	19.4196999999999989	32.2651469999999989	5.5483570000000002
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Se	16.0536740000000009	38.0049500000000009	5.5947610000000001
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Se	38.1093479999999971	6.3681099999999997	4.6593879999999999
Se	36.1063419999999979	9.2835959999999993	4.8340209999999999
Se	34.7472619999999992	12.4488190000000003	4.5207569999999997
Se	33.0385909999999967	15.3196779999999997	4.5658380000000003
Se	31.3397790000000001	18.1539199999999994	4.5731409999999997
Se	29.6826380000000007	20.9732580000000013	4.5809740000000003
Se	28.0163790000000006	23.8059620000000010	4.6174540000000004
Se	26.3687770000000015	26.6507690000000004	4.5856750000000002
Se	24.7687349999999995	29.5308260000000011	4.4160019999999998
Se	39.1319480000000013	-0.5875020000000000	1.9934580000000000
Se	37.6989629999999991	2.4229550000000000	1.8539770000000000
Se	36.1051100000000034	5.3406359999999999	2.0055250000000000
Se	34.5012630000000016	8.2950610000000005	2.2253609999999999
Se	32.8181760000000011	11.4076079999999997	1.7623009999999999
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Se	27.8715830000000011	19.9260480000000015	1.7083290000000000
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Se	22.8941769999999991	28.3243440000000000	1.6773199999999999
Se	21.2104050000000015	31.2738149999999990	1.8519330000000001
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Se	17.7304050000000011	37.1572710000000015	1.9462100000000000
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Se	10.9395469999999992	42.8561860000000010	1.9883839999999999
Se	16.4352489999999989	43.9458500000000001	4.6906920000000003
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Se	14.2902520000000006	40.7084639999999993	5.3543740000000000

Se	12.7014040000000001	43.6544019999999975	5.8319890000000001
Se	10.7557700000000001	46.6585120000000018	5.3023059999999997
Se	10.9934779999999996	40.8071240000000017	5.3768120000000001
Se	8.9964440000000003	43.9466529999999977	4.7589829999999997
Se	7.1953659999999999	41.2513959999999997	4.3673770000000003

W₁₀₅Se₂₁₀; $E_{tot}=-61\,508\,146.791\,805\,60$ eV; $E_{rel}=38.883\,347\,819\,0$ meV/f.u.

W	22.5141390000000001	-4.4299179999999998	3.1153559999999998
W	21.3062940000000012	-2.2227299999999999	3.0378560000000001
W	19.4774239999999992	1.0583530000000001	3.1848150000000000
W	17.9210570000000011	3.8644140000000000	3.3474260000000000
W	16.3448950000000011	6.6441150000000002	3.3560560000000002
W	14.7188479999999995	9.4458889999999993	3.3683109999999998
W	13.0832840000000008	12.2750769999999996	3.3374830000000002
W	11.4604479999999995	15.1244650000000007	3.2930500000000000
W	9.8440899999999996	17.9693970000000007	3.2671470000000000
W	8.2218879999999999	20.7857340000000015	3.2692350000000001
W	6.6140990000000004	23.5737850000000009	3.3142090000000000
W	5.0269399999999997	26.3988130000000005	3.2816649999999998
W	3.4204819999999998	29.3603670000000001	3.1384400000000001
W	1.7655270000000001	32.0181540000000027	3.1961539999999999
W	22.8181329999999996	0.3895180000000000	3.2364169999999999
W	24.1687130000000003	-1.9211190000000000	3.2935729999999999
W	20.6855919999999998	3.5456340000000002	3.2147690000000000
W	19.1205010000000009	6.3405360000000002	3.2871220000000001
W	17.5066470000000010	9.1928490000000007	3.3550040000000001
W	15.8480559999999997	12.0300659999999997	3.3649789999999999
W	14.2285810000000001	14.8747650000000000	3.3326050000000000
W	12.6198080000000008	17.7261829999999989	3.3088000000000002
W	10.9985809999999997	20.5567729999999997	3.2715660000000000
W	9.3724950000000007	23.3414830000000002	3.2424309999999998
W	7.7885119999999999	26.0894000000000013	3.2218830000000001

W	6.0855910000000000	29.4735109999999985	3.2452589999999999
W	4.8442239999999996	31.9286679999999983	3.1723729999999999
W	25.7855230000000013	0.7116220000000000	3.2895520000000000
W	24.6985910000000004	3.8225730000000002	3.3373599999999999
W	23.2347169999999998	6.6067070000000001	3.4751859999999999
W	21.5879440000000002	9.4380880000000005	3.4585050000000002
W	19.8809100000000001	12.4606390000000005	3.5751759999999999
W	18.2119639999999983	15.2702050000000007	3.5631960000000000
W	16.6172870000000010	18.0944250000000011	3.5437449999999999
W	14.9845360000000003	21.0129869999999990	3.5185330000000001
W	13.3296690000000009	23.8880429999999997	3.4716700000000000
W	11.6808870000000002	26.7065100000000015	3.4216039999999999
W	10.0392039999999998	29.4436570000000017	3.3196140000000001
W	7.9168550000000000	31.9890940000000015	3.1975340000000001
W	27.5375210000000017	3.3995270000000000	3.0456799999999999
W	26.0405039999999985	6.1824070000000004	3.2927450000000000
W	24.3638170000000009	9.4634990000000005	3.4432269999999998
W	22.9982940000000013	11.8868849999999995	3.4671989999999999
W	20.9512350000000005	15.0543200000000006	3.4887210000000000
W	19.4161940000000008	17.7732729999999997	3.4582449999999998
W	17.7510690000000011	20.6522299999999994	3.3960659999999998
W	16.0942630000000015	23.6822720000000011	3.3718349999999999
W	14.4130230000000008	26.4912840000000003	3.3172980000000001
W	12.7788869999999992	29.3175109999999997	3.2319410000000000
W	11.0596449999999997	32.1083959999999990	3.0501630000000000
W	29.5626199999999990	6.6907269999999999	3.2918020000000001
W	28.4252560000000010	9.2264490000000006	3.3709600000000002
W	26.0724519999999984	12.3926219999999994	3.6170870000000002
W	25.0230989999999984	14.9998939999999994	3.4945460000000002
W	22.8674959999999992	18.2762180000000001	3.5737500000000000
W	21.7590170000000001	20.8064590000000003	3.5346630000000001
W	19.8992380000000004	24.1076359999999994	3.4380950000000001
W	18.2831380000000010	26.3506700000000009	3.4583439999999999

W	16.5931840000000008	29.9546160000000015	3.3116580000000000
W	14.9550719999999995	32.2096119999999999	3.2475860000000001
W	31.2370310000000018	9.4580219999999997	3.4730409999999998
W	30.1237059999999985	11.9548190000000005	3.4321470000000001
W	27.7894210000000008	15.2187839999999994	3.6328960000000001
W	26.6295040000000007	17.8042629999999988	3.5310120000000000
W	24.7070739999999986	20.4599930000000008	3.6515089999999999
W	23.0341389999999997	24.0992099999999994	3.4603679999999999
W	21.4685200000000016	26.3819090000000003	3.5617489999999998
W	19.8171959999999991	30.0553060000000016	3.3724620000000001
W	18.1941339999999983	32.2658139999999989	3.4319080000000000
W	32.9162320000000008	12.2289589999999997	3.4712630000000000
W	31.7739420000000017	14.7685730000000000	3.4349020000000001
W	29.3771979999999999	18.0142950000000006	3.6044619999999998
W	28.0493510000000015	20.4815809999999985	3.5393490000000001
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W	24.6842289999999984	26.3847999999999985	3.5885870000000000
W	23.0727000000000011	30.0680019999999999	3.3887649999999998
W	21.4292580000000008	32.3334079999999986	3.4291999999999998
W	34.5421649999999971	15.0503219999999995	3.4540259999999998
W	33.3896280000000019	17.6026699999999998	3.3850989999999999
W	30.9144350000000010	20.7713509999999992	3.4778709999999999
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W	36.0981960000000015	17.8844400000000014	3.4131119999999999
W	34.9066589999999977	20.4451320000000010	3.3065190000000002
W	33.0368670000000009	24.0746469999999988	3.3371940000000002
W	31.3312530000000002	26.3173560000000002	3.5189610000000000
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W	27.9630949999999991	32.3115579999999980	3.3604219999999998
W	37.6724960000000024	20.7084170000000007	3.2037599999999999

W	36.291136000000016	24.060022000000000	3.218998000000000
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W	39.561058000000027	24.124227000000012	2.993091999999999
W	37.767369000000022	26.358533999999988	3.308513000000000
W	36.015766999999968	29.995083999999985	3.252339999999998
W	34.436712999999975	32.280517000000032	3.370531999999999
W	41.055957999999968	26.913495000000011	3.169709999999998
W	39.798352999999988	29.749321999999994	3.253928000000002
W	37.682457999999969	32.219023999999974	3.322852000000001
W	42.552449000000029	29.576149000000009	3.168291000000000
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W	44.182229999999970	32.183143999999986	3.215646000000000
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Se	6.270164000000003	25.273520999999988	5.154863999999999
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Se	21.150123000000007	5.509081000000001	4.764000000000002
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Se	21.4213079999999998	22.8465419999999995	5.1045439999999997
Se	19.7790309999999998	25.7658899999999988	5.3811590000000002

Se	18.137288000000016	28.669312000000015	4.8655939999999998
Se	16.455428000000013	31.712689000000010	5.2142689999999998
Se	31.679657999999999	11.054783000000005	5.3394800000000000
Se	29.774912000000005	14.021478000000001	4.9432489999999998
Se	28.089611999999989	16.897363999999996	5.4629700000000003
Se	26.407039999999985	19.726303000000015	5.3429390000000003
Se	24.720438000000015	22.773327999999993	4.9612540000000003
Se	23.061284000000006	25.770461000000010	5.4151790000000002
Se	21.423552999999983	28.699186999999984	4.8859690000000002
Se	19.795286999999983	31.840738999999992	5.2939400000000001
Se	33.353395999999965	13.868508000000003	5.3278710000000000
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Se	31.424783000000015	22.765805000000003	4.9873029999999998
Se	29.691537000000003	25.696187999999994	5.3575039999999996
Se	28.008209000000008	28.664327000000001	4.8779709999999996
Se	26.342030999999986	31.899570000000006	5.2465310000000001
Se	36.514865000000004	19.668831000000008	5.1872860000000003
Se	34.753537000000015	22.675929000000000	4.7400739999999999
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Se	17.7988369999999989	7.4923679999999999	1.4820640000000000
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Se	26.1915739999999992	4.4807560000000004	1.3388020000000000

Se	24.633203999999992	7.497656000000001	1.6388110000000000
Se	22.930568999999984	10.252506000000003	1.511670000000001
Se	21.389953999999995	13.171032000000003	1.7712260000000000
Se	19.664207999999986	16.037144999999989	1.5932839999999999
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Se	16.469664999999991	27.626000000000012	2.0130550000000000
Se	14.730741999999993	30.446066999999993	1.6103390000000000
Se	12.977622999999995	33.497587000000029	2.1909019999999999
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Se	19.7194280000000006	33.9512519999999967	2.4013380000000000
Se	35.1618130000000022	12.8090499999999992	2.4508150000000000
Se	33.0954169999999976	15.8760499999999993	1.5696120000000000
Se	31.3846379999999989	18.7622120000000017	2.0584739999999999
Se	29.5184110000000004	21.8180920000000000	1.7988590000000000
Se	28.0265249999999995	24.7039240000000007	1.6862040000000000
Se	26.3585589999999996	27.7415170000000018	2.0947420000000001
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Se	23.0455000000000005	34.0060939999999974	2.4306160000000001
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Se	34.6986800000000031	18.7400230000000008	1.4881770000000001
Se	32.9351630000000029	21.7283730000000013	2.0409120000000001
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Se	27.9718699999999991	30.6068500000000014	1.5198730000000000
Se	26.3395909999999986	33.9902930000000012	2.3913560000000000
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Se	22.7683749999999989	-1.2824590000000000	1.2994230000000000
Se	24.4785280000000007	-4.1794419999999999	1.8489819999999999
Se	20.3329689999999985	-4.5616000000000003	2.2561279999999999
Se	29.6058109999999992	33.9747509999999977	2.3628079999999998
Se	32.8299280000000024	31.8099090000000011	5.2163420000000000
Se	31.2190450000000013	30.6214009999999988	1.4683210000000000
Se	34.5376779999999997	28.6389950000000013	4.8021459999999996
Se	32.8981649999999988	27.7156219999999998	1.9744740000000001

Se	36.288355000000028	25.683883000000016	5.199316999999997
Se	34.617137999999971	24.688866000000009	1.458733000000001
Se	38.145037000000021	22.776154999999993	4.703800000000002
Se	36.247467000000003	21.811146000000008	1.590905000000000
Se	38.457794999999973	18.598248999999991	2.435696000000001
Se	39.663426999999987	25.734667999999992	4.952675000000002
Se	39.784070999999973	21.782063000000008	2.135663000000001
Se	37.926482999999975	24.734905000000013	1.313565000000001
Se	37.830218999999996	28.656328999999995	4.615832000000002
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Se	39.419659000000029	31.612563000000015	5.050065000000000
Se	39.438156999999968	27.691888999999998	1.620919000000000
Se	36.217914000000004	33.997281000000010	2.551539000000000
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Se	43.303893999999997	27.403465000000006	2.245550000000002
Se	42.751339000000015	31.460177000000016	5.032752000000003
Se	41.254693000000032	30.496584999999996	1.280143000000000
Se	39.539515999999990	33.803856000000032	2.287231999999999
Se	45.999820999999972	33.250773999999998	4.059281999999996
Se	42.852702000000007	33.630440999999976	1.927074000000000
Se	44.819386999999990	30.238497999999999	2.033262999999998

W₁₀₅Se₂₁₀; $E_{tot} = -61\,508\,147.850\,709\,12$ eV; $E_{rel} = 28.798\,552\,390\,4$ meV/f.u.

W	21.348023999999988	-1.124897000000000	3.346190000000000
W	19.478936000000009	1.688600000000001	3.400716000000001
W	17.814360000000006	4.472814999999998	3.420659999999998
W	16.178188999999997	7.244911000000001	3.383383999999999

W	14.5102250000000002	10.0008199999999992	3.3751000000000002
W	12.8664769999999997	12.7627699999999997	3.3704879999999999
W	11.2130890000000001	15.5466479999999994	3.2461859999999998
W	9.2173169999999995	18.8526449999999990	2.9834230000000002
W	7.5336499999999997	21.9166600000000003	3.2107450000000002
W	6.0813709999999999	24.6389659999999999	3.2367539999999999
W	4.5562220000000000	27.3046979999999984	3.1199450000000000
W	2.7449530000000002	30.7243759999999995	3.0530789999999999
W	1.2769260000000000	33.3747690000000006	3.1328630000000000
W	-0.2681410000000000	36.1196970000000022	3.0628299999999999
W	-1.9398560000000000	38.7172330000000002	3.0099170000000002
W	24.5718710000000016	-1.2379869999999999	3.4307960000000000
W	22.8631540000000015	1.0645950000000000	3.4572720000000001
W	20.6132910000000003	4.1785909999999999	3.3164440000000002
W	18.9791659999999993	6.9658629999999997	3.3416210000000000
W	17.2764960000000016	9.7867700000000006	3.3272979999999999
W	15.6002539999999996	12.5643750000000001	3.3021699999999998
W	13.9839800000000007	15.3295949999999994	3.3061090000000002
W	12.4524369999999998	18.8877580000000016	3.2659410000000002
W	10.9410249999999998	21.1673669999999987	3.3814289999999998
W	8.9962879999999998	24.6685550000000013	3.3559899999999998
W	7.6670639999999999	27.0012860000000003	3.3921039999999998
W	6.0482329999999997	30.6227760000000018	3.2345950000000001
W	2.4546489999999999	36.2893869999999978	3.2001230000000001
W	4.5069600000000003	32.9157579999999967	3.3044889999999998
W	1.1865960000000000	38.6442920000000001	3.0481889999999998
W	27.7907340000000005	-1.2841739999999999	3.5439560000000001
W	29.2581349999999993	1.0308780000000000	3.6105220000000000
W	26.0612239999999993	1.0149630000000001	3.5352779999999999
W	24.5706460000000000	4.6841109999999997	3.3556900000000001
W	23.0947279999999999	7.1545449999999997	3.4514469999999999
W	21.2442740000000008	10.3730039999999999	3.4668649999999999
W	19.6560260000000007	13.1213180000000005	3.5360779999999998

