

Supporting Information

Exploration of the potential energy surface in mixed Zintl Clusters applying an automatic Johnson Polyhedra generator: The case of Arachno $E_6M_2^{4-}$ (E = Si, Ge, Sn; M = Sb, Bi)

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Figure S1. Isosurface and contour plot for B_z^{ind} and the external field (NICS_{zz}). The isosurface value is set to $\pm 3,0$ ppm. Blue: long range shielding regions; Red: deshielding regions. PBE0/def2-TZVP.

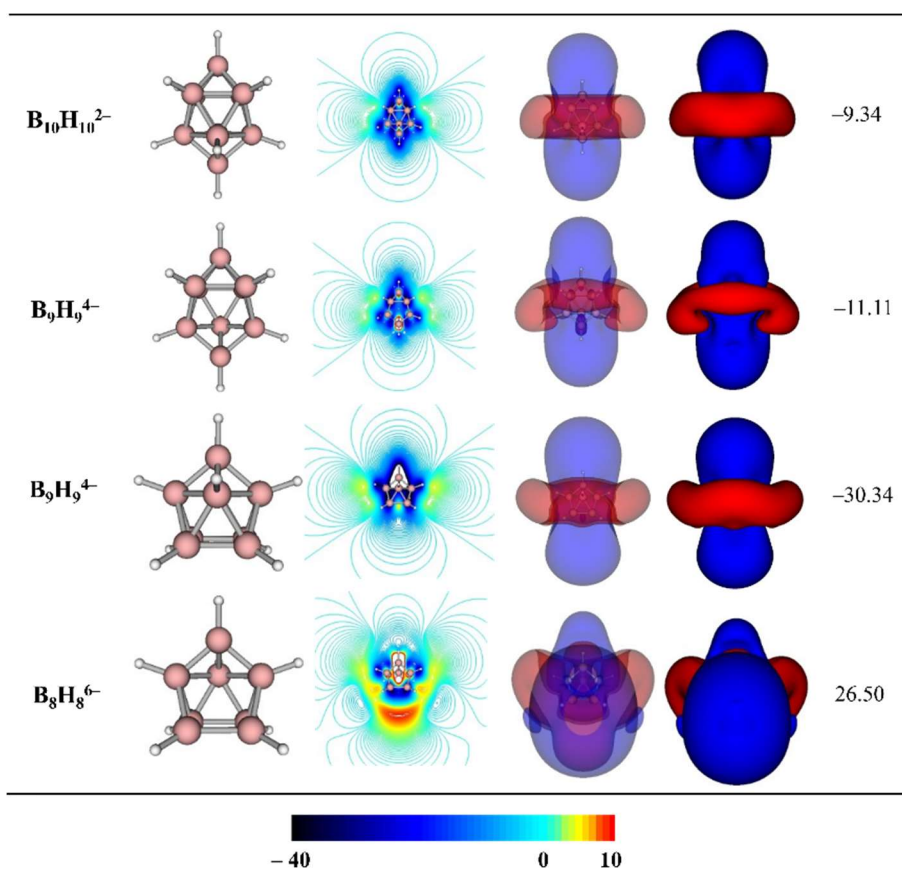
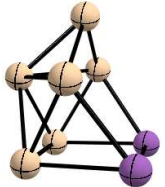
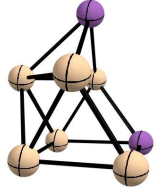
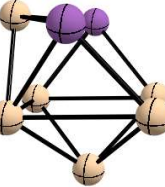
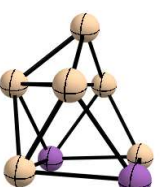
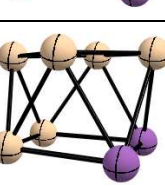
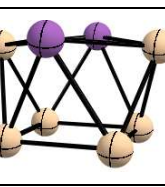
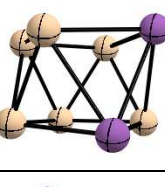
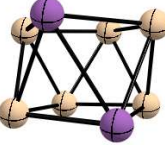

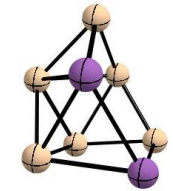
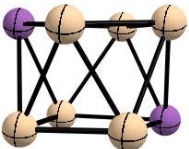
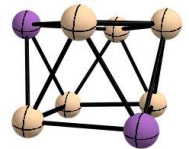


Table S1. Lower energy structures in the singlet state below 10 kcal·mol⁻¹ for the systems studied, with their respective coordinates. In addition the energy (kcal·mol⁻¹) at the PBE0-D3/Def2TZVP (PCM,Solvent=Water) level and in bold DLPNO-CCSD(T) def2-QZVPP/C CPCM(water).