W	17.9768630000000016	15.8030930000000005	3.4179750000000002
W	15.6482410000000005	18.9377339999999990	3.4014650000000000
W	14.1440819999999992	21.1751189999999987	3.5312640000000002
W	12.6820839999999997	24.7924250000000015	3.3850539999999998
W	10.9536320000000007	26.9761440000000015	3.5451760000000001
W	9.3192450000000004	30.6594939999999987	3.3161079999999998
W	7.6846509999999997	32.9045020000000008	3.4364390000000000
W	6.2331630000000002	36.5814200000000014	3.2520560000000001
W	4.5372219999999999	38.7835320000000010	3.2944049999999998
W	31.0163009999999986	-1.2634810000000001	3.5639539999999998
W	27.7684399999999982	4.6974739999999997	3.3628680000000002
W	26.1814210000000003	6.9610110000000001	3.4772729999999998
W	24.2208679999999994	10.2804529999999996	3.4388600000000000
W	22.6779879999999991	12.7848910000000000	3.4742959999999998
W	20.7921049999999994	15.9988550000000007	3.4611760000000000
W	19.4246890000000008	18.6556500000000014	3.4411440000000000
W	17.3694209999999991	21.1405010000000004	3.6059950000000001
W	15.8515020000000000	24.8332979999999992	3.4254190000000002
W	14.2252220000000005	27.0620300000000000	3.5627979999999999
W	12.5738939999999992	30.6850510000000014	3.3592800000000000
W	9.4191780000000005	36.6327399999999983	3.3044739999999999
W	10.9060570000000006	32.9254689999999997	3.4975520000000002
W	7.7557790000000004	38.8728740000000030	3.4100169999999999
W	34.4016360000000034	-1.2648070000000000	3.6991580000000002
W	36.2032340000000019	1.4274370000000001	3.7480210000000000
W	32.3664720000000017	1.0768240000000000	3.6487479999999999
W	30.9973530000000004	4.7316200000000004	3.4581130000000000
W	29.3811929999999997	6.9639949999999997	3.5559479999999999
W	27.2278780000000005	10.2136379999999996	3.4659149999999999
W	25.7431769999999993	12.7036180000000005	3.4510630000000000
W	23.8161169999999984	15.9085280000000004	3.4618679999999999
W	22.2517800000000001	18.5753960000000014	3.3952010000000001
W	20.6768520000000002	21.2260139999999993	3.4724100000000000

W	19.0491670000000006	24.8606200000000008	3.4885709999999999
W	17.4033599999999993	27.0987650000000002	3.6195230000000000
W	15.8561280000000000	30.7452480000000001	3.3635920000000001
W	14.1038460000000008	32.9435829999999967	3.5210919999999999
W	12.6619930000000007	36.6121509999999972	3.3513250000000001
W	10.9527920000000005	38.8997099999999989	3.4283489999999999
W	37.4602670000000018	-1.2648230000000000	3.9167860000000001
W	34.1974220000000031	4.7321910000000003	3.6510630000000002
W	32.6637219999999999	7.0081080000000000	3.7124039999999998
W	31.2232400000000005	10.5974350000000008	3.6220990000000000
W	29.6657319999999984	13.3767510000000005	3.5922000000000001
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W	14.1694499999999994	38.8392389999999992	3.4781800000000000
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W	37.4363699999999966	4.0176249999999998	3.7612860000000001
W	35.9094399999999965	6.9838190000000004	4.0043600000000001
W	33.9918890000000005	10.3636560000000006	3.7356560000000001
W	32.3729399999999998	13.1837350000000004	3.5262190000000002
W	30.7174779999999998	15.9573169999999998	3.4778319999999998
W	29.0648069999999983	18.7421210000000009	3.4720840000000002
W	27.4307300000000005	21.5505220000000008	3.4950350000000001
W	25.7694979999999987	24.3377009999999991	3.5614810000000001
W	24.0861030000000014	27.0925660000000015	3.6307920000000000
W	22.5131300000000003	29.9876259999999988	3.7724120000000001
W	20.6641629999999985	33.3906750000000017	3.7631060000000001

W	19.162109000000009	35.872411999999971	3.602945000000001
W	17.420815000000010	38.658912000000008	3.523321000000001
Se	22.507421000000008	-2.897829000000002	4.332774999999998
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Se	25.944790999999986	-2.983623999999998	4.407168000000004
Se	24.372363000000000	0.381616000000000	5.338315999999998
Se	22.700611999999996	3.366527000000000	4.712138000000004
Se	21.006789000000013	6.175163999999997	4.821056999999997
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Se	15.931426999999993	14.701783000000007	4.812913000000000
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Se	2.6545359999999998	32.3395679999999999	4.9847400000000004
Se	1.0177259999999999	35.0945109999999971	4.9813599999999996
Se	-0.5714980000000000	38.0031600000000012	4.8828370000000003
Se	5.9968070000000004	32.2591449999999966	5.2034760000000002
Se	4.4209280000000000	35.2230500000000006	4.5926410000000004
Se	2.7628480000000000	38.1670700000000025	4.9843970000000004
Se	-1.0083970000000000	33.9142719999999969	2.2250060000000000
Se	-2.5084460000000002	36.7531829999999999	1.8322630000000000
Se	-3.8035109999999999	39.7677490000000020	3.7693989999999999
Se	2.8731460000000002	34.2227519999999998	1.5934919999999999
Se	1.0601860000000001	37.0180519999999973	1.1776190000000000
Se	-0.5812820000000000	40.1623090000000005	1.7495920000000000
Se	29.2742520000000006	-2.9264850000000000	4.5879729999999999
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Se	10.9296260000000007	29.2880439999999993	4.8415249999999999
Se	32.6296749999999989	-3.0453410000000001	4.1944509999999999
Se	30.8834270000000011	0.3016500000000000	5.5047850000000000
Se	29.2946939999999998	3.3148700000000000	4.9247100000000001
Se	27.7480629999999984	6.3300510000000001	5.3460279999999996
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Se	9.3175299999999996	28.3538829999999997	1.9585750000000000
Se	7.7000500000000000	31.2730280000000000	1.4592680000000000
Se	29.4337389999999992	-0.7474499999999999	1.7011490000000000

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Se	17.489497000000001	19.518336999999989	1.753068000000001
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Se	9.339143000000000	38.364184000000016	5.268475999999997
Se	6.141899999999997	34.298510000000003	1.852139000000000
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Se	29.276071000000017	9.290805999999999	4.871825000000003
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Se	39.0216259999999977	-2.8510540000000000	5.1781350000000002
Se	37.5017420000000001	0.3924890000000000	5.7081400000000002
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Se	34.2619839999999982	6.3417399999999997	5.6551580000000001
Se	32.5720579999999984	9.2386730000000004	5.3383479999999999
Se	31.0169950000000014	12.2757430000000003	5.4632920000000000
Se	29.3025689999999983	15.1086229999999997	5.3871490000000000
Se	27.6136049999999997	17.9003750000000004	5.3513260000000002
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Se	24.2657160000000012	23.5973369999999996	5.4409500000000000
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Se	32.7418740000000028	-0.6764990000000000	1.8129700000000000
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Se	29.4270029999999991	5.3134639999999997	1.5764950000000000
Se	27.8050530000000009	8.2561040000000006	1.9052819999999999
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Se	14.2325370000000007	31.3336590000000008	1.5433690000000000
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Se	34.2795679999999976	2.4217170000000001	2.3420369999999999
Se	32.7272579999999991	5.3638560000000002	1.7345610000000000
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Se	17.624703000000002	31.326591000000005	1.6593880000000001
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Se	9.392932999999993	40.564884999999968	2.4128330000000000
Se	15.928145999999999	34.224679999999993	2.1277200000000001
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Se	12.775180000000006	40.563284000000030	2.4745539999999999
Se	42.206279000000021	-2.5927110000000000	3.0609459999999999
Se	41.046585000000003	0.4950340000000000	5.0563180000000001
Se	39.584808000000024	3.4524480000000000	4.8182590000000003
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Se	31.334831999999987	18.197486999999989	4.4573460000000003
Se	29.679952000000001	21.034973999999983	4.444487999999998
Se	27.994294000000000	23.881295999999990	4.5154040000000002
Se	26.287653999999999	26.697634000000008	4.5985750000000003
Se	24.676919000000016	29.523727999999984	4.6010629999999999
Se	39.153405999999968	-0.5703040000000000	1.9956790000000000
Se	37.723590999999990	2.4413550000000002	1.8696870000000001
Se	36.131684999999974	5.359035999999997	2.0311669999999999
Se	34.523356999999972	8.305037999999997	2.2416309999999999

Se	32.8337730000000008	11.4059460000000001	1.7498250000000000
Se	31.1645779999999988	14.2864190000000004	1.6438260000000000
Se	29.4742880000000014	17.0928289999999983	1.6157830000000000
Se	27.8295570000000012	19.9202730000000017	1.6241600000000000
Se	26.1672989999999999	22.7383750000000013	1.6702429999999999
Se	24.4990209999999990	25.5331370000000000	1.7262169999999999
Se	22.6916319999999985	28.3548250000000017	1.8937690000000000
Se	21.1075699999999991	31.3703989999999990	2.1119690000000002
Se	22.9197540000000011	32.4510799999999975	4.4343700000000004
Se	21.3979880000000016	35.5533769999999976	4.6380299999999997
Se	19.5880620000000008	38.3801520000000025	4.4785979999999999
Se	19.3256599999999992	34.1675219999999982	1.7855950000000000
Se	17.7683950000000017	36.9904480000000007	1.7331920000000001
Se	16.2707419999999985	40.4554070000000010	2.5619689999999999

$W_{105}Se_{210}$; $E_{tot} = -61\,508\,148.504\,960\,48$ eV; $E_{rel} = 22.567\,587\,057\,1$ meV/f.u.

W	58.8894689999999983	-66.5837760000000003	3.4730850000000002
W	57.0519620000000032	-63.7634400000000028	3.5693540000000001
W	60.3630130000000023	-64.3881959999999935	3.5313150000000002
W	55.3899809999999988	-60.9989709999999974	3.6146900000000000
W	53.7860200000000006	-58.2359709999999993	3.5935990000000002
W	52.2103490000000008	-55.4246679999999969	3.5212420000000000
W	50.6676349999999971	-52.4138990000000007	3.4023379999999999
W	62.1411900000000017	-66.7289779999999979	3.4695510000000001
W	58.1756639999999976	-61.2712860000000035	3.4637799999999999
W	56.5167369999999991	-58.4863059999999990	3.4425960000000000
W	54.9457889999999978	-55.6730670000000032	3.4371589999999999
W	53.3164299999999969	-52.1803829999999991	3.4935480000000001
W	52.1438940000000031	-49.5375190000000032	3.3557239999999999
W	65.4174390000000017	-66.7795990000000046	3.4500989999999998
W	63.5832899999999981	-64.4697879999999941	3.5185230000000001
W	62.0937509999999975	-60.8129989999999978	3.4379599999999999

W	60.507396000000000	-58.046914000000010	3.5430760000000001
W	58.927875999999977	-55.2146370000000033	3.5550600000000001
W	57.282635999999966	-52.4666080000000008	3.3868469999999999
W	54.8166840000000022	-49.338057999999966	3.4733480000000001
W	53.690353999999992	-46.729813999999975	3.3326769999999999
W	68.695650999999980	-66.7788610000000062	3.4354100000000001
W	66.914186999999983	-64.5090380000000039	3.4919250000000002
W	65.326702999999949	-60.797727999999993	3.2978679999999998
W	63.31589999999992	-58.405980999999970	3.3813290000000000
W	61.8458970000000008	-55.635649999999983	3.4186410000000000
W	59.992584999999983	-52.217250999999974	3.4764970000000002
W	58.8343220000000002	-49.6526470000000018	3.3227880000000001
W	56.4504710000000003	-46.4365900000000025	3.4604990000000000
W	55.307997999999978	-43.9270670000000010	3.3426540000000000
W	71.960044999999938	-66.785617999999995	3.4399950000000001
W	70.2550880000000006	-64.522132999999966	3.4888990000000000
W	68.5859760000000023	-60.8555130000000020	3.3410549999999999
W	67.1993750000000034	-58.4453590000000034	3.3795489999999999
W	65.016165999999983	-55.039991999999980	3.4506869999999998
W	63.957028999999986	-52.4908980000000014	3.3386860000000000
W	61.575656999999996	-49.3820630000000023	3.5038529999999999
W	60.4441410000000019	-46.8635980000000032	3.3293180000000002
W	58.177377999999974	-43.540433999999976	3.4862000000000002
W	56.9780810000000031	-41.1548530000000028	3.3861629999999998
W	75.2208250000000049	-66.7787720000000036	3.4854759999999998
W	73.582482999999963	-64.525452999999988	3.5177559999999999
W	71.9013900000000064	-60.855654999999987	3.3441960000000002
W	70.117650999999951	-58.556592999999994	3.4339100000000000
W	68.9507260000000031	-55.6222070000000031	3.3230160000000000
W	66.7362420000000043	-52.3321940000000012	3.4555030000000002
W	65.4963240000000013	-49.8729730000000018	3.3608520000000000
W	63.252214999999996	-46.5938620000000014	3.4753289999999999
W	62.0774850000000029	-44.1377960000000016	3.3967760000000000

W	59.877740000000029	-40.833154999999979	3.5180650000000000
W	58.742660000000008	-38.436670999999969	3.4435470000000001
W	78.469967999999944	-66.752696999999977	3.5450740000000001
W	76.895562999999957	-64.509033999999998	3.5934849999999998
W	75.329211000000008	-60.853642000000007	3.4414030000000002
W	73.725200999999984	-58.620817999999999	3.5555569999999999
W	71.764679999999985	-55.108679000000022	3.4070670000000001
W	70.064075000000025	-52.852431000000028	3.4138730000000002
W	68.240257999999972	-49.640639999999977	3.4323000000000001
W	67.169008000000052	-46.495266999999983	3.4518680000000002
W	65.295916000000054	-44.175837000000014	3.5824140000000000
W	63.724547999999986	-40.499003999999993	3.4656340000000001
W	62.114392999999997	-38.282401000000001	3.5725330000000000
W	81.687053000000059	-66.714662000000041	3.6187909999999999
W	80.185391999999931	-64.467394999999962	3.6589860000000001
W	78.535218999999979	-60.803710000000024	3.4919730000000002
W	76.978560999999991	-58.518920000000014	3.5848860000000000
W	75.427508000000031	-54.980887000000027	3.5043090000000001
W	73.898098000000045	-52.309046000000022	3.5085950000000001
W	72.278745000000007	-49.499355999999988	3.5019999999999998
W	70.317807999999994	-46.399994999999970	3.4581529999999998
W	68.579750000000042	-44.117511000000004	3.5772010000000001
W	66.960593000000029	-40.449339999999994	3.4653470000000000
W	65.312915000000038	-38.224870000000028	3.6270970000000000
W	84.876126999999968	-66.701854999999948	3.8800129999999999
W	83.425813000000051	-64.398053000000044	3.7545829999999998
W	81.706732999999998	-60.758924000000004	3.5514459999999999
W	80.083325999999996	-58.499290000000020	3.6062810000000001
W	78.194699999999974	-55.316715000000021	3.4610420000000000
W	76.649427000000029	-52.505713000000001	3.3975890000000000
W	75.035465000000021	-49.716104000000014	3.3706130000000001
W	73.349827000000048	-46.909270999999968	3.3459859999999999
W	71.752471999999974	-44.110881999999966	3.4956920000000000

W	70.3168830000000042	-40.4785230000000027	3.4454889999999998
W	68.4998489999999975	-38.1997349999999969	3.5836420000000002
W	88.7466830000000044	-66.8793610000000029	3.8112330000000001
W	86.6608980000000031	-63.8893879999999967	3.7409659999999998
W	90.3147419999999954	-64.3493770000000040	3.8600319999999999
W	85.4377379999999960	-61.0597449999999995	3.7219280000000001
W	83.8592170000000010	-58.4178739999999976	3.6342170000000000
W	82.1547269999999941	-54.9388829999999970	3.5844779999999998
W	80.6502859999999941	-52.1008950000000013	3.5435910000000002
W	79.0410590000000042	-49.2679830000000010	3.5281449999999999
W	77.3812139999999999	-46.4382540000000006	3.5015209999999999
W	75.6850309999999951	-43.6390469999999979	3.4923240000000000
W	73.5551719999999989	-40.5814620000000019	3.4183949999999999
W	71.7355089999999933	-38.2089879999999980	3.5102080000000000
W	88.1849119999999971	-61.0158470000000008	3.9325489999999999
W	86.5685270000000031	-58.3431879999999978	3.6939820000000001
W	84.9392529999999937	-55.2946579999999983	3.5245419999999998
W	83.3867709999999960	-52.4139849999999967	3.4542109999999999
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W	80.1884249999999952	-46.7311649999999972	3.4540920000000002
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W	76.8238079999999977	-41.1620849999999976	3.3841239999999999
W	74.9892080000000050	-38.3557449999999989	3.4468559999999999
Se	60.0627909999999972	-68.3607709999999997	4.4372550000000004
Se	58.5250630000000029	-64.9469490000000036	5.3103650000000000
Se	56.7265990000000002	-62.1290690000000012	5.4370830000000003
Se	55.0625179999999972	-59.3276279999999971	5.4430969999999999
Se	53.4553009999999986	-56.4946339999999978	5.4044179999999997
Se	51.9125119999999995	-53.5263769999999965	5.2427320000000002
Se	49.7068370000000002	-50.4703659999999985	4.2983430000000000
Se	63.5435459999999992	-68.4642869999999988	4.3821360000000000
Se	61.9509880000000024	-65.0961460000000045	5.3602390000000000
Se	60.2581240000000022	-62.1077709999999996	4.8381740000000004

Se	58.5462010000000035	-59.1925900000000027	4.9355989999999998
Se	56.9130249999999975	-56.3520019999999988	4.9125610000000002
Se	55.2466549999999970	-53.4303400000000011	4.7918370000000001
Se	53.4442969999999988	-50.4538840000000022	5.3030080000000002
Se	51.3821870000000018	-47.4162340000000029	4.3330669999999998
Se	66.9092129999999941	-68.4550969999999950	4.4101450000000000
Se	65.2720549999999946	-65.1267869999999931	5.3228669999999996
Se	63.661146999999997	-62.1823679999999968	4.8814229999999998
Se	61.8913539999999998	-59.2326189999999997	5.3475200000000003
Se	60.3055590000000024	-56.2942480000000032	5.3514499999999998
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Se	68.5906750000000045	-65.1047039999999981	5.3086490000000000
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Se	65.2732040000000069	-59.0957470000000029	5.0524490000000002
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Se	60.2156110000000027	-50.5068100000000015	5.3107410000000002
Se	58.4340860000000006	-47.5689390000000003	4.8370490000000004
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Se	54.7555529999999990	-41.5504800000000003	4.3253599999999999
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Se	60.190916000000014	-48.572445000000019	1.4982580000000001
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Se	75.3692920000000015	-39.9971200000000024	1.6196219999999999
Se	73.7724999999999937	-36.5822629999999975	2.5141760000000000

W₁₀₅Se₂₁₀; $E_{tot}=-61\,508\,148.650\,619\,92$ eV; $E_{rel}=21.180\,354\,295\,2$ meV/f.u.

W	21.0482750000000003	-0.7996410000000000	3.4312339999999999
W	19.2525440000000003	1.8973120000000001	3.3712640000000000
W	17.5476169999999989	4.6727340000000002	3.3055639999999999
W	15.909499999999995	7.5031309999999998	3.2760090000000002
W	14.2926380000000002	10.3258010000000002	3.2741400000000001
W	12.6819539999999993	13.1336929999999992	3.2829839999999999
W	11.0684050000000003	15.9318209999999993	3.2898209999999999
W	9.4517240000000005	18.7290080000000003	3.2869290000000002
W	7.8340600000000000	21.5293400000000013	3.2788670000000000
W	6.2178550000000001	24.3339819999999989	3.2755619999999999
W	4.6023430000000003	27.1411699999999989	3.2847070000000000
W	2.9828320000000001	29.9523870000000016	3.3036740000000000
W	1.3559600000000001	32.7713170000000034	3.3256480000000002
W	-0.2254140000000000	35.6185270000000003	3.3569870000000002
W	-1.6937480000000000	38.5158429999999967	3.3734820000000001
W	24.3751180000000005	-0.8866650000000000	3.5094129999999999
W	22.1392020000000009	1.6250610000000001	3.3544420000000001
W	20.4508180000000017	4.3060190000000000	3.2967689999999998
W	18.7922930000000008	7.1021939999999999	3.2794349999999999
W	17.1476110000000013	9.9383970000000001	3.2646530000000000
W	15.5109080000000006	12.7779150000000001	3.2609919999999999
W	13.8743289999999995	15.6148659999999992	3.2659690000000001
W	12.2375670000000003	18.4486020000000011	3.2696299999999998
W	10.6038730000000001	21.2790479999999995	3.2682340000000001
W	8.9737310000000008	24.1098159999999986	3.2640229999999999
W	7.3439969999999999	26.9433469999999993	3.2640359999999999
W	5.7099140000000004	29.7842689999999983	3.2733490000000001
W	2.4638309999999999	35.4880350000000035	3.3097880000000002

W	4.0741540000000001	32.6404489999999967	3.2914800000000000
W	0.9547450000000000	38.2699110000000005	3.3322940000000001
W	-0.1005090000000000	41.3843350000000001	3.5086179999999998
W	27.5408189999999991	-0.8832380000000000	3.5738259999999999
W	28.7834450000000004	1.6216219999999999	3.5337550000000002
W	26.0719759999999994	1.6625360000000000	3.5028060000000001
W	24.3414609999999989	4.9271250000000002	3.5122969999999998
W	22.7571310000000011	7.6532470000000004	3.5087570000000001
W	21.1416530000000016	10.4119030000000006	3.4802000000000000
W	19.5180800000000012	13.2167960000000004	3.4676390000000001
W	17.8867079999999987	16.0487390000000012	3.4678650000000002
W	16.2522200000000012	18.8875880000000009	3.4716119999999999
W	14.6226350000000007	21.7158240000000013	3.4743860000000000
W	12.9982070000000007	24.5340929999999986	3.4740799999999998
W	11.3714420000000000	27.3534679999999994	3.4729980000000000
W	9.7417040000000004	30.1765630000000016	3.4757330000000000
W	8.1162910000000004	33.0043039999999976	3.4866429999999999
W	6.5032189999999996	35.8326860000000025	3.5072820000000000
W	4.8950790000000000	38.6557919999999982	3.5216400000000001
W	3.1707999999999998	41.5292699999999968	3.5273639999999999
W	1.3343700000000001	43.9454459999999969	3.6653940000000000
W	30.6852739999999997	-0.9029550000000000	3.6888920000000001
W	27.1302349999999990	4.4825299999999997	3.3784100000000001
W	25.5413050000000013	7.3828750000000003	3.4004750000000001
W	23.9218750000000000	10.1640540000000001	3.4029720000000001
W	22.2946360000000006	12.9541699999999995	3.3858739999999998
W	20.6611830000000012	15.7740530000000003	3.3770859999999998
W	19.0264780000000009	18.6088309999999986	3.3795910000000000
W	17.3982680000000016	21.4382750000000009	3.3869060000000002
W	15.7753329999999998	24.2567559999999993	3.3912360000000001
W	14.1518979999999992	27.0721460000000000	3.3900899999999998
W	12.5246300000000002	29.8917819999999992	3.3881579999999998
W	9.2802450000000007	35.5361059999999966	3.3983629999999998

W	10.8992540000000009	32.7138840000000002	3.3910160000000000
W	7.6603070000000004	38.3609650000000002	3.3943159999999999
W	6.0362929999999997	41.1654880000000034	3.3921380000000001
W	4.4074910000000003	43.9428740000000033	3.5043820000000001
W	3.2031269999999998	47.2221440000000001	3.6784599999999998
W	33.9390569999999983	-0.8176030000000000	3.8801120000000000
W	35.3896099999999976	1.6951200000000000	3.9942910000000000
W	32.7033640000000005	1.5789310000000001	3.7406869999999999
W	31.0624150000000014	4.9812409999999998	3.6547109999999998
W	29.5387099999999982	7.7920100000000003	3.6114160000000002
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W	23.0448209999999989	19.0230670000000011	3.6323590000000001
W	21.4182559999999995	21.8453559999999989	3.6370700000000000
W	19.7948689999999985	24.6759290000000000	3.6380580000000000
W	18.1661290000000015	27.5054820000000007	3.6368399999999999
W	16.5365670000000016	30.3338590000000003	3.6363210000000001
W	14.9048060000000007	33.1581750000000000	3.6388479999999999
W	13.2811319999999995	35.9804930000000027	3.6420100000000000
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W	10.0524830000000005	41.5667329999999993	3.6395170000000001
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W	6.3213689999999998	47.4250589999999974	3.6320090000000000
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W	33.8118079999999992	4.6471320000000000	3.7052269999999998
W	32.2809579999999983	7.4931210000000004	3.5777220000000001
W	30.7246839999999999	10.3122640000000008	3.5912910000000000
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W	22.571898999999984	24.413018000000010	3.661886000000000
W	20.946045000000016	27.236401999999982	3.654312000000000
W	19.322462999999991	30.053415000000011	3.651863000000001
W	16.079647999999988	35.685943999999992	3.667908999999999
W	17.698359000000000	32.870167999999996	3.658469000000002
W	14.464456000000002	38.510382999999974	3.672556999999998
W	12.842494999999995	41.327517000000003	3.649134999999998
W	11.192021000000004	44.106309000000031	3.574183000000001
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Se	22.403067000000001	-2.521825000000002	4.366005999999996
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Se	4.199907999999998	28.791412000000011	5.158826000000004
Se	25.794713000000016	-2.644794999999998	4.326181000000001
Se	24.086117999999990	0.868964000000000	5.077421000000002
Se	22.403759000000009	3.695825000000001	4.876856000000001
Se	20.762819000000004	6.448982000000000	4.800495999999999
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Se	9.349240999999992	26.198070000000013	4.762588000000000
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Se	17.053179000000001	2.181922000000001	2.429476999999999
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Se	12.090408999999993	10.812630999999997	2.280330000000002
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Se	12.8916810000000002	31.9905539999999995	4.9183310000000002
Se	11.2707020000000000	34.8134190000000032	4.9235139999999999
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Se	18.1433779999999985	31.2533360000000009	1.7797410000000000
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Se	4.1016490000000001	51.9897589999999994	4.8685159999999996
Se	4.6117070000000000	46.0969139999999982	5.2185689999999996
Se	2.4038689999999998	49.2703080000000000	4.6756650000000004
Se	6.1124400000000003	54.5093510000000023	2.8339020000000001

W₁₀₅Se₂₁₀; $E_{tot} = -61\,508\,149.075\,138\,38$ eV; $E_{rel} = 17.137\,321\,342\,8$ meV/f.u.

W	20.8969769999999997	-0.8651890000000000	3.4378129999999998
W	19.1419819999999987	1.8501350000000001	3.4172050000000000
W	17.4571639999999988	4.6217280000000001	3.3862860000000001
W	15.8099100000000004	7.4411940000000003	3.3514759999999999
W	14.1780659999999994	10.2665179999999996	3.3185899999999999
W	12.5530050000000006	13.0924090000000000	3.2959309999999999
W	10.9290570000000002	15.9190939999999994	3.2961559999999999

W	9.313349999999998	18.7497240000000005	3.3162850000000001
W	7.7271400000000003	21.5808339999999994	3.3499270000000001
W	6.1825299999999999	24.3995929999999994	3.3734139999999999
W	4.6480110000000003	27.2370030000000014	3.2617240000000001
W	3.0593819999999998	30.1740560000000002	2.9817399999999998
W	1.4042319999999999	32.8225860000000011	2.9414030000000002
W	24.2191669999999988	-1.0144869999999999	3.3729589999999998
W	22.0450510000000008	1.5316740000000000	3.3505889999999998
W	20.3510710000000010	4.2390900000000000	3.3243350000000000
W	18.6636990000000011	7.0616000000000003	3.3041190000000000
W	16.9996119999999991	9.9198660000000007	3.2820649999999998
W	15.3632390000000001	12.7723289999999992	3.2718820000000002
W	13.7397150000000003	15.6098239999999997	3.2748560000000002
W	12.1192510000000002	18.4377700000000004	3.2859769999999999
W	10.5067140000000006	21.2704759999999986	3.2994050000000001
W	8.9232399999999998	24.0964129999999983	3.3065199999999999
W	7.3994460000000002	26.9067299999999996	3.2768730000000001
W	5.7530340000000004	30.3017900000000004	3.2093959999999999
W	4.5025919999999999	32.6853210000000018	3.0818219999999998
W	27.3714340000000007	-1.0666359999999999	3.3652950000000001
W	28.9487319999999997	1.1718519999999999	3.5594359999999998
W	25.7949570000000001	1.1996590000000000	3.4821200000000001
W	24.2913929999999993	4.8435920000000001	3.4464670000000002
W	22.6408260000000006	7.5809680000000004	3.4800130000000000
W	20.9995650000000005	10.3629840000000009	3.4527120000000000
W	19.3730070000000012	13.1897380000000002	3.4490690000000002
W	17.7523650000000011	16.0344480000000011	3.4607600000000001
W	16.1345400000000012	18.8719360000000016	3.4680240000000002
W	14.5240790000000004	21.6816129999999987	3.4646400000000002
W	12.9234130000000000	24.4919620000000009	3.4706969999999999
W	11.3365760000000009	27.4211920000000013	3.4903080000000002
W	9.6863019999999995	30.2615809999999996	3.3557039999999998
W	7.7772699999999997	32.7796250000000029	3.2301579999999999

W	30.522656999999988	-1.0914640000000000	3.6061369999999999
W	27.5226720000000000	4.8717370000000004	3.3656600000000001
W	25.4382120000000000	7.3374410000000001	3.3472040000000001
W	23.7747589999999995	10.0955490000000001	3.3216850000000000
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W	20.5232899999999994	15.7413779999999992	3.3406430000000000
W	18.9070169999999997	18.5851579999999998	3.3571819999999999
W	17.2957619999999999	21.4101089999999985	3.3611819999999999
W	15.6933279999999993	24.1988899999999987	3.3398379999999999
W	14.1202260000000006	26.9714179999999999	3.3229869999999999
W	12.4020700000000001	30.2092840000000002	3.3200539999999998
W	10.9207529999999995	32.7609390000000005	3.2611640000000000
W	34.3767580000000024	-1.0430219999999999	3.9274410000000000
W	35.4303129999999982	1.6284940000000001	3.6195539999999999
W	32.7414240000000021	1.6291350000000000	3.6234050000000000
W	30.7161830000000009	4.8157110000000003	3.4696669999999998
W	29.3676649999999988	7.3715650000000004	3.4488310000000002
W	27.7002540000000010	10.6524129999999992	3.5087199999999998
W	26.1417280000000005	13.4007740000000002	3.5556190000000001
W	24.5418909999999997	16.1750849999999993	3.5715189999999999
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W	16.4133420000000001	30.2776360000000011	3.4301010000000001
W	14.0533590000000004	32.8514479999999978	3.2103090000000001
W	37.5221540000000005	-0.8991770000000000	3.8341870000000000
W	33.7289349999999999	4.3284360000000000	3.4246590000000001
W	32.1123100000000008	7.2364119999999996	3.4210090000000002
W	30.4896749999999983	10.1698880000000003	3.3508100000000001
W	28.9295900000000010	13.0945879999999999	3.4182329999999999
W	27.3284340000000014	15.8962289999999999	3.4623480000000000
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W	24.0773790000000005	21.5409720000000000	3.4747319999999999
W	22.4427629999999994	24.3946719999999999	3.4654699999999998
W	20.8067150000000005	27.2444920000000010	3.4315730000000002
W	19.1618649999999988	30.0913930000000001	3.3523250000000000
W	17.5330189999999995	32.9211859999999987	3.0087039999999998
W	40.5797919999999976	-0.8702550000000000	3.9023010000000000
W	42.0198600000000013	1.7079040000000001	3.8977089999999999
W	39.3620170000000016	1.6023419999999999	3.7576540000000000
W	37.6473579999999970	4.9793930000000000	3.6935730000000002
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W	38.8402770000000004	7.4807670000000002	3.5835370000000002
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W	32.5375640000000033	18.8006589999999996	3.6120739999999998
W	30.9147019999999983	21.6338420000000013	3.6282169999999998
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Se	8.931608999999999	20.374372000000000	5.198100000000000
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Se	9.315855000000000	26.235126000000000	4.809962999999998
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Se	16.935539999999996	2.160501000000000	2.483114000000000
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Se	24.036992999999989	6.474078999999997	5.315796999999999
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Se	22.6378629999999994	20.7195299999999989	5.4220379999999997
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Se	39.0642429999999976	-2.5945570000000000	4.8090510000000002
Se	37.3676159999999982	0.9061020000000000	5.3654299999999999
Se	35.7022369999999967	3.7657829999999999	5.0569660000000001
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Se	39.0702649999999991	-0.2210480000000000	1.9699030000000000
Se	37.4534859999999981	2.7307760000000001	2.3357060000000001
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Se	34.1207539999999980	8.4002479999999995	2.0999070000000000
Se	32.5293559999999999	11.3163769999999992	2.0802030000000000
Se	30.9414620000000014	14.2040989999999994	2.1029450000000001
Se	29.3343039999999995	17.0404699999999991	2.1505470000000000
Se	27.7146569999999990	19.8631819999999983	2.1678470000000001
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Se	26.6215420000000016	32.4642550000000014	4.5663879999999999
Se	24.6699920000000006	35.0520339999999990	5.2025259999999998
Se	19.3993029999999997	34.2334049999999976	2.1956340000000001
Se	23.2625139999999995	34.1506139999999974	1.7632310000000000
Se	20.8018679999999989	35.6340160000000026	4.8547110000000000

W₁₀₅Se₂₁₀; $E_{tot} = -61\,508\,149.347\,597\,52$ eV; $E_{rel} = 14.542\,472\,390\,4$ meV/f.u.