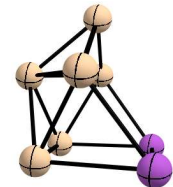
Si₆Sb₂⁴⁻					
	Sb	1.383577750	1.419815000	-1.788756000	0.00
	Sb	1.383577750	-1.419815000	-1.788756000	
	Si	-1.303477250	-1.249460000	-1.788756000	
	Si	-1.303477250	1.249460000	-1.788756000	
	Si	-0.040050250	0.000000000	1.788756000	
	Si	-0.096197250	-1.875011000	0.323650000	
	Si	-1.876266250	0.000000000	0.245938000	
	Si	-0.096197250	1.875011000	0.323650000	
	Sb	0.099144580	0.084714330	1.846922572	3.81
	Si	-0.191745784	2.025139370	0.105584114	
	Si	-1.405872548	1.171902703	-1.848297291	
	Si	-1.953003119	-0.053007702	0.201878910	
	Sb	1.264349813	1.245113878	-1.922045991	
	Si	-1.349004919	-1.364527591	-1.760213448	
	Si	0.065836433	-1.948440532	0.178708751	
	Si	1.093949332	-1.391346312	-1.857133560	
	Sb	-0.188282512	2.037353220	1.714808132	4.09
	Si	-1.691826889	-0.124064774	1.915917996	
	Sb	0.113860318	-2.040561927	1.717547155	
	Si	-1.637605286	1.120821066	-0.285942090	
	Si	-1.454513304	-1.350306793	-0.284282302	
	Si	1.655753269	-1.043976779	-0.179461776	
	Si	1.483834182	1.276354461	-0.181020278	
	Si	0.037211097	0.001604353	-1.716177643	
	Si	-0.331722000	-0.031426000	-1.919178000	5.43
	Sb	-2.016154000	-0.645360000	0.103100000	
	Si	-1.370476000	1.792461000	-0.604921000	
	Si	1.173888000	1.700534000	-0.980955000	
	Si	0.196552000	2.696781000	0.942367000	
	Sb	1.733989000	-0.913715000	-0.335516000	
	Si	0.039711000	-1.236992000	1.658215000	
	Si	1.319931000	0.758129000	1.751129000	
	Sb	-1.510894000	-1.045314000	-0.182058000	6.63
	Si	0.000048000	-0.244274000	2.007229000	
	Si	-1.691746000	1.249148000	1.076577000	
	Sb	1.510818000	-1.045408000	-0.182070000	
	Si	1.691813000	1.249057000	1.076591000	
	Si	0.000142000	2.729911000	0.101935000	
	Si	-1.207196000	1.316222000	-1.467866000	
	Si	1.207217000	1.316135000	-1.468000000	
	Sb	-1.981951000	0.314565000	0.000000000	7.34
	Si	-0.256904000	1.957799000	1.256365000	
	Si	-0.256904000	1.957799000	-1.256365000	
	Si	-0.256904000	-0.447502000	1.946329000	
	Si	1.820889000	0.757311000	1.256426000	
	Si	1.820889000	0.757311000	-1.256426000	
	Si	-0.256904000	-0.447502000	-1.946329000	
	Sb	1.264338000	-1.559526000	0.000000000	
	Si	0.113143000	-0.365500000	-2.014898000	7.52
	Si	1.464263000	-1.857283000	-0.547854000	
	Sb	-1.037959000	-1.437988000	0.259923000	
	Sb	-1.065423000	1.418209000	-0.260187000	
	Si	2.273050000	0.367027000	-1.186522000	
	Si	0.104223000	0.366705000	2.014216000	
	Si	1.428764000	1.884523000	0.548088000	
	Si	2.278877000	-0.323418000	1.187933000	
	Si	0.107634000	-0.366072000	2.014220000	7.52
	Si	1.442164000	-1.874192000	0.547973000	
	Si	2.276975000	0.340110000	1.187579000	
	Sb	-1.048454000	1.430648000	0.259884000	
	Sb	-1.055147000	-1.425873000	-0.259954000	
	Si	2.275509000	-0.350756000	-1.186892000	
	Si	1.450593000	1.867618000	-0.547964000	
	Si	0.110244000	0.365899000	-2.014659000	
	Si	0.107634000	-0.366072000	2.014220000	5.67
	Si	1.442164000	-1.874192000	0.547973000	
	Si	2.276975000	0.340110000	1.187579000	
	Sb	-1.048454000	1.430648000	0.259884000	
	Sb	-1.055147000	-1.425873000	-0.259954000	
	Si	2.275509000	-0.350756000	-1.186892000	
	Si	1.450593000	1.867618000	-0.547964000	
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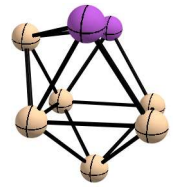
	Sb	-1.778158000	-0.459141000	-0.194476000	7.81
	Si	-0.187173000	-0.149822000	1.981644000	
	Si	-0.226293000	2.200704000	1.176682000	
	Si	-1.302882000	1.978026000	-1.011928000	8.02
	Sb	0.803128000	-1.590779000	-0.125414000	
	Si	1.857176000	0.997680000	1.140353000	
	Si	1.043657000	2.194205000	-1.005044000	
Si	2.367412000	0.246775000	-1.116394000		

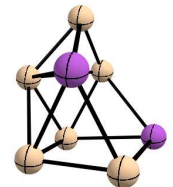
	Sb	-2.093481000	-0.459934000	-0.122534000	9.19
	Si	-0.104650000	-1.344843000	1.370872000	
	Si	-0.792920000	0.983701000	1.764092000	
	Si	0.104648000	-1.344791000	-1.370921000	6.64
	Sb	2.093446000	-0.459980000	0.122528000	
	Si	1.034241000	2.036658000	0.587797000	
	Si	-1.034203000	2.036609000	-0.587734000	
Si	0.793012000	0.983784000	-1.764087000		

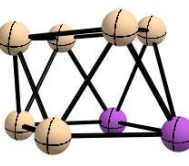
	Si	0.792868000	0.983761000	1.764032000	9.19
	Si	1.034322000	2.036614000	-0.587613000	
	Si	-1.034290000	2.036599000	0.587613000	
	Sb	2.093484000	-0.459955000	-0.122510000	6.17
	Si	-0.792847000	0.983761000	-1.764034000	
	Sb	-2.093495000	-0.459937000	0.122504000	
	Si	0.104613000	-1.344839000	1.370875000	
Si	-0.104625000	-1.344858000	-1.370849000		

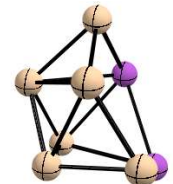
Si₆Bi₂⁴⁻

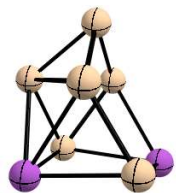
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	Bi	1.454089440	-1.503453000	-1.801919477	
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	Si	-1.319510427	1.247278000	-1.783371677	0.00
	Si	-0.067289506	0.000000000	1.792645577	
	Si	-0.163542401	-1.886406000	0.344750481	
	Si	-1.906749766	0.000000000	0.246134304	
Si	-0.163542401	1.886406000	0.344750481		

	Bi	-0.283537000	-0.687153000	1.959120000	5.99
	Si	-1.832827000	0.623113000	-0.000000000	
	Bi	-0.283537000	-0.687153000	-1.959120000	
	Si	-0.283537000	1.961836000	1.347494000	3.51
	Si	-0.283537000	1.961836000	-1.347494000	
	Si	2.069983000	0.501001000	-1.189789000	
	Si	2.069983000	0.501001000	1.189789000	
Si	1.621868000	2.598883000	-0.000000000		

	Bi	-2.184593000	-0.433916000	-0.277234000	6.66
	Si	-0.054736000	-1.750522000	0.762949000	
	Si	0.778267000	0.007927000	2.202335000	
	Si	-1.188750000	1.335492000	1.633191000	4.01
	Bi	2.085699000	-0.498775000	-0.253081000	
	Si	0.898151000	2.218095000	0.846613000	
	Si	-1.040622000	1.968527000	-0.803309000	
Si	1.193988000	1.750006000	-1.497765000		

	Si	-1.609517000	-1.474633000	1.204856000	6.97
	Si	-3.057987000	0.051561000	0.000000000	
	Si	-1.609517000	-1.474633000	-1.204856000	
	Si	-1.609517000	1.083345000	1.683109000	4.84
	Si	-1.609517000	1.083345000	-1.683109000	
	Bi	0.814511000	-0.113707000	-1.592943000	
	Bi	0.814511000	-0.113707000	1.592943000	
Si	-0.161720000	2.079251000	0.000000000		

	Bi	-1.476354000	-0.898696000	-0.085730000	7.43
	Si	-1.244476000	2.143682000	1.117172000	
	Si	-0.036998000	2.737452000	-1.055729000	
	Si	-2.060456000	1.540758000	-1.099657000	5.87
	Si	0.014541000	0.217716000	2.039307000	
	Si	1.147701000	2.221866000	1.130283000	
	Si	2.022513000	1.606605000	-1.063182000	
Bi	1.502865000	-0.867004000	-0.094447000		