W	20.6990189999999998	-0.8685420000000000	3.2590990000000000
W	19.0347359999999988	1.8955569999999999	3.4338030000000002
W	17.3474809999999984	4.6572449999999996	3.4175730000000000
W	15.6831929999999993	7.4798450000000001	3.3767429999999998
W	14.0605750000000000	10.3444699999999994	3.3451480000000000
W	12.4639860000000002	13.2137949999999993	3.3306399999999998
W	10.9065159999999999	16.0859150000000000	3.3309359999999999
W	9.4028369999999999	18.9396549999999984	3.3228730000000000
W	7.8630519999999997	21.7829610000000002	3.2119719999999998
W	6.2542220000000004	24.7168559999999999	2.9700920000000002
W	4.5986510000000003	27.3728319999999989	2.9236320000000000
W	24.2055240000000005	-1.3810810000000000	3.2370109999999999
W	21.8374600000000001	1.6738270000000000	3.3167830000000000
W	20.1429149999999986	4.3998290000000004	3.3617349999999999
W	18.4822319999999998	7.1937249999999997	3.3630439999999999
W	16.8485890000000005	10.0382140000000000	3.3500420000000002
W	15.2542380000000009	12.8935040000000001	3.3373940000000002
W	13.6839110000000002	15.7442430000000009	3.2995619999999999
W	12.1330550000000006	18.6184979999999989	3.2458550000000002

W	10.6210710000000006	21.460409999999995	3.2083800000000000
W	8.9380860000000002	24.823458999999997	3.1148080000000000
W	7.7281659999999999	27.2298860000000005	2.9486770000000000
W	27.0157209999999992	-0.9327720000000000	3.4345889999999999
W	28.6839930000000010	1.9042669999999999	3.4208210000000001
W	25.9012810000000009	1.9111350000000000	3.3765399999999999
W	24.2073110000000007	4.8487629999999999	3.5363039999999999
W	22.4915750000000010	7.6477610000000000	3.5327809999999999
W	20.8457340000000002	10.4495410000000000	3.5168499999999998
W	19.2467609999999993	13.2772810000000003	3.5315370000000001
W	17.7002969999999991	16.1635570000000008	3.5403950000000002
W	16.0994160000000015	19.0005999999999986	3.4002370000000002
W	14.5655809999999999	21.4758519999999997	3.2872640000000000
W	12.7249839999999992	25.0066330000000008	3.2024249999999999
W	11.0945870000000006	27.2607759999999999	3.1914549999999999
W	31.1284939999999999	-1.2310120000000000	3.2580179999999999
W	27.3045259999999992	4.3196380000000003	3.4148250000000000
W	25.2608940000000004	7.4559829999999998	3.4135080000000002
W	23.6105310000000017	10.1802720000000004	3.4013439999999999
W	22.0332949999999990	12.9545119999999994	3.4117389999999999
W	20.5100349999999985	15.7296800000000001	3.4485649999999999
W	18.9128070000000008	19.0736799999999995	3.4727830000000002
W	17.6013039999999990	21.4502920000000010	3.4518909999999998
W	15.9499980000000008	25.1134860000000018	3.2636599999999998
W	14.3288659999999997	27.3192100000000018	3.3234290000000000
W	33.9156550000000010	-0.9517660000000000	3.3412120000000001
W	35.5458830000000034	1.8300790000000000	3.4101309999999998
W	32.7543160000000029	1.5865910000000001	3.3426369999999999
W	30.4156820000000003	4.8922200000000000	3.5439099999999999
W	29.3503849999999993	7.4674240000000003	3.4589370000000002
W	27.5909879999999994	10.6844380000000001	3.5721569999999998
W	25.9725430000000017	13.4252179999999992	3.6360920000000001
W	24.4364880000000007	16.2650439999999996	3.6628069999999999

W	22.705097999999996	19.169259000000003	3.5270269999999999
W	20.912580999999994	21.4656239999999983	3.5799919999999998
W	19.223017999999997	25.1590750000000014	3.3463090000000002
W	17.5512489999999985	27.3989459999999987	3.3706480000000001
W	34.4384060000000005	4.4095779999999998	3.3953530000000001
W	32.0993700000000004	7.6659189999999997	3.5747650000000002
W	30.8240470000000002	10.1230790000000006	3.4957989999999999
W	28.718030999999999	13.1977460000000004	3.4937830000000001
W	27.215158999999999	15.847094999999995	3.5330189999999999
W	25.6260440000000003	19.2052769999999988	3.5586250000000001
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W	22.5202939999999998	25.1987670000000001	3.3964330000000000
W	20.7934079999999994	27.4465199999999996	3.4056259999999998
W	37.1865710000000007	4.6273020000000002	3.4566780000000001
W	36.1169000000000011	7.2780240000000003	3.4138549999999999
W	33.7071090000000027	10.4992450000000002	3.6124809999999998
W	32.6876809999999978	13.5057620000000007	3.6095709999999999
W	31.1310299999999991	16.3368129999999994	3.6654730000000000
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W	27.4532309999999988	21.5360370000000003	3.6473870000000002
W	25.8591209999999982	25.2200600000000001	3.4113620000000000
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W	38.8410190000000028	7.4348330000000002	3.4780080000000000
W	37.7773180000000011	10.1576850000000007	3.4107599999999998
W	35.3983029999999985	13.2855609999999995	3.5058769999999999
W	33.8567099999999996	16.0528100000000009	3.4398059999999999
W	32.2717140000000029	18.8312239999999989	3.4420030000000001
W	30.6649799999999999	21.5758979999999987	3.5153189999999999
W	29.1841819999999998	25.2124859999999984	3.3945870000000000
W	27.3376599999999996	27.5070459999999990	3.4351189999999998
W	40.4614690000000010	10.2546710000000001	3.4805450000000002
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W	37.8247959999999992	16.4355629999999984	3.4875710000000000

W	36.2753159999999966	19.275549999999991	3.5029640000000000
W	34.6205539999999985	22.0497990000000001	3.4795150000000001
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W	42.0006160000000008	13.1163340000000002	3.4683660000000001
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Se	13.6403820000000007	11.9970040000000004	5.2013619999999996
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Se	15.6577620000000000	15.0002220000000008	4.8088470000000001
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Se	10.8534740000000003	23.7161320000000018	4.5243460000000004
Se	9.2883169999999993	26.6971960000000017	4.8838640000000000
Se	18.4687710000000003	-0.5077420000000000	2.4932189999999999

Se	16.804864999999995	2.354290999999999	2.415366000000001
Se	15.083615000000000	5.196705999999998	2.434343000000001
Se	13.422879000000000	8.071597000000006	2.406860000000000
Se	11.813731000000006	10.961116999999998	2.358970999999999
Se	10.201624000000007	13.837811000000003	2.388100000000001
Se	8.663339999999998	16.754747999999993	2.328541000000000
Se	7.059548999999996	19.632231000000009	2.418400999999998
Se	5.539431999999997	22.543965000000000	2.159854999999999
Se	4.025449000000001	25.441672000000005	1.709878000000000
Se	2.745070000000001	28.455863999999983	3.662370000000001
Se	22.317689999999989	-0.202038000000000	1.601839000000000
Se	20.447338999999995	2.669235000000000	1.488715000000000
Se	18.786611000000006	5.473497000000001	1.522143999999999
Se	17.150327999999982	8.308659999999997	1.517029000000000
Se	15.541888999999994	11.168981999999997	1.496678000000000
Se	13.948404999999993	14.016391999999997	1.470288000000000
Se	12.353588000000002	16.862386999999982	1.440133000000001
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Se	9.263306999999993	22.750671000000005	1.473184000000000
Se	7.581871999999997	25.614602000000014	1.089704999999999
Se	5.993831000000001	28.808522000000000	1.690411000000001
Se	29.091331000000003	-2.037841999999999	4.739943000000002
Se	27.288730000000010	0.786323000000000	5.242638000000004
Se	25.614209999999999	3.641115000000001	5.237142000000004
Se	23.883659999999990	6.546829999999999	5.363747000000000
Se	22.179954999999996	9.342157000000003	5.365896000000002
Se	20.569396999999986	12.150185999999997	5.364722000000004
Se	19.007688000000017	15.010184999999999	5.372906000000004
Se	17.466751999999996	17.947029000000006	5.292306000000000
Se	15.885476999999998	20.800111999999986	5.255499000000004
Se	14.272221000000000	23.708804000000007	4.749635999999997
Se	12.630146999999991	26.750833000000001	5.115274999999996
Se	32.674492999999982	-2.128026999999999	5.185933000000003

Se	30.7024560000000015	0.8019849999999999	4.7829480000000002
Se	28.9947809999999997	3.6692209999999998	5.2454000000000001
Se	27.2986329999999988	6.5378600000000002	4.8066560000000003
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Se	23.9931449999999984	12.2461739999999999	4.9593790000000002
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Se	20.8119230000000002	17.9304789999999983	4.8592240000000002
Se	19.2004689999999982	20.8498400000000004	5.3210720000000000
Se	17.5575650000000003	23.7611460000000001	4.7868990000000000
Se	15.9081480000000006	26.8629290000000012	5.2045329999999996
Se	25.6209859999999985	-0.0571760000000000	1.5888270000000000
Se	23.8759709999999998	2.7275730000000000	1.9628460000000001
Se	22.1672909999999987	5.5025729999999999	2.0578520000000000
Se	20.4700869999999995	8.3235550000000007	2.0211320000000002
Se	18.8318610000000000	11.1739210000000000	2.0129120000000000
Se	17.2453630000000011	14.0515810000000005	2.0329890000000002
Se	15.6907499999999995	16.8770279999999993	1.9551470000000000
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Se	12.6306209999999997	22.6528370000000017	1.9013110000000000
Se	10.9228780000000008	25.5531369999999995	1.4724670000000000
Se	9.2736359999999998	28.9016489999999990	2.1291810000000000
Se	29.1033590000000011	-0.1567700000000000	1.9165710000000000
Se	27.3416649999999990	2.6916920000000002	1.4548140000000001
Se	25.6998449999999998	5.5905500000000004	1.7093920000000000
Se	23.9173930000000006	8.4483130000000006	1.5501210000000001
Se	22.2816490000000016	11.2665810000000004	1.5544830000000001
Se	20.6752250000000011	14.0846789999999995	1.5657200000000000
Se	19.1302440000000011	17.0363170000000004	1.7349239999999999
Se	17.5165380000000006	19.8509799999999998	1.4875840000000000
Se	15.9927720000000004	22.8311080000000004	1.8390409999999999
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Se	12.5623509999999996	29.0225310000000007	2.4213600000000000
Se	36.2009129999999999	-0.3728660000000000	2.3903040000000000

Se	34.3039300000000011	0.6506810000000000	5.2421889999999998
Se	32.4001140000000021	3.6641300000000001	4.8455190000000004
Se	30.7328800000000015	6.5461760000000000	5.4064690000000004
Se	29.0348940000000013	9.3877679999999994	5.2143730000000001
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Se	25.7610390000000002	15.1241800000000008	5.5001239999999996
Se	24.1602260000000015	18.0728369999999998	5.3737380000000003
Se	22.5146739999999994	20.9010420000000003	5.4146720000000004
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Se	27.4911349999999999	18.0354309999999991	4.9522120000000003
Se	25.8289019999999994	20.9456750000000014	5.4432029999999996
Se	24.1647210000000001	23.8574659999999987	4.8968280000000002
Se	22.4287370000000017	27.0030059999999992	5.2805249999999999
Se	32.4793099999999981	-0.0959160000000000	1.4575370000000001
Se	30.7453690000000002	2.7279860000000000	2.0147330000000001
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Se	23.9931979999999996	14.1530810000000002	2.1159300000000001
Se	22.4381979999999999	16.9549309999999984	2.0995029999999999
Se	20.8456629999999983	19.7629459999999995	1.8059380000000000
Se	19.2402440000000006	22.8396819999999998	2.0105749999999998
Se	17.6092499999999994	25.7533439999999985	1.4717300000000000
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Se	27.3466600000000000	14.2085779999999993	1.6185210000000001
Se	25.8039829999999988	17.1417420000000007	1.8255880000000000
Se	24.1522539999999992	19.9503179999999993	1.6150450000000001
Se	22.5137539999999987	22.8835020000000000	2.0854180000000002
Se	20.8886889999999994	25.7689500000000002	1.5373500000000000
Se	19.1904240000000001	29.0881749999999997	2.3871869999999999
Se	37.5934859999999986	6.2846440000000001	5.3201479999999997
Se	35.7542970000000011	9.3686229999999995	4.8893199999999997
Se	34.0632420000000025	12.2940140000000007	5.3992940000000003
Se	32.4966599999999985	15.2057830000000003	5.4541009999999996
Se	30.8704689999999999	18.0823630000000009	5.4663190000000004
Se	29.1682279999999992	20.9200869999999988	5.4326520000000000
Se	27.4864770000000007	23.8815500000000007	4.8943760000000003
Se	25.7164749999999991	27.0192979999999991	5.2868579999999996
Se	39.2183360000000008	9.1276189999999993	5.3276830000000004
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Se	30.7759099999999997	23.8478850000000016	4.9251750000000003
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Se	35.7940690000000004	5.5526600000000004	1.5799220000000000
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Se	32.2987630000000010	11.4624740000000003	1.8545840000000000
Se	30.6786230000000018	14.2536869999999993	2.1091210000000000
Se	29.1060729999999985	17.0119439999999997	2.1309450000000001
Se	27.5343310000000017	19.8216070000000002	1.9044239999999999
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Se	35.775970999999984	11.268985000000007	2.046943999999999
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Se	32.488796000000007	17.114453000000010	1.624907000000001
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Se	36.061428999999968	21.068013000000005	5.310546999999997
Se	34.152737000000019	23.969174999999999	5.091383999999997
Se	32.290987999999987	26.949531000000003	5.286214000000002
Se	42.901395999999983	15.111795000000008	4.356717999999999
Se	41.388336999999999	18.251432999999987	4.168527000000001
Se	39.685681000000024	21.227152000000002	4.271383000000002
Se	37.984765000000030	24.210972999999992	4.135785000000003
Se	36.043300000000021	27.108902000000005	4.309123999999997
Se	41.245372000000033	8.163997000000002	2.558965000000002
Se	39.166258999999966	11.247474000000004	1.580677000000001
Se	37.446328999999986	14.222505999999992	2.106587999999999
Se	35.838568999999997	17.153293000000015	2.035302000000002
Se	34.222912999999984	19.978729000000013	2.030978999999999
Se	32.515058000000033	22.855419999999987	2.111768999999998
Se	30.812505000000016	25.840212000000011	1.546513000000000
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Se	42.925536999999985	11.191535000000000	2.517230000000001
Se	40.779215000000007	14.264754999999992	1.635284000000000
Se	39.289842999999976	17.249549999999993	1.501057000000001
Se	37.712825000000023	20.093384000000004	1.478939000000000
Se	36.056449999999981	22.893903000000017	1.485690000000000
Se	34.232934999999977	25.697247999999983	1.606128999999999

Se	32.676220000000007	29.1130719999999990	2.4498310000000001
W	30.6924010000000003	-6.5247880000000000	3.2031239999999999
W	32.3217130000000026	-3.7303419999999998	3.3095420000000000
W	29.5585470000000008	-3.9870310000000000	3.1854030000000000
W	27.4703780000000002	-12.1718670000000007	2.9919060000000002
W	28.9391269999999992	-9.4036000000000008	2.9937520000000002
W	27.5038820000000008	-7.1548550000000004	3.1410730000000000
W	25.5500079999999983	-3.7389519999999998	3.2714010000000000
W	26.0062910000000009	-9.4561360000000008	3.0193889999999999
W	24.4080009999999987	-6.8127230000000001	3.0846469999999999
W	22.7157680000000006	-4.1806320000000001	2.9731139999999998
Se	34.5473690000000033	-3.1969430000000001	2.2964289999999998
Se	32.9521519999999981	-6.1125520000000000	2.4378370000000000
Se	30.9238350000000004	-2.9525450000000002	1.3589460000000000
Se	31.1614140000000006	-8.9144620000000003	2.1330950000000000
Se	29.1292070000000010	-5.8460109999999998	1.4748220000000001
Se	27.5272970000000008	-2.9243619999999999	1.8139840000000000
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Se	29.3779350000000008	-11.6998979999999992	1.7043349999999999
Se	27.4334820000000015	-8.7454450000000001	1.1319079999999999
Se	25.8914329999999993	-5.7870929999999996	1.5411090000000001
Se	24.0500779999999992	-3.0683850000000001	1.2775190000000001
Se	27.4988950000000010	-14.3012840000000008	3.7781440000000002
Se	25.4618639999999985	-11.7324929999999998	1.8289489999999999
Se	23.7354740000000000	-9.0234380000000005	2.1412010000000001
Se	22.0342270000000013	-6.3402289999999999	2.1855000000000002
Se	20.5285699999999984	-3.2501970000000000	2.2071779999999999
Se	29.3153919999999992	-7.7831910000000004	4.9122659999999998
Se	27.5165340000000000	-4.9327980000000000	4.5523959999999999
Se	27.5465400000000002	-10.6098750000000006	4.8448520000000004
Se	25.7835169999999998	-7.8185399999999996	4.9405250000000001
Se	24.0748029999999993	-5.0851340000000000	4.9128829999999999

$W_{105}Se_{210}$; $E_{tot} = -61\,508\,149.350\,902\,72$ eV; $E_{rel} = 14.510\,994\,295\,2$ meV/f.u.

W	19.413647999999985	1.3328660000000001	3.2947229999999998
W	17.785744999999986	4.1688000000000001	3.2792560000000002
W	16.1546050000000001	6.9987009999999996	3.2920110000000000
W	14.5007280000000005	9.8221319999999999	3.3221750000000001
W	12.8665269999999996	12.6493420000000008	3.3583840000000000
W	11.2909509999999997	15.4743239999999993	3.3728419999999999
W	9.6996219999999997	18.2936900000000016	3.2135159999999998
W	7.8235760000000001	21.7045220000000008	3.0743689999999999
W	6.3357910000000004	24.4429809999999996	3.2505630000000001
W	4.8256930000000002	27.1459210000000013	3.2374730000000000
W	3.1719819999999999	29.7497560000000014	3.2583579999999999
W	6.3009259999999996	29.6731000000000016	3.1960959999999998
W	22.2026609999999991	1.0676980000000000	3.3042899999999999
W	20.5819049999999990	3.8941509999999999	3.3013729999999999
W	18.9590040000000002	6.7172200000000002	3.3039730000000000
W	17.3044270000000004	9.5497879999999995	3.3348010000000001
W	15.6369209999999992	12.3857230000000005	3.3427090000000002
W	14.0128029999999999	15.2048939999999995	3.3224010000000002
W	12.4727890000000006	18.0322619999999993	3.2810310000000000
W	11.1006230000000006	21.6346670000000003	3.2424830000000000
W	9.6015519999999999	23.9249340000000004	3.3540040000000002
W	7.5597640000000004	27.3106289999999987	3.3043279999999999
W	28.9632289999999983	1.2964070000000001	3.3841090000000000
W	26.2189140000000016	1.5076440000000000	3.4905339999999998
W	24.6064480000000003	4.2860740000000002	3.5005959999999998
W	22.9941379999999995	7.1475450000000000	3.5321210000000001
W	21.3537379999999999	9.9238180000000007	3.5312260000000002
W	19.6577370000000009	12.8397629999999996	3.5725140000000000
W	18.0041270000000004	15.6579590000000000	3.5436260000000002
W	16.4546150000000004	18.3820580000000007	3.4205350000000001
W	14.3587579999999999	21.6662110000000006	3.3273679999999999

W	12.7924290000000003	23.9060370000000013	3.4467590000000001
W	11.3336210000000008	27.5732339999999994	3.2842110000000000
W	9.6703460000000003	29.7933990000000009	3.3468550000000001
W	27.3882230000000000	3.9895179999999999	3.3404850000000001
W	25.7938699999999983	6.7672369999999997	3.3895360000000001
W	24.1436470000000014	9.7979889999999994	3.4850010000000000
W	22.6451449999999994	12.3671749999999996	3.4967229999999998
W	20.7334670000000010	15.5866910000000001	3.4944150000000000
W	19.3218919999999983	18.1492919999999991	3.4829880000000002
W	17.6291040000000017	21.6449630000000006	3.3889360000000002
W	16.0492260000000009	23.9227200000000018	3.4940210000000000
W	14.5186060000000001	27.6126490000000011	3.3045339999999999
W	12.9022830000000006	29.8602319999999999	3.3969250000000000
W	32.8519170000000003	0.8361070000000000	3.3968029999999998
W	31.2915090000000014	4.5475370000000002	3.3869319999999998
W	29.8479010000000002	7.1836070000000003	3.5871800000000000
W	28.2548980000000007	9.8286239999999996	3.5233590000000001
W	25.6284990000000015	12.6675559999999994	3.5645539999999998
W	24.7001379999999990	15.7594989999999999	3.5251160000000001
W	22.4309890000000003	18.0890750000000011	3.5231520000000001
W	21.1136960000000009	21.7474799999999995	3.4119180000000000
W	19.3722589999999997	23.9507289999999990	3.5544500000000001
W	17.7713539999999988	27.6261410000000005	3.3376690000000000
W	16.1075039999999987	29.8882919999999999	3.3683450000000001
W	34.5545400000000029	4.4354760000000004	3.2528329999999999
W	32.9712120000000013	6.7076300000000000	3.4542790000000001
W	30.9846590000000006	10.0576690000000006	3.5843769999999999
W	29.7250869999999985	12.6363249999999994	3.5051960000000002
W	27.8152879999999989	15.9160799999999991	3.5532960000000000
W	26.3150620000000011	18.4363540000000015	3.5310750000000000
W	24.3312449999999991	21.7003360000000001	3.4553400000000001
W	22.6627830000000010	23.9925919999999984	3.5681609999999999
W	21.0793630000000007	27.6473680000000002	3.3652519999999999

W	19.3383670000000016	29.9054159999999989	3.3762680000000000
W	36.1319919999999968	7.3615719999999998	3.4255480000000000
W	35.0064550000000025	9.9196369999999998	3.3960669999999999
W	32.4380930000000021	12.8256759999999996	3.5434230000000002
W	30.7213080000000005	15.5798220000000001	3.4237730000000002
W	29.0935780000000008	18.3919579999999989	3.4437310000000001
W	27.4155559999999987	21.1697430000000004	3.4053770000000001
W	25.8521450000000002	23.9539459999999984	3.5164860000000000
W	24.3943140000000014	27.6335279999999983	3.3724249999999998
W	22.5896459999999983	29.9229519999999987	3.4021940000000002
W	37.6742180000000033	10.1094290000000004	3.5174840000000001
W	36.4570870000000014	12.7044090000000001	3.4116710000000001
W	34.7336179999999999	16.0817760000000014	3.5517650000000001
W	33.1045530000000028	18.8769430000000007	3.5840869999999998
W	31.4414760000000015	21.6774410000000017	3.5804100000000001
W	29.7628570000000003	24.4623320000000000	3.5544220000000002
W	27.6161239999999992	27.5309670000000004	3.4097759999999999
W	25.8416609999999984	29.8884369999999997	3.4264839999999999
W	39.0974440000000030	12.9605599999999992	3.4840939999999998
W	37.4709410000000034	15.8901459999999997	3.4578110000000000
W	35.8487330000000028	18.6672499999999992	3.4726469999999998
W	34.2204490000000021	21.4318489999999997	3.5178929999999999
W	32.5726429999999993	24.1895330000000008	3.4757319999999998
W	30.9005660000000013	26.9464280000000009	3.4588510000000001
W	29.0805030000000002	29.7472490000000001	3.4629189999999999
Se	20.6037469999999985	0.1657380000000000	5.1847110000000001
Se	18.9674639999999997	2.9712529999999999	5.1563530000000002
Se	17.3408739999999995	5.7916889999999999	5.1550750000000001
Se	15.6944510000000008	8.6090780000000002	5.1777899999999998
Se	14.0559419999999999	11.4375630000000008	5.2096260000000001
Se	12.4584949999999992	14.2968750000000000	5.2319009999999997
Se	10.8853740000000005	17.2370459999999994	5.1720069999999998
Se	9.2580139999999993	20.3411870000000015	4.7474420000000004

Se	7.7411519999999996	23.3098929999999989	5.0367800000000003
Se	6.1708509999999999	26.1226050000000001	5.1235530000000002
Se	4.6024940000000001	29.0305870000000006	5.0784750000000001
Se	24.2162199999999999	0.3440270000000000	4.8186380000000000
Se	22.5834079999999986	3.1526960000000002	4.8079559999999999
Se	20.9585320000000017	5.9766810000000001	4.8055770000000004
Se	19.3188800000000001	8.7986939999999993	4.8252689999999996
Se	17.6360519999999994	11.6442990000000002	4.8385069999999999
Se	15.9851299999999998	14.4945000000000004	4.8481759999999996
Se	14.3665669999999999	17.3417950000000012	4.8248680000000004
Se	12.6524940000000008	20.2526149999999987	4.7377620000000000
Se	11.1114569999999997	23.2599629999999991	5.2255649999999996
Se	9.5408890000000000	26.2280970000000018	4.6579360000000003
Se	7.9309209999999997	29.1873910000000016	5.0804489999999998
Se	17.1554549999999999	1.9205950000000001	2.3059180000000001
Se	15.5395850000000006	4.7677680000000002	2.2703350000000002
Se	13.8894610000000007	7.5945660000000004	2.3061919999999998
Se	12.2249940000000006	10.4312339999999999	2.3510460000000002
Se	10.6030029999999993	13.3242379999999994	2.3249710000000001
Se	8.9130230000000008	16.1749790000000004	2.4542999999999999
Se	7.5787190000000004	19.3556409999999985	2.1900879999999998
Se	5.5782239999999996	22.1549769999999988	2.3570199999999999
Se	4.0637090000000002	24.9579309999999985	2.3625250000000002
Se	2.5508080000000000	27.7948179999999994	2.0889169999999999
Se	20.8888700000000007	2.1859989999999998	1.4502440000000001
Se	19.2700150000000008	5.0203840000000000	1.4449010000000000
Se	17.6430450000000008	7.8664370000000003	1.4667330000000001
Se	15.9861109999999993	10.6880229999999994	1.4907079999999999
Se	14.3104030000000009	13.4985590000000002	1.4840450000000001
Se	12.6801139999999997	16.3447449999999996	1.4462680000000001
Se	11.1089199999999995	19.3988739999999993	1.5905879999999999
Se	9.4342720000000000	22.2992770000000000	1.3644810000000001
Se	7.9256219999999997	25.2476729999999989	1.6823230000000000

Se	6.1080620000000003	28.0542219999999993	1.3268169999999999
Se	4.4929990000000002	31.1973890000000011	1.9607479999999999
Se	27.5812880000000007	0.4100270000000000	5.3448859999999998
Se	25.9640340000000016	3.2053859999999998	5.3299409999999998
Se	24.3325159999999983	6.0039189999999998	5.3409630000000003
Se	22.6812760000000004	8.8163370000000008	5.3754600000000003
Se	21.0027919999999995	11.6797319999999996	5.3489209999999998
Se	19.3337760000000003	14.5416399999999992	5.3861220000000003
Se	17.6907089999999982	17.4322979999999994	5.3540150000000004
Se	15.9837760000000006	20.3678130000000017	4.9525550000000003
Se	14.3964110000000005	23.3021050000000010	5.2997670000000001
Se	12.8448200000000003	26.2164329999999985	4.8119490000000003
Se	11.2596900000000009	29.2808640000000011	5.2266849999999998
Se	30.9253490000000006	0.3227660000000000	4.9030790000000000
Se	29.4502479999999984	3.3134070000000002	4.8816629999999996
Se	27.8137289999999986	6.0517040000000000	4.8680050000000001
Se	26.1879510000000018	8.8783689999999993	4.8901399999999997
Se	24.2849089999999990	11.6551919999999996	5.3612520000000004
Se	22.7268989999999995	14.5941949999999991	4.8258669999999997
Se	20.9443869999999990	17.3715750000000000	5.3668790000000000
Se	19.3734339999999996	20.3761779999999995	4.8434119999999998
Se	17.7056089999999990	23.3103839999999991	5.3240850000000002
Se	16.0958140000000007	26.2361350000000009	4.8180209999999999
Se	14.5087419999999998	29.3798470000000016	5.2411050000000001
Se	24.2025630000000014	2.1975600000000002	1.9709280000000000
Se	22.5763120000000015	5.0544900000000004	2.0013130000000001
Se	20.9590360000000011	7.8673289999999998	1.9854730000000000
Se	19.3180909999999990	10.7194830000000003	2.0569340000000000
Se	17.6469960000000015	13.5510719999999996	2.0436429999999999
Se	15.9957320000000003	16.3664379999999987	1.9890150000000000
Se	14.4290649999999996	19.3211280000000016	2.0062609999999999
Se	12.7517750000000003	22.2689319999999995	1.4649040000000000
Se	11.2170310000000004	25.2935620000000014	1.8809199999999999

Se	9.4710789999999996	28.1106690000000015	1.6102909999999999
Se	7.7999879999999999	31.3796689999999998	2.3241070000000001
Se	27.6677779999999984	2.2707869999999999	1.4930040000000000
Se	26.0166560000000011	5.0880150000000004	1.5250459999999999
Se	24.4370569999999994	7.9993960000000000	1.6573410000000000
Se	22.7493669999999995	10.7405089999999994	1.5725760000000000
Se	21.1166860000000014	13.6517339999999994	1.7873810000000001
Se	19.3675759999999997	16.4905760000000008	1.5569530000000000
Se	17.8581789999999998	19.4363039999999998	1.7519119999999999
Se	16.0303679999999993	22.2624120000000012	1.5346910000000000
Se	14.4645050000000008	25.3067659999999997	1.9753930000000000
Se	12.8805060000000005	28.2671950000000010	1.4375389999999999
Se	11.1273879999999998	31.5684949999999986	2.5559010000000000
Se	32.9683560000000000	3.1030300000000000	4.7760809999999996
Se	31.3677250000000001	6.1266530000000001	5.3435379999999997
Se	29.6371919999999989	8.9268180000000008	5.4261210000000002
Se	27.7276540000000011	11.7810159999999993	5.0249930000000003
Se	26.1260559999999984	14.6416380000000004	5.1856450000000001
Se	24.3823749999999997	17.5813150000000000	5.1569190000000003
Se	22.6310970000000005	20.3734360000000017	4.9478689999999999
Se	21.0289889999999993	23.3771270000000015	5.3876499999999998
Se	19.3874279999999999	26.2700609999999983	4.8398969999999997
Se	17.7296130000000005	29.4298169999999999	5.2359700000000000
Se	34.8188910000000007	6.0788229999999999	5.1703150000000004
Se	33.0257829999999970	8.9682449999999996	4.8227469999999997
Se	31.1805340000000015	11.8143379999999993	5.4436109999999998
Se	29.3461679999999987	14.6239200000000000	5.2177379999999998
Se	27.7555319999999988	17.6014100000000013	5.4589020000000001
Se	25.9152449999999988	20.4133829999999996	5.1829409999999996
Se	24.3324609999999986	23.3611150000000016	5.4057550000000001
Se	22.6867340000000013	26.2949039999999989	4.8755839999999999
Se	20.9707550000000005	29.4537939999999985	5.2512290000000004
Se	31.0791019999999989	2.2453699999999999	2.0432500000000000