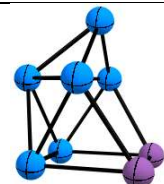


Bi	-1.877552000	-0.686237000	-0.189730000
Si	-1.201937000	1.099112000	1.849615000
Si	-1.199731000	1.968453000	-0.934090000
Si	-0.019051000	-0.953188000	1.776276000
Si	-0.066895000	2.968984000	0.898674000
Si	1.363998000	1.972698000	-0.719341000
Si	0.187026000	0.208171000	-1.958519000
Bi	2.035531000	-0.539055000	0.035795000

7.73

5.05

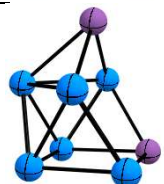
Ge₆Sb₂₄⁴⁻



Ge	0.023415500	0.000000000	1.885793500
Ge	-0.062010500	-1.981044000	0.343793500
Ge	-0.062010500	1.981044000	0.343793500
Ge	-1.997286500	0.000000000	0.318286500
Sb	1.350791500	-1.420509000	-1.885793500
Sb	1.350791500	1.420509000	-1.885793500
Ge	-1.397622500	1.318185000	-1.885793500
Ge	-1.397622500	-1.318185000	-1.885793500

0.00

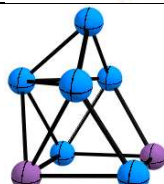
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Ge	0.598449000	1.813404000	1.315277000
Ge	1.216729000	-0.768666000	1.695957000
Sb	1.940656000	-0.937275000	-0.938437000
Ge	1.313786000	1.684432000	-1.183086000
Ge	-1.272352000	0.033989000	1.634093000
Ge	-0.240387000	-2.177322000	0.017698000
Ge	-1.118069000	1.851383000	-0.688457000
Sb	-2.253225000	-0.591962000	-0.813082000

1.48

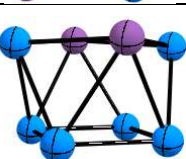
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Sb	1.322350118	1.272645046	-1.968838757
Ge	0.066084084	1.995470431	0.302016779
Ge	1.245927881	-1.440841323	-1.873707630
Ge	-1.420362395	1.405056317	-1.827988299
Ge	0.077632078	0.037279800	1.878518176
Ge	0.184712678	-1.953357764	0.346833144
Sb	-1.458443915	-1.385979238	-1.843538019
Ge	-2.002827747	0.173427519	0.469875511

2.34

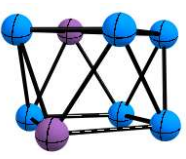
2.78



Ge	0.460542000	1.764981000	1.333565000
Sb	2.171897000	0.042398000	0.000000000
Ge	0.460542000	1.764981000	-1.333565000
Ge	-1.760147000	0.481106000	1.332740000
Ge	0.460542000	-0.795724000	2.028020000
Ge	0.460542000	-0.795724000	-2.028020000
Ge	-1.760147000	0.481106000	-1.332740000
Sb	-1.118954000	-1.862462000	0.000000000

6.09

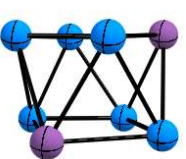
4.92



Ge	-0.385291000	-1.659014000	-1.371440000
Ge	-1.219037000	0.810177000	-1.659863000
Sb	2.053180000	-0.666996000	-0.535914000
Ge	0.387033000	-1.658893000	1.370539000
Sb	-2.051938000	-0.669824000	0.535810000
Ge	0.949929000	1.914721000	-0.839503000
Ge	1.217901000	0.809953000	1.659948000
Ge	-0.952513000	1.913612000	0.840484000

7.35

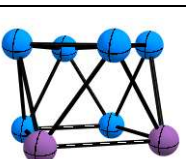
7.16



Ge	1.407423000	0.216218000	-1.655076000
Sb	-0.365621000	2.091847000	-0.672158000
Ge	0.365621000	1.214032000	1.913167000
Ge	2.016992000	-0.420969000	0.813161000
Ge	-1.407423000	-0.216218000	-1.655076000
Ge	-2.016992000	0.420969000	0.813161000
Ge	-0.365621000	-1.214032000	1.913167000
Sb	0.365621000	-2.091847000	-0.672158000

7.37

7.03



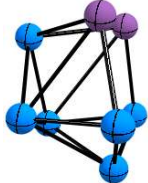
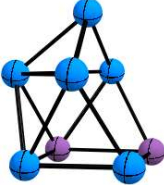
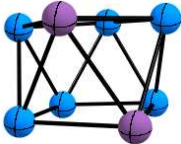
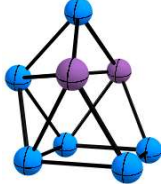
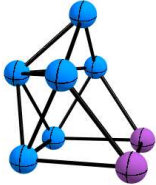
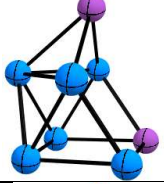
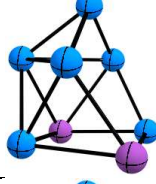
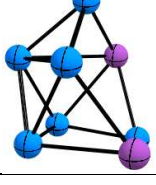
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Ge	-1.859115000	-0.071650000	1.279295000
Ge	-1.859115000	-0.071650000	-1.279295000
Sb	0.526363000	-1.455783000	-1.547124000
Ge	0.526363000	1.226232000	1.778282000
Ge	-1.172389000	2.086234000	-0.000000000
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Ge	2.160111000	0.244910000	0.000000000

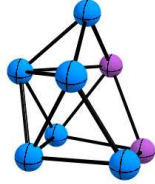
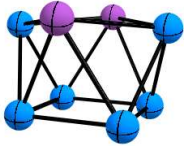
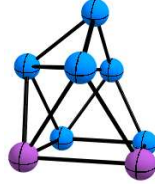
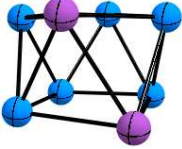
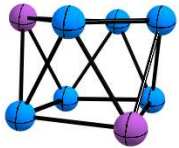
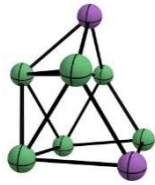
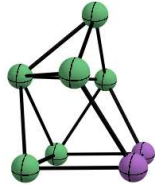
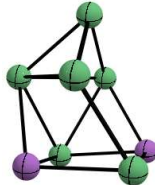
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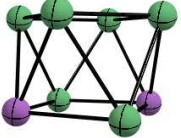
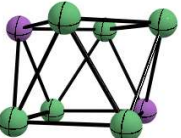
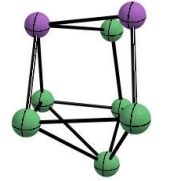
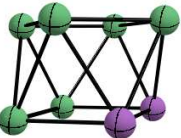
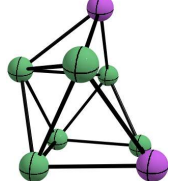
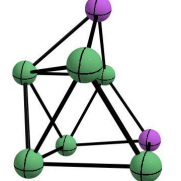
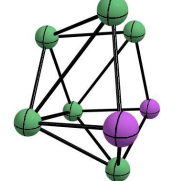
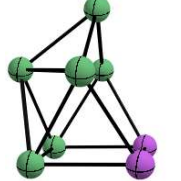
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Sb	0.063170000	-2.120296000	-0.365351000
Ge	-1.663400000	-0.192715000	1.349246000
Ge	-1.533401000	1.548283000	-0.837793000
Sb	2.165500000	-0.246700000	-0.610737000

8.00

	Ge 0.925696000 -0.606268000 1.840206000 Ge -0.019931000 1.800604000 1.362340000 Ge 0.900036000 2.076893000 -1.057227000		8.37
	Ge -1.947494000 1.177463000 -0.513788000 Ge -1.491207000 -0.980937000 1.204679000 Ge -0.428292000 1.440840000 1.636178000 Ge -1.957123000 -1.220910000 -1.266877000 Ge 0.413976000 -1.941864000 -0.967729000 Sb 1.272072000 -0.801697000 1.454150000 Ge 0.251756000 2.346860000 -0.703114000 Sb 1.964561000 0.286276000 -1.070997000		8.75 8.73
	Ge 1.784914000 1.045849000 1.002910000 Sb 0.809131000 1.212893000 -1.556482000 Ge -1.784914000 1.186082000 -0.427962000 Ge -0.661224000 1.138797000 1.905695000 Ge 1.784914000 -1.186082000 -0.427962000 Sb -0.809131000 -1.212893000 -1.556482000 Ge -1.784914000 -1.045849000 1.002910000 Ge 0.661224000 -1.138797000 1.905695000		8.89 7.17
	Ge -2.462659000 0.178948000 0.000000000 Sb -0.827807000 -0.409517000 2.021251000 Ge -0.652366000 2.010500000 0.000000000 Sb -0.827807000 -0.409517000 -2.021251000 Ge 1.438415000 1.088012000 1.305456000 Ge 1.438415000 1.088012000 -1.305456000 Ge 1.438415000 -1.530069000 -1.256271000 Ge 1.438415000 -1.530069000 1.256271000		9.20 30.36
Ge₆Bi₂⁴⁻			
	Ge -1.306505025 -1.317126375 -1.948698343 Ge -1.315102029 1.318384625 -1.941689500 Ge -2.035899104 -0.006846375 0.214599395 Bi 1.520652136 1.514666625 -1.835310942 Bi 1.529685426 -1.497479375 -1.844525250 Ge -0.114088939 -1.990219375 0.350533603 Ge -0.127191628 1.988034625 0.360417541 Ge -0.107182627 -0.004611375 1.892556009		0.00 0.00
	Ge 0.088844679 2.076150677 0.173158315 Bi -0.017037327 -0.063635823 1.957333052 Ge -2.096104705 0.110884129 0.094452584 Ge 1.313284943 1.424181954 -1.889219966 Bi 1.424820400 -1.377195370 -1.914978350 Ge -0.285176198 -2.146240705 0.135802748 Ge -1.277577223 1.443897421 -1.985147450 Ge -1.392378812 -1.236340714 -2.039986441		3.27 3.19
	Bi 1.224482548 -1.384371808 -2.072229661 Ge -1.615544531 -1.273785307 -1.773722827 Ge 1.391502179 1.403388123 -1.836916131 Ge -0.123941422 -2.004724014 0.275224282 Bi -1.380777254 1.609690450 -1.852783880 Ge 0.387624799 1.919894916 0.403304459 Ge -2.011302542 0.005091142 0.513441170 Ge 0.095084265 -0.088730365 1.883913125		3.78 3.91
	Ge -0.173699267 1.967571985 0.328224944 Ge -0.201267068 0.064982481 1.932899456 Bi 1.601649981 1.477180633 -1.755440589 Ge -2.042235584 -0.026135647 0.155695495 Ge -1.209001769 1.071334242 -2.006010118 Ge 1.489868198 -1.286524785 -2.020560994 Bi 0.503588551 -2.123654912 0.390394507 Ge -1.077448136 -1.521920014 -1.949586124		3.98 3.86
	Ge -2.055181000 -1.230014000 -1.202322000 Ge -1.993512000 -0.373026000 1.238465000 Ge -0.892674000 1.955042000 1.290768000 Ge -2.044523000 1.256379000 -1.032207000 Bi 0.372407000 -1.990078000 -0.172540000		7.92

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	Bi 0.375858000 2.198419000 -0.574563000 Ge -0.375858000 1.199477000 2.081809000 Ge 2.015083000 0.404235000 0.940908000 Ge -1.423805000 0.200287000 -1.532445000 Ge 0.375858000 -1.199477000 2.081809000 Ge 1.423805000 -0.200287000 -1.532445000 Ge -2.015083000 -0.404235000 0.940908000 Bi -0.375858000 -2.198419000 -0.574563000		9.91 8.44
Sn₆Sb₂⁴⁻			
	Sn -1.558449935 -1.536133171 -2.082684193 Sn -2.306440199 -0.085592181 0.452427217 Sn -1.561041600 1.467732328 -2.074905180 Sn 1.407260093 -1.161571642 -2.242826615 Sn -0.165967605 2.280923538 0.519587037 Sn 0.326324310 -2.278955281 0.166230218 Sb 0.096261530 -0.123319474 2.071613884 Sb 1.327185323 1.723250381 -1.886039548		0.00 0.91
	Sn -2.243411500 0.000000000 0.450878500 Sn 0.021373500 -2.235127000 0.322436500 Sn 0.165914500 0.000000000 2.144210500 Sn 0.021373500 2.235127000 0.322436500 Sn -1.625954500 -1.500316000 -2.144210500 Sb 1.294125500 -1.423029000 -2.144210500 Sb 1.294125500 1.423029000 -2.144210500 Sn -1.625954500 1.500316000 -2.144210500		1.66 0.00
	Sn 1.368090850 -1.413652375 -2.183004093 Sn 0.095250583 -2.267241375 0.285814560 Sb -1.541488078 -1.436131375 -2.100925782 Sb 1.460863083 1.487791625 -2.058817311 Sn 0.037218192 -0.038427375 2.138448648 Sn -1.436338624 1.515701625 -2.2111047404 Sn 0.040731690 2.260313625 0.363641936 Sn -2.280942771 0.134656625 0.410142849		2.57 1.97
	Sn 0.639054000 1.876467000 1.480849000 Sn 0.639054000 1.876467000 -1.480849000 Sn -1.956491000 0.297839000 -1.480300000 Sn -1.956491000 0.297839000 1.480300000		5.60