Se	29.402142999999988	5.1753790000000004	1.9299050000000000
Se	27.8254750000000008	7.8691709999999997	2.0221950000000000
Se	26.187833999999987	10.7583050000000000	2.0804499999999999
Se	24.294357999999990	13.6866140000000005	1.8409050000000000
Se	22.691981999999994	16.4190180000000012	1.8238660000000000
Se	21.0529520000000012	19.4887200000000007	2.0091540000000001
Se	19.3714990000000000	22.3369560000000007	1.6340690000000000
Se	17.758123999999987	25.303243999999994	2.0273919999999999
Se	16.1461770000000016	28.2261510000000015	1.4779420000000001
Se	14.4698410000000006	31.542712999999991	2.3649580000000001
Se	34.459505999999975	2.1606429999999999	1.7653740000000000
Se	32.911876999999969	5.0435860000000003	1.4965830000000000
Se	31.3396250000000016	8.0809619999999995	1.8550420000000001
Se	29.5271410000000003	10.889488999999993	1.6472140000000000
Se	27.6829110000000007	13.6927280000000007	2.2160600000000001
Se	26.1278080000000017	16.6129590000000000	1.6946749999999999
Se	24.3178930000000015	19.3947700000000012	2.1755949999999999
Se	22.7340990000000005	22.3711790000000015	1.5923060000000000
Se	21.062554999999997	25.340817999999987	2.0502270000000000
Se	19.4268670000000014	28.219052999999988	1.5168779999999999
Se	17.7842370000000010	31.5597190000000012	2.3624040000000002
Se	36.442394999999977	8.9596499999999999	5.3463570000000002
Se	34.5311110000000028	11.9005559999999999	4.9667399999999997
Se	32.809179999999978	14.887278999999995	4.9702180000000000
Se	31.131851999999985	17.6630660000000006	4.9246610000000004
Se	29.4299420000000005	20.535803999999988	4.9212090000000002
Se	27.802931999999984	23.331590999999995	4.9728029999999999
Se	25.9585940000000015	26.2410180000000004	4.9141199999999996
Se	24.226935999999985	29.4223940000000006	5.2715329999999998
Se	37.959839999999998	11.8306670000000000	5.3597370000000000
Se	36.1838720000000009	14.758264999999997	5.1749960000000002
Se	34.508338999999994	17.770241999999996	5.4104799999999997
Se	32.793411999999965	20.586622999999995	5.4210589999999996

Se	31.1380380000000017	23.4388089999999991	5.4046709999999996
Se	29.2893979999999985	26.3574979999999996	5.1820399999999998
Se	27.4879679999999986	29.3360100000000017	5.3024969999999998
Se	36.6237270000000024	5.1453660000000001	2.1582520000000001
Se	34.5592510000000033	8.0261669999999992	1.7119860000000000
Se	32.9559089999999983	10.9202910000000006	2.0088970000000002
Se	31.0737519999999989	13.7864319999999996	1.6577560000000000
Se	29.3705630000000006	16.6334909999999994	1.6251329999999999
Se	27.6926230000000011	19.4709220000000016	1.6134649999999999
Se	26.0053120000000000	22.3148899999999983	1.6181530000000000
Se	24.3539610000000017	25.3498160000000006	2.0302530000000001
Se	22.7312089999999998	28.2524489999999986	1.5396220000000000
Se	21.0958709999999989	31.5892799999999987	2.4075750000000000
Se	38.4234349999999978	7.9220050000000004	2.5608540000000000
Se	36.3650960000000012	10.9893009999999993	1.5513090000000000
Se	34.4595130000000012	13.8792290000000005	2.1521629999999998
Se	32.7427449999999993	16.7480340000000005	2.0962459999999998
Se	31.0811619999999991	19.5638649999999998	2.1036410000000001
Se	29.4130310000000001	22.3791060000000002	2.0923550000000000
Se	27.6996690000000001	25.2328690000000009	2.1163430000000001
Se	26.0573750000000004	28.2447189999999999	1.5540339999999999
Se	24.4472260000000006	31.6051220000000015	2.4609570000000001
Se	39.9168239999999983	14.9547260000000009	4.4322809999999997
Se	38.2638359999999977	17.9784770000000016	4.3172180000000004
Se	36.5030670000000015	20.8361310000000017	4.5197180000000001
Se	34.7862709999999993	23.7139249999999997	4.5321680000000004
Se	33.1251790000000028	26.6364120000000000	4.3070740000000001
Se	31.2212420000000002	29.5222979999999993	4.4293370000000003
Se	40.0579430000000016	11.0196710000000007	2.5510730000000001
Se	37.8277190000000019	14.0800269999999994	1.6661120000000000
Se	36.2042220000000015	16.9845609999999994	1.6076490000000001
Se	34.6050990000000027	19.8013049999999993	1.6412780000000000
Se	32.9770889999999994	22.5543480000000010	1.6436010000000001

Se	31.262346999999983	25.302690999999994	1.6125560000000001
Se	29.475322999999995	28.0895490000000017	1.6572279999999999
Se	27.9159310000000005	31.5179119999999990	2.4753300000000000
W	26.1382750000000001	-9.8523589999999999	2.9249260000000001
W	22.7132930000000002	-4.2411040000000000	3.3689629999999999
W	24.402138999999982	-6.9946979999999996	3.2439460000000002
W	27.591370999999988	-7.6029890000000000	3.1637279999999999
W	25.496342999999995	-4.4447380000000001	3.2748260000000000
W	29.5616780000000006	-4.2059709999999999	3.3613729999999999
W	21.054445999999987	-1.4784539999999999	3.3377970000000001
W	23.8340560000000004	-1.7232970000000001	3.3136890000000001
W	27.8989620000000009	-1.2790750000000000	3.5077080000000000
W	31.045716999999998	-1.8184670000000001	3.3742540000000001
Se	25.6841720000000002	-12.1056500000000007	1.5699770000000000
Se	23.914864999999989	-9.3631150000000005	2.1046550000000002
Se	27.641736999999991	-9.115892999999998	1.0981620000000001
Se	22.1307690000000008	-6.6207250000000002	2.4784649999999999
Se	25.9612200000000009	-6.2603049999999998	1.5313829999999999
Se	29.2302460000000011	-6.2040579999999999	1.6079520000000000
Se	20.474450999999984	-3.7613010000000000	2.3490929999999999
Se	24.126319999999998	-3.4409660000000000	1.4335990000000001
Se	27.5736400000000010	-3.3850760000000002	1.9240459999999999
Se	31.032703999999990	-3.5256609999999999	1.4381860000000000
Se	25.7875170000000011	-8.2950429999999997	4.9113150000000001
Se	24.037355999999991	-5.4184479999999997	5.1746930000000004
Se	27.548535999999986	-5.3998840000000001	4.6042180000000004
Se	22.505759999999987	-0.6423170000000000	1.4586410000000001
Se	25.8779240000000001	-0.6281530000000000	2.0224940000000000
Se	29.4405690000000000	-0.5513209999999999	1.7018960000000001
Se	32.713191999999994	-0.8453730000000000	1.5586949999999999
Se	22.2779880000000006	-2.6255199999999999	5.2223819999999996
Se	25.8681480000000015	-2.4668570000000001	4.8293499999999998
Se	29.300028999999985	-2.5310069999999998	5.1952439999999998

Se	18.795073999999996	-0.924335000000000	2.334649000000000
W	29.047201000000012	-9.885597999999999	2.986731999999999
W	27.598115000000000	-12.617312000000001	2.833565999999998
W	30.748221999999984	-7.151737999999999	3.179117999999999
Se	27.596979999999985	-14.778988999999993	3.527585000000000
Se	27.548024999999991	-11.128909999999994	4.749965000000000
Se	29.593278999999990	-12.113879000000007	1.682600000000001
Se	29.337258999999995	-8.321747000000002	4.942433000000003
Se	31.348380999999998	-9.422757000000007	2.213282000000000
Se	30.894549000000014	-5.541281999999998	5.094593999999998
W	32.343398000000005	-4.496133000000004	3.294023999999998
Se	33.050344000000026	-6.677196999999996	2.355208999999999
Se	32.608682000000017	-2.816803000000002	5.217185999999999
W	33.981095000000034	-1.784772999999999	3.446403999999998
Se	34.785781999999975	-3.904785000000000	2.571085000000001
Se	34.266105000000031	-0.111268000000000	5.374850999999996
W	35.565758000000024	0.995803000000000	3.606094999999998
Se	36.500956000000022	-0.982360000000000	2.751459000000001
Se	36.616711999999997	2.873330999999999	4.552876999999996
Se	1.346671000000000	30.807486000000008	4.096724000000000

$W_{105}Se_{210}$; $E_{tot} = -61\,508\,150.632\,896\,76\text{ eV}$; $E_{rel} = 2.301\,527\,247\,6\text{ meV/f.u.}$

W	21.057976000000000	-1.058972000000000	3.398898000000000
W	19.254743000000013	1.794567000000000	3.450320000000001
W	17.596253000000008	4.579385000000003	3.443712000000001
W	15.973129999999994	7.385234999999998	3.388507000000002
W	14.345271000000003	10.208968999999997	3.371602999999999
W	12.738538000000001	13.031805000000003	3.381319000000000
W	11.169057000000005	15.842776000000006	3.361079000000001
W	9.571175000000002	18.647604999999987	3.168499999999999
W	7.658809999999999	22.037537000000004	2.985002000000002
W	6.148854000000000	24.749504000000017	3.119339999999998

W	4.6142390000000004	27.4592339999999986	3.0571009999999998
W	2.9440450000000000	30.0541230000000006	3.0114770000000002
W	24.2936259999999997	-1.2381340000000001	3.4020480000000002
W	22.5746080000000013	1.1183170000000000	3.4746720000000000
W	20.4075829999999989	4.2835510000000001	3.3652340000000001
W	18.7815970000000014	7.0524269999999998	3.3547400000000001
W	17.1528889999999983	9.8928340000000006	3.3643790000000000
W	15.5071209999999997	12.7462140000000002	3.3552900000000001
W	13.8873449999999998	15.5744600000000002	3.3163600000000000
W	12.3525600000000004	18.3971839999999993	3.2580930000000001
W	10.9428280000000004	21.9898130000000016	3.1857210000000000
W	9.4196100000000005	24.2658869999999993	3.2818450000000001
W	7.3443589999999999	27.6359020000000015	3.1817020000000000
W	6.0717939999999997	29.9865379999999995	3.0356990000000001
W	27.5253319999999988	-1.3174370000000000	3.3996640000000000
W	29.1060769999999991	0.9264990000000000	3.5021830000000000
W	25.7824670000000005	0.9860200000000000	3.4957560000000001
W	24.3545839999999991	4.6819160000000002	3.3914080000000002
W	22.8237409999999983	7.4591609999999999	3.5334819999999998
W	21.1767099999999999	10.2742059999999995	3.5164149999999998
W	19.5419230000000006	13.1798409999999997	3.5641470000000002
W	17.8936169999999990	16.0090469999999989	3.5315880000000002
W	16.3405290000000001	18.7393220000000014	3.4045550000000002
W	14.2168019999999995	22.0303879999999985	3.2901639999999999
W	12.6144029999999994	24.2612160000000010	3.4086660000000002
W	11.1150110000000009	27.9189599999999984	3.2292109999999998
W	9.4290430000000001	30.1288599999999995	3.2621799999999999
W	27.5563019999999987	4.6180430000000001	3.3701099999999999
W	25.9466740000000016	6.9063400000000001	3.5273650000000001
W	23.9829229999999995	10.2587019999999995	3.4976600000000002
W	22.5831909999999993	12.6795760000000008	3.5256479999999999
W	20.6359899999999996	15.9649049999999999	3.5013869999999998
W	19.2040730000000011	18.4981119999999990	3.4718849999999999

W	17.5222160000000002	22.0253009999999989	3.3675329999999999
W	15.8878710000000005	24.2920669999999994	3.4736910000000001
W	14.2937449999999995	27.9784199999999998	3.2864830000000000
W	12.6555710000000001	30.2175970000000014	3.3643120000000000
W	35.5761540000000025	1.0299240000000001	3.5494080000000001
W	32.3836119999999994	0.9388649999999999	3.5271910000000002
W	30.8010410000000014	4.6157029999999999	3.4036190000000000
W	29.1887960000000000	6.8556910000000002	3.5786509999999998
W	27.6976270000000007	10.5069409999999994	3.4762140000000001
W	25.9299989999999987	12.6802600000000005	3.6566109999999998
W	24.3969139999999989	16.3090779999999995	3.4898189999999998
W	22.5504299999999986	18.4804299999999984	3.6254119999999999
W	20.9117630000000005	22.1407820000000015	3.4070930000000001
W	19.1864670000000004	24.3566290000000016	3.5245099999999998
W	17.5343410000000013	28.0274229999999989	3.3358960000000000
W	15.8516539999999999	30.2747250000000001	3.3739270000000001
W	34.0542230000000004	4.6497549999999999	3.4445760000000001
W	32.4714039999999997	6.8792080000000002	3.5937999999999999
W	30.8162179999999992	10.5482569999999996	3.4290790000000002
W	29.1788729999999994	12.7956020000000006	3.6133620000000000
W	27.5916740000000011	16.4261589999999984	3.4450740000000000
W	25.8610350000000011	18.6273580000000010	3.6018789999999998
W	24.1335049999999995	22.2159699999999987	3.4080910000000002
W	22.4354839999999989	24.4437730000000002	3.5452370000000002
W	20.8276420000000009	28.0934980000000003	3.3636230000000000
W	19.0714149999999982	30.3312309999999989	3.4028800000000001
W	42.4972980000000007	1.8512150000000001	3.6482250000000001
W	39.4587590000000006	1.5884469999999999	3.6918039999999999
W	37.3219810000000010	4.7110620000000001	3.5853860000000002
W	35.7125720000000015	6.9410330000000000	3.6230419999999999
W	33.9794229999999970	10.6084010000000006	3.4439829999999998
W	32.3348480000000009	12.8357969999999995	3.5767300000000000
W	30.8371940000000002	16.4907070000000004	3.4260419999999998

W	29.144795999999995	18.709578000000005	3.585205999999999
W	27.455999999999995	22.349374000000001	3.358034000000000
W	25.622999000000001	24.503609000000009	3.532408999999999
W	24.125109999999994	28.130167000000001	3.361537000000002
W	22.318000000000014	30.392610000000012	3.428658000000000
W	40.893866000000027	4.031672999999996	3.639104999999998
W	38.821795000000016	7.361056999999997	3.642863999999999
W	37.733888999999978	10.327427000000001	3.587060000000001
W	36.127302000000002	12.977672000000001	3.487708000000000
W	34.038651000000015	16.473243000000001	3.468631999999999
W	32.448273999999978	18.762651999999992	3.594612999999998
W	30.755960000000017	22.374765000000000	3.448411999999998
W	29.302461999999985	24.657830000000006	3.487257000000001
W	27.329847999999984	28.069133999999983	3.377831000000000
W	25.575603000000010	30.390194999999985	3.447719999999999
W	45.618231999999990	1.885520000000001	3.603368000000001
W	43.918109000000012	4.311010999999997	3.748146000000002
W	42.350659999999978	6.900731000000004	3.825464000000002
W	40.458958000000026	10.279604000000009	3.698595000000001
W	38.856020999999984	13.004528999999998	3.437695999999999
W	37.268729999999979	16.035952999999992	3.497548000000001
W	35.779707000000019	18.640461999999994	3.667612999999998
W	33.900424999999985	22.083926000000017	3.668110000000000
W	32.277866000000031	24.720013000000016	3.540814000000001
W	30.690574000000016	27.397904000000005	3.498492000000002
W	28.832104999999985	30.249618999999991	3.454575999999999
Se	22.228304999999989	-2.850791000000001	4.354104000000004
Se	20.693145999999987	0.597186000000000	5.216310000000000
Se	18.898178000000015	3.433241999999999	5.302652000000001
Se	17.197814000000010	6.227890000000004	5.271177999999999
Se	15.545159999999992	9.018739000000001	5.242653999999999
Se	13.928794999999991	11.840303999999997	5.242968000000003
Se	12.339242000000005	14.694570000000006	5.238597000000004