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	Sn 2.230061000 -0.788487000 -1.339469000 Sb 1.255412000 1.945351000 -1.178475000 Sb 0.532924000 1.695088000 1.560060000 Sn 1.606032000 -1.078614000 1.527736000 Sn -2.520341000 -0.788046000 -1.032138000 Sn -1.589254000 1.899908000 -0.573014000 Sn -0.109627000 -2.366730000 -0.628400000 Sn -1.440973000 -0.591278000 1.656069000	8.81 8.03
	Sb -1.352833000 -1.426615000 -1.387933000 Sn 1.743557000 1.396962000 -1.102623000 Sn 1.600515000 -1.555400000 -1.101904000 Sb -1.206017000 1.553085000 -1.382772000 Sn -0.291141000 -2.092152000 1.259397000 Sn -2.297323000 0.109336000 1.019769000 Sn -0.085654000 2.105987000 1.263136000 Sn 1.940073000 -0.093733000 1.488346000	8.92 5.20
Sn₆Bi₂⁴⁻		
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	Sn 0.182759069 2.296512595 0.383426843 Sn 1.345317048 1.525203966 -2.121316746 Sn -1.624719144 1.690173581 -1.968118531 Bi 0.084115436 -0.111031294 2.117465636 Sn -1.520997836 -1.305465296 -2.265791625 Sn -2.331485169 -0.054279346 0.381085854 Sn -0.137309616 -2.363762537 0.215551351 Bi 1.463938189 -1.465787076 -2.114635643	0.04 0.00
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	Sn -0.011786355 -0.122789722 2.146042384 Sn -0.098758768 2.247593014 0.479518169 Sn -2.304015224 -0.002940032 0.376878488 Sn 0.212539280 -2.264033613 0.207556247	2.07

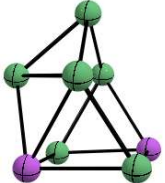
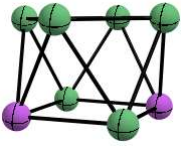
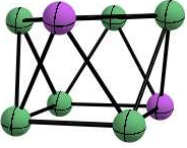
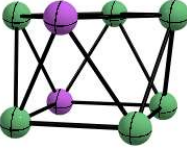
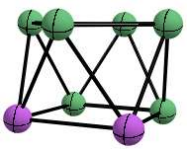
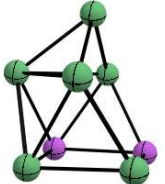
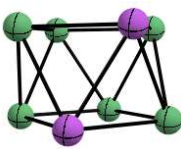
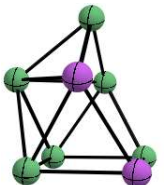
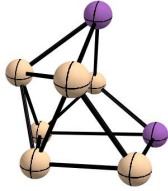
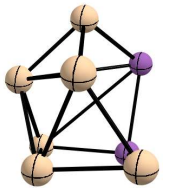
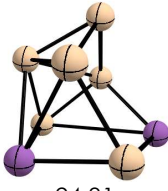
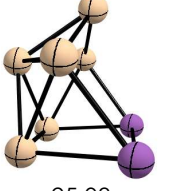
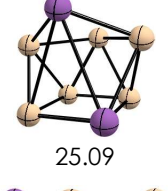
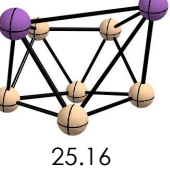
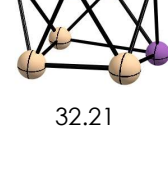
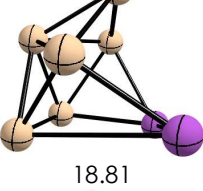
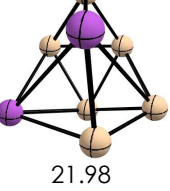
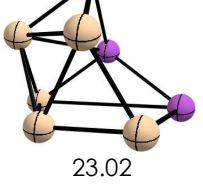
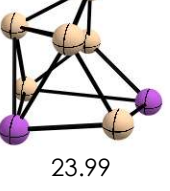
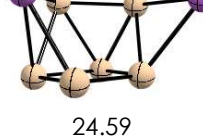
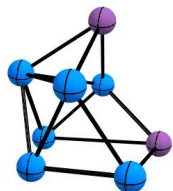
	Bi 1.484420928 1.676675541 -1.987266205 Sn -1.505062705 1.585179060 -2.134893696 Sn 1.523584724 -1.314661222 -2.203376508 Bi -1.455797525 -1.456034491 -2.258633127		1.97
	Sn 1.081299000 -2.210459000 0.000000000 Sn -1.461470000 -1.527740000 1.477797000 Sn -1.461470000 -1.527740000 -1.477797000 Bi 1.108833000 -0.000468000 -2.110772000 Bi 1.108833000 -0.000468000 2.110772000 Sn -1.461470000 1.529451000 -1.478246000 Sn 1.083256000 2.208590000 -0.000000000 Sn -1.461470000 1.529451000 1.478246000		5.01 1.67
	Sn -2.294483000 -0.538619000 0.936647000 Bi 0.412960000 2.291222000 -0.723828000 Sn -1.537471000 0.259748000 -1.862158000 Sn -0.412960000 1.412621000 2.127065000 Sn 1.537471000 -0.259748000 -1.862158000 Bi -0.412960000 -2.291222000 -0.723828000 Sn 0.412960000 -1.412621000 2.127065000 Sn 2.294483000 0.538619000 0.936647000		5.80 2.17
	Sn 2.294035000 -0.539871000 0.937559000 Bi -0.411546000 2.290779000 -0.723447000 Sn 0.411546000 1.412897000 2.126346000 Sn 1.538277000 0.258557000 -1.862984000 Sn -0.411546000 -1.412897000 2.126346000 Bi 0.411546000 -2.290779000 -0.723447000 Sn -1.538277000 -0.258557000 -1.862984000 Sn -2.294035000 0.539871000 0.937559000		5.80 2.09
	Sn 1.905017000 0.766712000 -1.520989000 Bi -2.055590000 -0.797266000 -0.727472000 Sn -0.826928000 1.881871000 -1.513585000 Bi 0.898017000 -2.005969000 -0.733905000 Sn 0.996842000 2.418362000 0.791389000 Sn 2.144286000 -0.293987000 1.376877000 Sn -0.575350000 -1.413239000 1.906289000 Sn -1.722296000 1.293649000 1.385906000		7.48 3.04
	Bi 1.415093000 -0.721092000 1.574713000 Bi 2.130005000 0.152800000 -1.216808000 Sn 0.323440000 2.536458000 -1.022223000 Sn -0.357358000 1.766924000 1.750341000 Sn 0.418829000 -2.266675000 -0.893077000 Sn -2.315669000 -1.451912000 -1.325584000 Sn -2.289022000 1.364083000 -0.571359000 Sn -1.665084000 -1.005512000 1.467780000		7.53 6.81
	Sn 2.264963000 0.629432000 1.108704000 Bi 1.521014000 -0.253072000 -1.694006000 Sn 0.398394000 2.364868000 -0.504742000 Sn -0.398394000 1.457491000 2.208088000 Bi -1.521014000 0.253072000 -1.694006000 Sn 0.398394000 -1.457491000 2.208088000 Sn -0.398394000 -2.364868000 -0.504742000 Sn -2.264963000 -0.629432000 1.108704000		7.87 4.48
	Sn 1.730339000 -0.733922000 1.537275000 Bi -0.607789000 -2.187868000 -0.222781000 Sn 2.080395000 -1.602085000 -1.250738000 Sn 2.171706000 1.265269000 -1.008349000 Bi -2.365335000 0.203194000 -0.731372000 Sn -0.460120000 2.430208000 -1.235128000 Sn 0.653874000 2.092594000 1.509794000 Sn -1.240809000 -0.157505000 2.031039000		8.84 7.19

Table S1. Lower energy structures in the triplet state below 10 kcal·mol⁻¹ for the systems studied, with their respective coordinates. In addition the energy (kcal·mol⁻¹) at the PBE0-D3/Def2TZVP (PCM,Solvent=Water) level and in bold DLPNO-CCSD(T) def2-QZVPP/C CPCM(water).

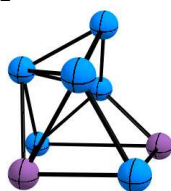
Si₆Sb₂⁴⁻							
	Sb 1.935623000	-0.917008000	-0.011734000		Sb -2.066244000	0.069899000	0.000229000
	Si -0.072601000	-0.762193000	1.689296000		Si 1.458962000	-0.375831000	1.970721000
	Sb -1.882502000	-0.947028000	-0.245140000		Si 1.087393000	1.892653000	1.259010000
	Si 0.402853000	1.572127000	2.076015000		Si -0.907642000	2.357478000	0.002060000
	Si -1.572733000	1.437671000	0.789370000		Sb 0.203609000	-1.640418000	0.001932000
	Si -0.941192000	1.141996000	-1.693231000		Si 2.611828000	0.342246000	-0.002173000
	Si 1.480991000	0.912961000	-1.732537000		Si 1.078685000	1.886296000	-1.265665000
	Si 0.509170000	2.487851000	-0.193157000		Si 1.456090000	-0.381666000	-1.971827000
22.87				24.51			
	Sb 2.073215000	-0.692179000	-0.178480000		Sb -1.781305000	-1.158504000	-0.163265000
	Si 0.071779000	-1.645684000	1.221523000		Sb 1.782325000	-1.157424000	-0.163231000
	Si -0.595723000	0.831677000	-2.085964000		Si 1.253499000	0.628079000	1.731939000
	Si 1.286471000	1.665967000	-0.808104000		Si -1.254305000	0.627935000	1.731765000
	Sb -1.842898000	-0.779409000	-0.310994000		Si -0.000881000	1.950261000	-1.767279000
	Si -1.224575000	1.984500000	-0.071600000		Si 2.018766000	1.402141000	-0.548348000
	Si 0.562401000	2.175390000	1.461656000		Si -0.000611000	2.427431000	0.589446000
	Si -0.939367000	0.348934000	2.065569000		Si -2.020186000	1.400747000	-0.548145000
24.81				25.08			
	Si 0.015578000	0.623192000	-1.898160000		Sb -2.022114000	-0.738185000	-0.032789000
	Si 1.486096000	-1.241437000	-1.331543000		Si 0.701712000	0.268391000	1.899549000
	Si -0.974566000	-1.656290000	-1.427597000		Si -1.337366000	1.437998000	1.250578000
	Sb -1.644369000	1.035786000	0.088111000		Sb 1.393701000	-1.333052000	-0.108162000
	Si 1.687742000	0.917824000	0.262109000		Si 2.457950000	1.038016000	0.418147000
	Si 0.386143000	-2.620039000	0.356626000		Si 0.485284000	2.512559000	0.025096000
	Si -1.639578000	-1.384678000	1.052325000		Si -1.180025000	1.436473000	-1.360129000
	Si 0.568327000	-0.837467000	1.972546000		Si 1.161661000	0.851785000	-1.719777000
25.09				25.16			
	Sb 2.452186000	-0.348392000	0.161452000				
	Si 0.407904000	-1.447357000	-1.145587000				
	Si 0.956355000	0.841522000	-1.723847000				
	Si -0.407826000	-1.447382000	1.145499000				
	Sb -2.452203000	-0.348397000	-0.161432000				
	Si -1.005904000	1.875020000	-0.669720000				
	Si 1.005876000	1.875041000	0.669728000				
	Si -0.956344000	0.841459000	1.723851000				
32.21							
Si₆Bi₂⁴⁻							
	Bi -1.733329000	-0.568506000	-0.001018000		Bi 1.832017000	-0.755271000	-0.120629000
	Bi 1.202423000	-1.236597000	-0.000355000		Si 1.487685000	1.796275000	0.820277000
	Si 2.015621000	1.013538000	1.306432000		Si -0.569081000	1.997933000	1.992718000
	Si -0.151571000	1.876264000	1.996646000		Si -0.016708000	-0.328614000	1.878286000
	Si -0.124296000	1.876333000	-2.002667000		Si 1.013867000	1.425931000	-1.696719000
	Si 2.037192000	1.016167000	-1.283263000		Si -0.489272000	2.881753000	-0.302603000
	Si 0.905151000	2.839236000	0.005304000		Bi -1.838809000	-0.767081000	-0.032488000
	Si -1.534586000	2.080141000	-0.014311000		Si -1.386227000	1.252098000	-1.784191000
18.81				21.98			
	Bi -1.945471000	-0.063888000	0.000142000		Bi -1.942784000	-0.644466000	-0.180255000
	Si 0.943026000	2.345529000	1.261149000		Si -0.916290000	0.736582000	2.117953000
	Si 0.939486000	2.342350000	-1.263117000		Si -1.280339000	2.224573000	-0.139447000
	Si -1.099051000	2.446954000	0.000964000		Si 0.075496000	-1.329524000	1.460082000
	Si 1.762765000	0.209086000	1.986351000		Si 0.535453000	2.529382000	1.328311000
	Si 2.739713000	1.127664000	-0.001527000		Si 1.212326000	1.847490000	-0.903054000
	Si 1.760526000	0.206713000	-1.987804000		Si -0.683657000	0.981622000	-2.099337000
	Bi 0.756911000	-1.399922000	0.000530000		Bi 2.121075000	-0.534591000	-0.117373000
23.02				23.99			
	Bi 2.195263000	-0.851751000	-0.204209000				
	Si 0.980911000	-0.074298000	2.104226000				
	Bi -2.566108000	-0.562240000	-0.035063000				
	Si 2.068602000	1.681268000	0.864835000				
	Si -0.946333000	1.105501000	1.315976000				
	Si -1.134453000	1.342668000	-1.321933000				
	Si 1.255103000	1.410108000	-1.579306000				
	Si -0.025252000	2.917700000	0.034740000				
24.59							

Ge₆Sb₂⁴⁻



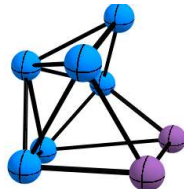
23.54

Ge	0.624961000	2.006460000	0.895817000
Ge	0.112385000	0.017557000	2.458101000
Sb	1.946199000	-1.406457000	-0.367135000
Ge	1.933804000	1.085622000	-1.127932000
Ge	-1.790225000	0.759888000	0.935579000
Ge	-0.436591000	-1.893333000	0.821643000
Ge	-0.587240000	1.602121000	-1.411167000
Sb	-1.856533000	-0.838760000	-1.246695000