Se	10.7513100000000001	17.617823999999998	5.1437590000000002
Se	9.0977420000000002	20.698139999999997	4.6811080000000000
Se	7.5389790000000003	23.6514850000000010	4.9385100000000000
Se	5.9212829999999999	26.4464720000000000	4.9750470000000000
Se	4.3285429999999998	29.3549219999999984	4.8782680000000003
Se	25.7089140000000000	-2.9673959999999999	4.3741450000000004
Se	24.1166039999999988	0.3732490000000000	5.3158019999999997
Se	22.4715190000000007	3.4169269999999998	4.7608730000000001
Se	20.7979109999999991	6.3029039999999998	4.8607500000000003
Se	19.1710969999999996	9.1402750000000008	4.8483060000000000
Se	17.5098360000000000	12.0024409999999992	4.8359430000000003
Se	15.8657979999999998	14.8667829999999999	4.8412309999999996
Se	14.2404279999999996	17.7215519999999991	4.8086099999999998
Se	12.5035360000000004	20.6250099999999996	4.6978770000000001
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Se	9.3085249999999995	26.5702779999999983	4.5778299999999996
Se	7.6607630000000002	29.5176249999999989	4.9611570000000000
Se	18.9088120000000011	-0.7849590000000000	2.4692259999999999
Se	17.0377760000000009	2.1085340000000001	2.6208179999999999
Se	15.3881470000000000	5.0355939999999997	2.4341070000000000
Se	13.7458580000000001	7.9194040000000001	2.3827769999999999
Se	12.1063880000000008	10.7914720000000006	2.3654869999999999
Se	10.4777269999999998	13.6764820000000000	2.3426779999999998
Se	8.8014130000000002	16.5253410000000009	2.4063829999999999
Se	7.4415699999999996	19.6799019999999985	2.1268470000000002
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Se	3.8891260000000001	25.2575199999999995	2.1851460000000000
Se	2.3674309999999998	28.0855589999999999	1.8432180000000000
Se	1.0878350000000001	31.1112059999999992	3.7817409999999998
Se	22.6368280000000013	-0.6480640000000000	1.5469560000000000
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Se	19.0427579999999992	5.2914339999999997	1.5076290000000001
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Se	12.5579870000000007	16.7023569999999992	1.4308149999999999
Se	10.9883690000000005	19.7488320000000002	1.5501220000000000
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Se	5.9355409999999997	28.3580159999999992	1.1679459999999999
Se	4.2918050000000001	31.4937439999999995	1.7355000000000000
Se	29.1330820000000017	-0.8122170000000000	1.5480959999999999
Se	27.4375709999999984	0.3086200000000000	5.3068809999999997
Se	25.8315780000000004	3.2521390000000001	4.8789030000000002
Se	24.2253140000000009	6.2978139999999998	5.3141280000000002
Se	22.5596180000000004	9.1585029999999996	5.3458139999999998
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Se	19.2273539999999983	14.8970649999999996	5.3687430000000003
Se	17.5707570000000004	17.7892420000000016	5.3418720000000004
Se	15.8509279999999997	20.7355319999999992	4.9103490000000001
Se	14.2146489999999996	23.6652799999999992	5.2634850000000002
Se	12.6192940000000000	26.5717660000000002	4.7755830000000001
Se	10.9910499999999995	29.6282339999999991	5.1693569999999998
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Se	29.1285470000000011	3.2076920000000002	4.8736819999999996
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Se	17.5319530000000015	23.6949350000000010	5.3063159999999998
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Se	24.2176979999999986	2.4217740000000001	1.9763610000000000

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Se	17.5235449999999986	13.9030980000000000	2.0394850000000000
Se	15.8751929999999994	16.7295979999999993	1.9802839999999999
Se	14.3080250000000007	19.6893619999999991	1.9779920000000000
Se	12.6141640000000006	22.6333969999999987	1.4233070000000001
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Se	30.8168119999999988	6.2341189999999997	5.3952330000000002
Se	29.2286709999999985	9.1369589999999992	4.9867059999999999
Se	27.5922480000000014	12.0958740000000002	5.4652120000000002
Se	25.9575560000000003	15.0013150000000000	4.9936309999999997
Se	24.2366530000000004	17.9459319999999991	5.4358919999999999
Se	22.5357480000000017	20.8024500000000003	4.9239499999999996
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Se	29.2041739999999983	15.0821609999999993	4.9518540000000000
Se	27.5374060000000007	18.0671859999999995	5.4185540000000003
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Se	20.7075279999999999	29.8717469999999992	5.2728330000000003
Se	30.7903270000000013	2.3347549999999999	2.0459010000000002
Se	29.1847689999999993	5.2518430000000000	1.5673990000000000
Se	27.6044119999999999	8.2835560000000008	2.0534189999999999
Se	25.8547060000000002	11.0767260000000007	1.7853470000000000
Se	24.2831709999999994	14.0522460000000002	2.0952280000000001
Se	22.5333399999999990	16.8449179999999998	1.7961140000000000
Se	20.9317549999999990	19.8591809999999995	2.0518950000000000
Se	19.2113489999999985	22.7326310000000014	1.5954109999999999
Se	17.5565660000000001	25.7170909999999999	2.0056500000000002
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Se	39.0645730000000029	3.3948670000000001	5.2959079999999998
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Se	34.0816560000000024	8.3011049999999997	2.0937030000000001
Se	32.4328259999999986	11.2425719999999991	1.5804990000000001
Se	30.7961419999999997	14.1974370000000008	2.0527000000000002
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Se	25.7560690000000001	22.8751779999999982	1.5689869999999999
Se	24.0858899999999991	25.8388320000000000	2.0035750000000001
Se	22.4588010000000011	28.7523589999999984	1.5393289999999999
Se	20.8022850000000012	32.0594180000000009	2.4651369999999999
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Se	39.2072580000000031	5.3298290000000001	2.0808890000000000
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Se	29.1373399999999982	22.9207749999999990	1.5900140000000000
Se	27.4087460000000007	25.8024610000000010	2.0953080000000002
Se	25.7745530000000009	28.7850290000000015	1.5355129999999999
Se	24.1562570000000001	32.1024639999999977	2.4992549999999998
Se	46.1431490000000011	3.8078660000000002	4.9074460000000002
Se	44.5772929999999974	6.5715570000000003	4.6759399999999998
Se	42.6200440000000000	9.2166599999999992	4.6782349999999999
Se	41.2107120000000009	12.3775739999999992	4.5040769999999997
Se	39.6040050000000008	15.2948540000000008	4.1533470000000001
Se	38.0393889999999999	18.2257530000000010	4.4526329999999996
Se	36.0167379999999966	21.0883150000000015	4.5702319999999999
Se	34.6042259999999970	24.2443680000000015	4.4908659999999996
Se	32.9121430000000004	27.0826999999999991	4.3626170000000002
Se	31.0648139999999984	29.9562729999999995	4.2638660000000002
Se	44.1648110000000003	2.5582140000000000	1.7961220000000000
Se	42.4658829999999980	5.2941820000000002	1.8999550000000001
Se	40.8855130000000031	8.2591750000000008	2.1527340000000001
Se	39.2808050000000009	11.2498050000000003	1.6806270000000001
Se	37.5295139999999989	14.2307120000000005	1.6939000000000000
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Se	34.3254120000000000	20.0591909999999984	2.0797279999999998
Se	32.5823570000000018	22.9222450000000002	1.7180690000000001
Se	30.8462059999999987	25.7339389999999995	1.6716190000000000
Se	29.2393859999999997	28.5693139999999985	1.6800459999999999
Se	27.6496470000000016	31.9965510000000002	2.4517000000000002
W	30.7535479999999986	-1.3313330000000001	3.3910019999999998
Se	29.0858740000000004	-3.0082320000000000	4.3668269999999998

Se	32.346220999999999	-0.757520000000000	1.528581000000000
W	33.938648000000000	-1.270254000000000	3.355449999999999
Se	32.467187000000002	-2.993332000000001	4.366111000000001
Se	35.580053999999970	-0.586145000000000	1.512635000000000
W	37.158633999999993	-1.138906999999999	3.320195000000000
Se	35.945687999999970	-2.974896999999999	4.146917000000002
Se	39.293906999999973	-0.991592000000000	2.354693999999998
Se	47.498368999999967	0.958187000000000	2.732791999999999

W₁₀₅Se₂₁₀; $E_{tot} = -61\,508\,150.655\,888\,57$ eV; $E_{rel} = 2.082\,557\,628\,5$ meV/f.u.

W	20.843405000000006	-0.998712000000000	3.496475000000002
W	19.054894000000009	1.708074000000001	3.482997000000001
W	17.352078999999998	4.482440999999997	3.469028999999999
W	15.709467999999993	7.310793000000003	3.463448000000001
W	14.124167999999992	10.150539999999995	3.479039999999999
W	12.605484000000006	12.989945000000005	3.459571000000000
W	11.074690999999996	15.822920999999991	3.259799999999998
W	9.219621999999993	19.231871999999992	3.006937000000002
W	7.743517999999999	22.055061999999995	3.125150000000001
W	6.274531999999998	24.717568000000000	3.042934999999999
W	4.666665000000001	27.332499999999996	3.012294999999999
W	24.196173999999992	-1.134927000000000	3.384903000000000
W	21.967562999999984	1.405499000000001	3.377545000000000
W	20.239515999999983	4.102674999999996	3.361870999999998
W	18.545434000000002	6.927547999999998	3.370505999999998
W	16.898468999999986	9.801529999999996	3.376819999999999
W	15.317064999999995	12.661509000000006	3.369383000000000
W	13.836316999999993	15.518777000000000	3.320955000000001
W	12.483992999999999	19.144702999999998	3.227024999999998
W	11.019992000000002	21.461611999999988	3.292411000000000
W	9.031454000000001	24.876030000000001	3.168574000000000
W	7.803124999999996	27.236504000000000	3.024744000000001

W	27.393036999999996	-1.1550100000000001	3.3243369999999999
W	29.001063999999995	1.0897330000000001	3.4850180000000002
W	25.7744140000000002	1.1074340000000000	3.4477000000000002
W	24.165870999999992	4.7222119999999999	3.4305560000000002
W	22.5210110000000014	7.4406100000000004	3.4832000000000001
W	20.8948229999999988	10.2218339999999994	3.4833229999999999
W	19.3363160000000001	13.0261940000000003	3.5068009999999998
W	17.8141439999999989	15.8072800000000004	3.4294850000000001
W	15.762971999999995	19.1261930000000007	3.3212079999999999
W	14.217838999999997	21.3883629999999982	3.4315289999999998
W	12.8212620000000008	25.0707510000000013	3.2061240000000000
W	11.1760020000000004	27.315927999999995	3.2331759999999998
W	30.5458640000000017	-1.1269849999999999	3.3328240000000000
W	27.4165670000000006	4.8122499999999997	3.3014169999999998
W	25.3772750000000009	7.1512830000000003	3.3652289999999998
W	23.7044020000000017	9.9137489999999993	3.3324769999999999
W	22.0892139999999984	12.7130379999999992	3.3576380000000001
W	20.5851720000000000	15.5096969999999992	3.3819870000000001
W	19.0882259999999988	19.0605539999999998	3.3755370000000000
W	17.5135509999999996	21.3443860000000001	3.5030880000000000
W	15.9929159999999992	25.0540769999999995	3.2661330000000000
W	14.4224200000000007	27.3408160000000002	3.3129780000000002
W	33.7839129999999983	-1.0159629999999999	3.3505259999999999
W	36.2182310000000030	1.6918500000000001	3.7627769999999998
W	32.1958690000000018	1.1504859999999999	3.5109599999999999
W	30.6621880000000004	4.7710119999999998	3.3708459999999998
W	29.1794809999999991	7.0830650000000004	3.4526729999999999
W	27.5871110000000002	10.4915959999999995	3.4744820000000001
W	26.0641430000000014	13.1819190000000006	3.5380970000000000
W	24.5336660000000002	15.9400209999999998	3.5239829999999999
W	22.4716820000000013	19.1231560000000016	3.4106510000000001
W	20.8249299999999984	21.3418889999999983	3.5409549999999999
W	19.2178889999999996	25.0291749999999986	3.3182640000000001

W	17.6428580000000004	27.3259289999999986	3.3031809999999999
W	33.8499460000000028	4.7693390000000004	3.5316960000000002
W	32.2353579999999980	7.0394530000000000	3.4997500000000001
W	30.3733600000000017	10.1125959999999999	3.3808829999999999
W	28.8459429999999983	12.9176020000000005	3.3781240000000001
W	27.3014329999999994	15.6199030000000008	3.4254069999999999
W	25.6280280000000005	19.0213999999999999	3.4615149999999999
W	24.1153869999999984	21.3579660000000011	3.5660390000000000
W	22.4905560000000015	25.0271229999999996	3.3656139999999999
W	20.8881279999999983	27.3099330000000009	3.3367810000000002
W	42.4222699999999975	1.9213860000000000	3.7838630000000002
W	39.3020119999999977	1.9035210000000000	3.7901150000000001
W	37.7571110000000019	4.3668740000000001	3.6230449999999998
W	35.9530320000000003	7.6814260000000001	3.5941860000000001
W	34.4063710000000000	10.5022190000000002	3.5828929999999999
W	32.8292879999999982	13.3511450000000007	3.5743980000000000
W	31.1628340000000001	16.2014190000000013	3.5798540000000001
W	29.4613429999999994	18.9746330000000007	3.5350700000000002
W	27.4059099999999987	21.3158439999999985	3.5960969999999999
W	25.7686379999999993	25.0289189999999984	3.3929079999999998
W	24.1368749999999999	27.2972360000000016	3.4034740000000001
W	40.4691600000000022	4.4329049999999999	3.6287630000000002
W	38.7539749999999970	7.2865560000000000	3.4514440000000000
W	37.1771109999999965	10.1796729999999993	3.4420080000000000
W	35.5931259999999980	13.0279650000000000	3.4356870000000002
W	33.9680669999999978	15.8827549999999995	3.4240529999999998
W	32.3022050000000007	18.6937719999999992	3.4063949999999998
W	30.6397079999999988	21.4177810000000015	3.4548269999999999
W	29.0340379999999989	25.0090779999999988	3.4143859999999999
W	27.3648899999999990	27.2778060000000018	3.4888070000000000
W	48.7895060000000029	1.9648289999999999	3.9949300000000001
W	45.6917720000000003	2.0636800000000002	3.8896329999999999
W	44.4042400000000015	4.4307040000000004	3.7490910000000000

W	42.709086999999967	7.8217220000000003	3.6498409999999999
W	41.1702200000000005	10.6319250000000007	3.6009050000000000
W	39.5761600000000016	13.4695459999999994	3.5760079999999999
W	37.9488360000000000	16.3383019999999988	3.5625100000000001
W	36.2785000000000011	19.2092899999999993	3.5509490000000001
W	34.5629220000000004	22.0433519999999987	3.5388060000000001
W	32.8166909999999987	24.7437949999999987	3.5075400000000001
W	30.5964330000000011	27.2545849999999987	3.4804119999999998
W	47.0979549999999989	4.5942959999999999	3.9531480000000001
W	45.4651840000000007	7.5124110000000002	3.6607150000000002
W	43.9098380000000006	10.3363110000000002	3.5280990000000001
W	42.3546049999999994	13.1494289999999996	3.5197360000000000
W	40.76364800000000034	15.9819499999999994	3.5101950000000000
W	39.1345049999999972	18.8200399999999988	3.4891980000000000
W	37.4731400000000008	21.6523579999999995	3.4646029999999999
W	35.7539310000000015	24.4375259999999983	3.4381590000000002
W	33.9498269999999991	27.1384380000000007	3.4056600000000001
Se	22.1776920000000004	-2.7061060000000001	4.4347159999999999
Se	20.4250760000000007	0.5967150000000000	5.3328020000000000
Se	18.6670179999999988	3.3546830000000001	5.3157199999999998
Se	16.9762570000000004	6.1400189999999997	5.3089089999999999
Se	15.3560909999999993	8.9636800000000001	5.3205020000000003
Se	13.7864780000000007	11.8329170000000001	5.3254440000000001
Se	12.2443410000000004	14.7818249999999995	5.2344970000000002
Se	10.6261910000000004	17.9028759999999991	4.7412729999999996
Se	9.1065819999999995	20.8774639999999998	4.9362529999999998
Se	7.6013460000000004	23.7392910000000015	4.9771619999999999
Se	6.0647320000000002	26.6395489999999988	4.8677469999999996
Se	25.6297089999999983	-2.8781520000000000	4.2218999999999998
Se	23.9133770000000005	0.5604900000000000	5.0945600000000004
Se	22.2804539999999989	3.4728409999999998	4.8726750000000001
Se	20.5790199999999999	6.2513930000000002	4.8385090000000002
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Se	16.8413809999999984	2.0315129999999999	2.5539679999999998
Se	15.1215150000000005	4.9422699999999997	2.5377239999999999
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Se	10.2502410000000008	13.7131039999999995	2.5166740000000001
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Se	6.9799020000000001	19.7167780000000015	2.3102770000000001
Se	5.5210290000000004	22.5356710000000007	2.1457790000000001
Se	4.0366150000000003	25.3717630000000014	1.8516180000000000
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Se	20.5220419999999990	2.3433269999999999	1.5489590000000000
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Se	7.6078409999999996	25.6008670000000009	1.1636169999999999
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Se	29.0255669999999988	-2.8046150000000001	4.3878389999999996
Se	27.3513190000000002	0.4190400000000000	5.2990870000000001
Se	25.7320959999999985	3.3768389999999999	4.8640429999999997
Se	23.9347710000000014	6.3343629999999997	5.3176769999999998
Se	22.2707709999999999	9.1345720000000004	5.3144039999999997