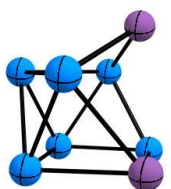
24.58

Sb	-1.738862000	-1.617438000	0.439387000
Ge	-1.974164000	0.991884000	0.334711000
Ge	0.771415000	-2.206962000	-0.350881000
Ge	-0.059682000	1.233248000	2.075486000
Ge	-0.956521000	1.034995000	-2.046861000
Ge	1.279786000	-0.241268000	-1.865222000
Sb	1.983035000	-0.184203000	0.905622000
Ge	0.550014000	2.059469000	-0.290841000



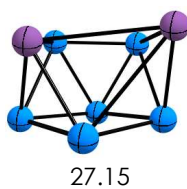
26.60

Ge	0.292008000	-1.095355000	-2.125670000
Ge	-1.842660000	0.157074000	-1.369742000
Ge	1.738243000	-1.437409000	0.004680000
Ge	-0.941542000	-1.975746000	-0.001412000
Sb	-0.611012000	2.127604000	-0.000514000
Sb	2.067385000	1.189416000	0.001363000
Ge	0.283758000	-1.091626000	2.128394000
Ge	-1.850902000	0.156559000	1.362396000



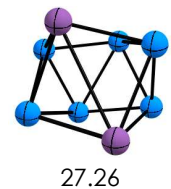
26.76

Sb	0.744867000	2.143218000	0.263840000
Ge	2.271362000	-0.000477000	0.472876000
Ge	0.915853000	-0.249751000	-1.986176000
Ge	-1.271504000	1.254768000	-1.279882000
Ge	0.431083000	-0.962739000	2.031718000
Ge	0.946998000	-2.145637000	-0.219934000
Ge	-1.340693000	-1.361103000	-1.203856000
Sb	-1.970341000	0.030861000	1.107300000



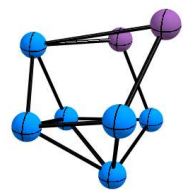
27.15

Sb	-2.273221000	-1.158221000	-0.309042000
Ge	-1.430797000	1.280315000	-1.198826000
Ge	1.079902000	0.809599000	-1.730560000
Sb	1.351276000	-1.710857000	-0.604355000
Ge	-1.522743000	0.662316000	1.505845000
Ge	0.356559000	2.166575000	0.443798000
Ge	2.416823000	0.475924000	0.586270000
Ge	0.569606000	-0.822138000	1.849200000



27.26

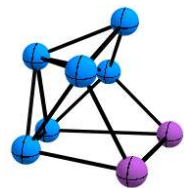
Ge	2.040075000	1.115985000	0.323227000
Sb	1.580555000	-1.311047000	-0.816897000
Ge	0.174572000	1.682457000	-1.444364000
Ge	-0.174698000	1.681523000	1.445425000
Ge	0.869559000	-0.708663000	1.897808000
Ge	-0.869442000	-0.707443000	-1.898385000
Ge	-2.040166000	1.115922000	-0.322614000
Sb	-1.580492000	-1.311561000	0.816209000



30.14

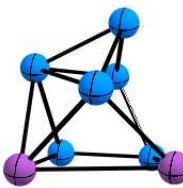
Ge	-0.237953000	-0.931456000	-2.165133000
Sb	1.253375000	-1.611735000	-0.001485000
Ge	-1.743175000	-1.348609000	-0.001320000
Ge	-1.734239000	0.933553000	-1.341455000
Sb	2.325019000	0.997050000	0.001023000
Ge	-0.238699000	-0.937333000	2.162981000
Ge	-1.732482000	0.931463000	1.343969000
Ge	-0.016517000	2.332035000	0.001693000

Ge₆Bi₂⁴⁻



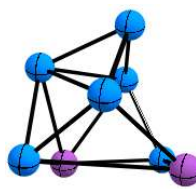
16.58

Ge	-0.946267000	1.074951000	2.123729000
Ge	-1.506832000	-1.340794000	1.368485000
Ge	-2.438134000	0.776278000	-0.000199000
Bi	0.862163000	-1.888294000	-0.000633000
Bi	2.056743000	0.872781000	0.000383000
Ge	-0.227362000	2.384577000	0.001154000
Ge	-1.506878000	-1.338619000	-1.369458000
Ge	-0.945440000	1.077592000	-2.123064000



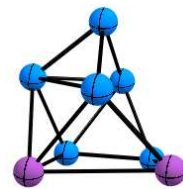
19.19

Bi	-2.211367000	-0.864389000	-0.279739000
Ge	0.529356000	0.931708000	-2.189558000
Ge	-0.060787000	-2.006726000	1.052639000
Ge	-1.424567000	1.705032000	-0.694131000
Bi	1.919596000	-0.909844000	-0.515614000
Ge	1.017389000	0.000574000	2.133958000
Ge	1.277376000	1.988093000	0.026982000
Ge	-0.581986000	1.983236000	1.733055000



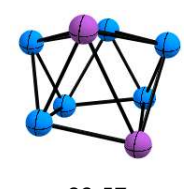
20.43

Bi	-2.211367000	-0.864389000	-0.279739000
Ge	0.529356000	0.931708000	-2.189558000
Ge	-0.060787000	-2.006726000	1.052639000
Ge	-1.424567000	1.705032000	-0.694131000
Bi	1.919596000	-0.909844000	-0.515614000
Ge	1.017389000	0.000574000	2.133958000
Ge	1.277376000	1.988093000	0.026982000
Ge	-0.581986000	1.983236000	1.733055000



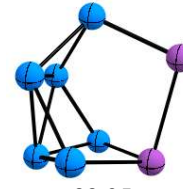
21.84

Ge	-0.935892000	0.165755000	-2.128782000
Ge	1.427427000	1.153082000	-1.796363000
Bi	2.220243000	-0.313353000	0.393140000
Bi	-0.910398000	-1.911902000	-0.218887000
Ge	-0.046950000	-0.323209000	2.049160000
Ge	-2.362661000	0.509411000	0.140764000
Ge	-0.390521000	2.338701000	-0.548467000
Ge	-1.088813000	1.928014000	1.831718000



22.57

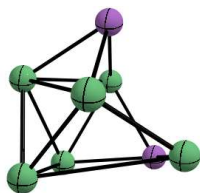
Ge	-1.877949000	-1.378705000	0.910878000
Ge	-0.566490000	-1.952965000	-1.317947000
Ge	0.566429000	-1.952766000	1.318227000
Bi	-1.787280000	1.136381000	-0.336861000
Ge	0.280039000	0.383994000	-2.133746000
Ge	1.877897000	-1.378838000	-0.910717000
Ge	-0.280114000	0.384376000	2.133619000
Bi	1.787352000	1.136353000	0.336740000



22.85

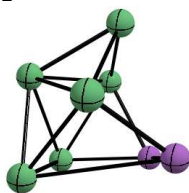
Ge	0.971628000	-2.407128000	-0.001056000
Ge	-1.097823000	-1.793212000	1.363641000
Ge	-2.606864000	-0.000061000	0.001105000
Ge	-1.108464000	-1.799489000	-1.354889000
Bi	2.355662000	-0.085293000	-0.000544000
Ge	-1.271684000	0.644336000	2.087128000
Ge	-1.272556000	0.636035000	-2.088135000
Bi	0.106319000	1.904867000	-0.002461000

Sn₆Sb₂⁴⁻



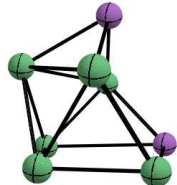
15.51

Sn	1.079733000	0.382396000	2.374570000
Sn	0.805901000	2.169692000	0.036539000
Sn	-1.665016000	1.011685000	1.537999000
Sn	0.274604000	-2.813281000	-0.030018000
Sn	-1.676316000	0.965265000	-1.547205000
Sn	2.338361000	-0.764648000	-0.019570000
Sb	1.074717000	0.477776000	-2.319351000
Sb	-2.209292000	-1.410236000	0.013160000



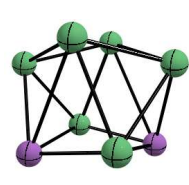
17.29

Sn	-0.415709000	-0.000870000	2.157091000
Sn	-2.459738000	0.001432000	-0.217570000
Sn	-0.952545000	-2.446845000	0.540925000
Sn	1.862830000	-1.546455000	0.682687000
Sn	-0.948909000	2.447205000	0.543816000
Sb	-0.848972000	0.002452000	-2.549370000
Sb	1.877625000	-0.000073000	-1.756386000
Sn	1.864844000	1.543107000	0.684923000



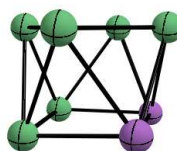
18.56

Sn	-2.579632000	-0.649251000	-0.596494000
Sb	-1.788409000	2.023005000	-0.808135000
Sb	1.812110000	-0.188907000	-1.974732000
Sn	-0.044714000	-2.213040000	-1.060388000
Sn	0.324470000	1.147135000	2.308146000
Sn	1.085663000	2.130621000	-0.400073000
Sn	-0.850533000	-1.468505000	1.731016000
Sn	2.040570000	-0.817739000	0.856317000



21.43

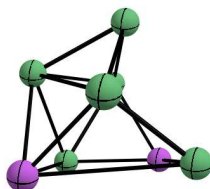
Sn	-0.328312000	-1.706151000	1.631607000
Sn	-2.320753000	-1.016515000	-0.415343000
Sn	0.317911000	-1.693002000	-1.644719000
Sn	2.313475000	-1.031982000	0.409424000
Sb	-1.356197000	1.551158000	-1.405916000
Sn	1.543362000	1.150895000	-1.545182000
Sb	1.365812000	1.535540000	1.416259000
Sn	-1.535491000	1.148325000	1.553664000



22.39

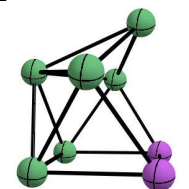
Sb	2.436462000	-1.093436000	-1.209089000
Sn	-1.148630000	1.712342000	-1.268707000
Sn	1.777894000	1.662746000	-0.662463000
Sb	-1.663252000	-1.145968000	-1.638438000
Sn	1.881110000	-0.570743000	1.535623000
Sn	-0.512643000	-2.163010000	0.826708000
Sn	-2.604612000	-0.019541000	0.854190000
Sn	-0.181792000	1.662399000	1.619126000

Sn₆Bi₂⁴⁻



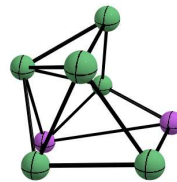
14.27

Sn	-0.272052000	2.794115000	0.470688000
Sn	1.493695000	1.485030000	-1.482692000
Sn	-1.578555000	1.037955000	-1.508454000
Sn	-1.699941000	0.588360000	1.773194000
Bi	2.480931000	-0.762170000	0.223223000
Sn	0.455803000	-1.371670000	-1.893303000
Sn	0.816629000	-0.573411000	2.647288000
Bi	-2.008389000	-1.623601000	-0.227271000



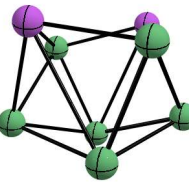
16.26

Sn	-0.679264000	-2.709951000	0.000000000
Sn	-0.740964000	-0.952825000	2.321023000
Sn	-2.523123000	0.029755000	0.000000000
Sn	-0.740964000	-0.952825000	-2.321023000
Bi	1.857302000	0.204267000	1.501998000
Sn	-0.740964000	1.953840000	1.481807000
Sn	-0.740964000	1.953840000	-1.481807000
Bi	1.857302000	0.204267000	-1.501998000



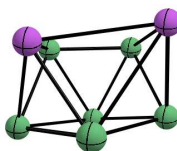
16.47

Sn	0.102777000	-2.104625000	0.967447000
Bi	-2.386282000	-1.253018000	-0.499107000
Bi	2.080853000	-1.228028000	-1.085201000
Sn	-0.600846000	0.225836000	2.671504000
Sn	-1.825063000	1.353598000	-1.550439000
Sn	1.183631000	1.587167000	-1.576534000
Sn	2.023875000	0.572870000	1.296334000
Sn	-0.377362000	2.483691000	0.821639000



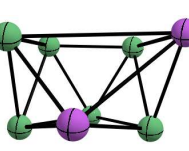
18.93

Sn	1.959103000	1.366247000	1.229824000
Bi	1.959103000	-0.001774000	-1.421605000
Sn	-0.059641000	2.281345000	-0.832920000
Sn	-0.883277000	1.354789000	1.962960000
Bi	-1.959103000	0.001774000	-1.421605000
Sn	0.883277000	-1.354789000	1.962960000
Sn	0.059641000	-2.281345000	-0.832920000
Sn	-1.959103000	-1.366247000	1.229824000



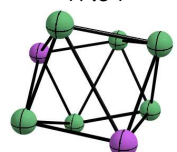
19.34

Sn	1.254884000	0.951278000	-1.922268000
Bi	-2.335611000	-1.315811000	-0.386876000
Sn	-1.659532000	1.423063000	-1.372957000
Bi	1.502246000	-1.792230000	-0.657570000
Sn	0.386155000	2.484196000	0.554008000
Sn	2.717077000	0.542897000	0.747638000
Sn	0.529653000	-0.987716000	2.065567000
Sn	-1.844851000	0.745629000	1.661793000



19.60

Sn	2.605783000	-0.112836000	0.763378000
Bi	0.508832000	-2.254600000	0.507698000
Sn	1.795801000	-1.014026000	-1.912195000
Sn	1.414626000	1.848852000	-1.356228000
Bi	-2.813865000	-0.547022000	-0.718456000
Sn	-1.440537000	2.039442000	-0.495085000
Sn	0.715098000	2.109360000	1.566605000
Sn	-1.264416000	-0.220099000	1.783383000



22.85

Sn	-0.647612000	-0.223811000	-2.364665000
Bi	2.038163000	-1.348005000	-0.057287000
Sn	-0.805792000	-2.314634000	-0.161748000
Sn	1.719454000	1.328502000	-1.455879000
Sn	-0.691729000	-0.540835000	2.326810000
Bi	-2.482511000	0.201759000	0.004295000
Sn	-0.479615000	2.486989000	0.095023000
Sn	1.642910000	1.166559000	1.648424000