Se	20.663482999999994	11.929354999999993	5.3364240000000001
Se	19.0981759999999987	14.7985310000000005	5.3317059999999996
Se	17.3882359999999991	17.8101999999999983	4.9286320000000003
Se	15.8070819999999994	20.7699509999999989	5.2874400000000001
Se	14.2784969999999998	23.7125729999999990	4.7755820000000000
Se	12.7473410000000005	26.7997200000000007	5.1303369999999999
Se	32.5278190000000009	-2.8155380000000001	4.2043309999999998
Se	30.6472520000000017	0.4098260000000000	5.3281000000000001
Se	28.9697530000000008	3.4066399999999999	4.8383070000000004
Se	27.2936329999999998	6.4777920000000000	5.1053509999999998
Se	25.6992100000000008	9.2863509999999998	4.8715760000000001
Se	24.0887090000000015	12.0380450000000003	4.8704989999999997
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Se	19.1504329999999996	20.7221709999999995	5.3247530000000003
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Se	16.0124430000000011	26.8636079999999993	5.1723129999999999
Se	25.7444859999999984	-0.6041299999999999	1.4953230000000000
Se	23.9999649999999995	2.4612579999999999	2.0541489999999998
Se	22.1907129999999988	5.2694879999999999	1.9725590000000000
Se	20.5190589999999986	8.0761330000000005	1.9893630000000000
Se	18.8799250000000001	10.9392829999999996	1.9981199999999999
Se	17.3019379999999998	13.7931580000000000	2.0102250000000002
Se	15.7985489999999995	16.7821609999999986	2.0162149999999999
Se	14.1647069999999999	19.7462510000000009	1.4587460000000001
Se	12.6774629999999995	22.7817730000000012	1.8277000000000001
Se	10.9788650000000008	25.6218159999999990	1.5064900000000001
Se	9.3472190000000008	28.9076559999999994	2.1468590000000001
Se	28.9824330000000003	-0.5901210000000000	1.4806660000000000
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Se	25.6854690000000012	5.3755509999999997	1.5315909999999999
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Se	22.3330810000000000	11.0167389999999994	1.5121760000000000

Se	20.7467140000000008	13.8568390000000008	1.5149410000000001
Se	19.1984379999999994	16.8445460000000011	1.6960270000000000
Se	17.4577889999999982	19.7026170000000000	1.5455000000000001
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Se	14.3872319999999991	25.7306600000000003	1.3697809999999999
Se	12.6665790000000005	29.0708200000000012	2.4633280000000002
Se	35.9496129999999994	-0.9134470000000000	2.4468019999999999
Se	34.1494459999999975	0.5783130000000000	5.1680080000000004
Se	32.2836900000000000	3.3801530000000000	4.9378919999999997
Se	30.6808210000000017	6.3874740000000001	5.3700859999999997
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Se	27.4541329999999988	12.1111780000000007	5.3806669999999999
Se	25.8460239999999999	14.9074840000000002	5.4001320000000002
Se	24.0794660000000000	17.8406909999999996	5.1221389999999998
Se	22.4586359999999985	20.7658629999999995	5.3810599999999997
Se	20.8270209999999985	23.6682440000000014	4.8409909999999998
Se	19.2428029999999985	26.8769670000000005	5.1890260000000001
Se	37.6939479999999989	0.3172830000000000	5.0564410000000004
Se	35.7455259999999981	3.6135440000000001	5.1719379999999999
Se	34.0269899999999978	6.5398310000000004	5.2333639999999999
Se	32.3875710000000012	9.3264390000000006	4.8746910000000003
Se	30.8392969999999984	12.1843789999999998	4.8819809999999997
Se	29.2336020000000012	14.9857289999999992	4.9742509999999998
Se	27.5025469999999999	17.8223589999999987	4.8357500000000000
Se	25.7834479999999999	20.7025870000000012	5.3848599999999998
Se	24.1339520000000007	23.6673319999999983	4.8817539999999999
Se	22.4805390000000003	26.8677069999999993	5.2392880000000002
Se	32.2278809999999964	-0.4989040000000000	1.5078149999999999
Se	30.6862400000000015	2.4926550000000001	1.9824390000000001
Se	29.0586459999999995	5.4065040000000000	1.5178190000000000
Se	27.3451799999999992	8.2970559999999995	2.0584570000000002
Se	25.6535210000000014	11.1279310000000002	1.9368060000000000
Se	24.0570440000000012	13.9113939999999996	2.0352549999999998

Se	22.503067999999990	16.806917999999996	2.0763760000000002
Se	20.7978379999999987	19.7062169999999988	1.6033390000000001
Se	19.197279999999992	22.7180749999999989	2.0132710000000000
Se	17.6266740000000013	25.6433299999999988	1.4353579999999999
Se	15.993432999999996	28.996708999999992	2.2858890000000001
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Se	32.4002580000000009	5.3355740000000003	1.5912880000000000
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Se	39.1396009999999990	3.5557249999999998	5.6126540000000000
Se	37.3600449999999995	6.3697410000000003	5.2846050000000000
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Se	34.1640480000000011	12.2206469999999996	5.4085089999999996
Se	32.5432750000000013	15.0846000000000000	5.3901009999999996
Se	30.8689760000000000	17.9415399999999998	5.3794649999999997
Se	29.1519930000000009	20.7458789999999986	5.3643390000000002
Se	27.4273759999999989	23.6569989999999990	4.8934699999999998
Se	25.7247379999999986	26.8154439999999994	5.3068039999999996
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Se	40.7656619999999990	6.5894190000000004	5.0277029999999998
Se	39.1901989999999998	9.4142250000000001	4.9144569999999996
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Se	35.9735349999999983	15.1813979999999997	4.9151109999999996
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Se	32.6281529999999975	20.8617060000000016	4.9171709999999997

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Se	37.6475819999999999	2.4131070000000001	1.8812000000000000
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Se	32.4229010000000031	11.2231930000000002	2.0780979999999998
Se	30.8196890000000003	14.0577089999999991	2.0651290000000002
Se	29.1768500000000017	16.8350940000000016	2.0297570000000000
Se	27.5224730000000015	19.6437640000000009	1.8056760000000001
Se	25.8328980000000001	22.7020349999999986	2.0811549999999999
Se	24.1575799999999994	25.6092189999999995	1.5363970000000000
Se	22.5561010000000017	28.9673529999999992	2.3726240000000001
Se	40.9169190000000000	2.5704400000000001	1.9076489999999999
Se	39.1534570000000031	5.4745130000000000	1.7431360000000000
Se	37.4179760000000030	8.4136849999999992	1.6369800000000001
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Se	34.2463679999999968	14.1535519999999995	1.6068009999999999
Se	32.5948599999999971	16.9785830000000004	1.5963590000000001
Se	30.8988970000000016	19.7932899999999989	1.5748380000000000
Se	29.0781099999999988	22.7396150000000006	2.0082339999999999
Se	27.4472980000000000	25.6539159999999988	1.5653120000000000
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Se	45.7385220000000032	3.6534209999999998	5.7927239999999998
Se	44.0714479999999966	6.5259080000000003	5.3855659999999999
Se	42.5197170000000000	9.5294270000000001	5.4775140000000002
Se	40.9071789999999993	12.3563740000000006	5.4243160000000001
Se	39.2932169999999985	15.2100170000000006	5.3956730000000004
Se	37.6528619999999989	18.0834319999999984	5.3765109999999998
Se	35.9906879999999987	20.9588199999999993	5.3605859999999996
Se	34.2666719999999998	23.8018749999999990	5.3477639999999997
Se	32.3524799999999999	26.6452899999999993	5.2473900000000002
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Se	49.3121920000000031	3.8764379999999998	5.2574639999999997
Se	47.7918590000000023	6.7629080000000004	4.7539939999999996
Se	46.2646769999999989	9.6639990000000004	4.4347760000000003
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Se	37.9670399999999972	24.1356670000000015	4.3505609999999999
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Se	34.2651409999999998	19.8771449999999987	2.0678800000000002
Se	32.5396280000000004	22.6560109999999995	2.0211579999999998
Se	30.9011980000000008	25.5575699999999983	1.7695620000000001
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Se	45.8771810000000002	5.6523040000000000	1.9858720000000001
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Se	41.1407540000000012	14.3309540000000002	1.6582790000000001
Se	39.5256159999999994	17.1610270000000007	1.6482550000000000
Se	37.8683720000000008	19.9860679999999995	1.6330960000000001
Se	36.1610360000000028	22.7834879999999984	1.6095020000000000
Se	34.3944109999999981	25.5412640000000017	1.5755999999999999
Se	32.6274250000000023	28.8403829999999992	2.4445510000000001

$\mathbf{W}_{105}\mathbf{Se}_{210}$; $E_{tot} = -61\,508\,150.874\,557\,12$ eV; $E_{rel} = 0$ meV/**f.u.**

W	20.9423579999999987	-1.0462370000000001	3.4031669999999998
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W	19.2611750000000015	1.6877489999999999	3.3841139999999998
W	17.5685250000000011	4.4702960000000003	3.3366829999999998
W	15.8955210000000005	7.2866190000000000	3.2911500000000000
W	14.2393549999999998	10.1190320000000007	3.2759190000000000
W	12.5938859999999995	12.9536540000000002	3.3007330000000001
W	10.9791650000000001	15.7891069999999996	3.3632360000000001
W	9.4269700000000007	18.6203380000000003	3.4020220000000001
W	7.8629129999999998	21.4448490000000014	3.2398250000000002
W	5.9989359999999996	24.8593940000000018	3.0153680000000000
W	4.5307779999999998	27.6138259999999995	3.1294070000000000
W	3.0450770000000000	30.3312379999999990	3.0493340000000000
W	1.4182150000000000	32.9435920000000024	2.9970460000000001
W	23.7176699999999983	-1.2636959999999999	3.3051930000000000
W	22.0552419999999998	1.4787980000000001	3.3511950000000001
W	20.3560920000000003	4.2507859999999997	3.3497830000000000
W	18.6759279999999990	7.0597279999999998	3.3047110000000002
W	17.0246740000000010	9.8749079999999996	3.2814700000000001
W	15.3872020000000003	12.6911740000000002	3.2862200000000001
W	13.7497380000000007	15.5117989999999999	3.3072720000000002
W	12.1479099999999995	18.3291569999999986	3.3255910000000002
W	10.6324109999999994	21.1586220000000012	3.3083019999999999
W	9.2754729999999999	24.7703099999999985	3.2275820000000000
W	7.8100009999999997	27.0729949999999988	3.3057650000000001
W	5.7843429999999998	30.4724700000000013	3.1767210000000001
W	4.5442419999999997	32.8349779999999996	3.0188980000000001
W	27.7817730000000012	-0.9544890000000000	3.4140419999999998
W	28.9322440000000007	1.8301559999999999	3.4124490000000001
W	26.1370410000000000	1.8443149999999999	3.4877440000000002
W	24.3982239999999990	4.7375939999999996	3.5651109999999999
W	22.6542420000000000	7.5434000000000001	3.5141300000000002
W	21.0332700000000017	10.3323070000000001	3.4902570000000002
W	19.4119010000000003	13.1395239999999998	3.4937170000000002
W	17.7776749999999986	15.9463259999999991	3.4961880000000001

W	16.167000999999991	18.728206000000001	3.514746000000001
W	14.607286000000002	21.507747999999994	3.469703000000000
W	12.539920000000004	24.764496999999986	3.335280000000000
W	11.008530999999996	27.022715000000016	3.441279000000002
W	9.555281000000008	30.697427000000011	3.231383000000001
W	7.910929999999996	32.936010000000031	3.239433000000000
W	30.797357999999991	-1.546448000000000	3.339761999999999
W	27.391590000000008	4.286768000000004	3.435927000000000
W	25.381468999999992	7.387436000000001	3.404853999999998
W	23.784749999999989	10.111148999999993	3.383248000000000
W	22.179857999999994	12.890957999999995	3.394314000000001
W	20.551819999999993	15.694556999999996	3.398054000000001
W	18.936685000000007	18.468928999999993	3.391395000000002
W	17.367903999999993	21.199849000000004	3.399586999999999
W	15.716468000000008	24.629345000000007	3.436808999999998
W	14.264438999999994	26.986529000000009	3.525299000000000
W	12.730442000000000	30.696283000000011	3.303710000000001
W	11.148021000000000	32.970649000000016	3.352548999999998
W	34.092742999999987	-0.912836000000000	3.508899000000000
W	35.697026000000010	1.807482000000000	3.624937000000001
W	32.967333000000036	1.568813999999999	3.418022999999998
W	30.469792000000018	4.643614999999996	3.527420999999999
W	29.391904000000003	7.673853000000003	3.546091000000001
W	27.844601000000008	10.486625999999993	3.594927999999999
W	26.225753000000010	13.308681999999992	3.618856000000001
W	24.577173999999994	16.147881999999992	3.633436000000001
W	22.921793999999984	18.987704000000008	3.631686000000002
W	21.254417000000001	21.806588000000014	3.611721000000002
W	19.575585000000002	24.556934999999993	3.551476000000001
W	17.525200000000017	26.933569999999996	3.584295000000000
W	15.949998000000008	30.667822000000010	3.371931000000000
W	14.352643000000005	32.955213000000005	3.391109000000002
W	34.525199999999981	4.315062000000002	3.457695999999999

W	32.1272170000000017	7.4437319999999998	3.4590770000000002
W	30.5916050000000013	10.2191170000000007	3.4219550000000001
W	29.0038379999999982	13.0193379999999994	3.4636070000000001
W	27.3631749999999982	15.8497760000000003	3.4866700000000002
W	25.7040049999999987	18.7002020000000009	3.4914990000000001
W	24.0422380000000011	21.5392079999999986	3.4749539999999999
W	22.3861460000000001	24.3176430000000003	3.4364819999999998
W	20.7395020000000017	27.0237170000000013	3.4716700000000000
W	19.1945230000000002	30.6271909999999998	3.4228770000000002
W	17.5532439999999994	32.9141090000000034	3.4833550000000000
W	37.2351299999999981	4.5646829999999996	3.5667789999999999
W	36.1250840000000011	7.7139930000000003	3.5521750000000001
W	34.6246679999999998	10.5386810000000004	3.5690469999999999
W	33.0196929999999966	13.4181450000000009	3.5871719999999998
W	31.3713930000000012	16.2863119999999988	3.6125660000000002
W	29.7124769999999998	19.1365170000000013	3.6245470000000002
W	28.0498699999999985	21.9862900000000003	3.6167250000000002
W	26.3700450000000011	24.8377760000000016	3.5927970000000000
W	24.6557700000000004	27.6630679999999991	3.5699939999999999
W	22.9235720000000001	30.3609599999999986	3.5317750000000001
W	20.7604949999999988	32.8713010000000025	3.5008330000000001
W	38.7722329999999999	7.5140750000000001	3.4721500000000001
W	37.3005270000000024	10.3966139999999996	3.4794200000000002
W	35.7359440000000035	13.2397100000000005	3.4986609999999998
W	34.1179910000000035	16.0632510000000011	3.5232600000000001
W	32.4874719999999968	18.8744410000000009	3.5411790000000001
W	30.8517599999999987	21.6790640000000003	3.5417090000000000
W	29.2117429999999985	24.4832140000000003	3.5220880000000001
W	27.5598719999999986	27.2844709999999999	3.4919699999999998
W	25.8661029999999990	30.0520239999999994	3.4693179999999999
W	24.0854800000000004	32.7519149999999968	3.4474459999999998
Se	22.2550649999999983	-2.2275130000000001	5.2147059999999996
Se	20.5063579999999988	0.5612360000000000	5.2623689999999996

Se	18.776883999999990	3.329677999999999	5.229795000000000
Se	17.094812000000000	6.124659000000000	5.177041000000000
Se	15.442795000000000	8.934945000000000	5.146256000000000
Se	13.801940000000000	11.747932000000000	5.151333000000000
Se	12.188603999999998	14.572765999999997	5.195845000000000
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