SUPPLEMENTARY MATERIALS

Theoretical study for stabilizing group 14 elements E= (C,Si, Ge, and Sn) by five different ligands (NHC, cAAC, PHC, PNHC, and cPAC) as L-E-E-L complexes

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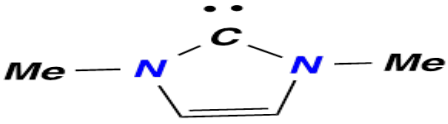
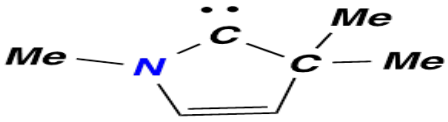
Carbene structures



NHC^{Me}



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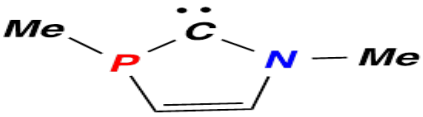

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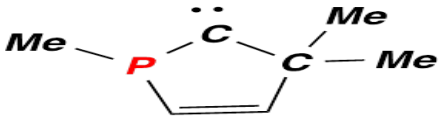
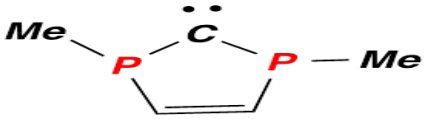


cPAC^{Me}



PHC^{Me}

Cartesian Coordinates

All geometries listed have been optimized at the **M06-2X/def2-tzvp** level of theory. Coordinates are enumerated in angstroms, SCF (E_0) energy and is expressed in Hartrees.

Cartesian coordinates of reactant optimized geometries

Group 14

2C

2Si
0 1

14	0.000000	-0.000000	1.029317
14	0.000000	-0.000000	-1.029317

2Ge
0 1

32	-0.000000	-0.000000	1.215646
32	0.000000	-0.000000	-1.215646

2Sn
0 1

50	0.000000	0.000000	1.403973
50	0.000000	0.000000	-1.403973

2Pb
0 1

82	-0.000000	-0.000000	1.468110
82	0.000000	0.000000	-1.468110

Ligands

CPAC^{Me}

0 1

C	0.04064200	-1.15690500	-0.00070400
C	-0.56855300	1.53507000	0.00049500
C	0.75495900	1.31691800	0.00080500
H	-1.07763500	2.49169900	0.00072400
H	1.49896300	2.11313400	0.00151600
P	-1.25366800	-0.12577700	-0.00151600
C	1.20011700	-0.14605600	-0.00000900
C	2.05492300	-0.39959800	-1.25733500
H	2.92375400	0.26969200	-1.27081100
H	2.40314000	-1.43588500	-1.25908400
H	1.46872900	-0.22970200	-2.16623900
C	2.05345500	-0.40091200	1.25810300
H	2.40201000	-1.43708300	1.25899600
H	2.92202600	0.26867500	1.27338600
H	1.46609900	-0.23229100	2.16650000
C	-3.03897000	-0.46088400	0.00088900
H	-3.51392700	-0.04965000	0.89419800

H	-3.51657900	-0.04974100	-0.89104000
H	-3.15099900	-1.54798800	0.00112500

PNHC^{Me}

0 1

C	0.29487700	-1.12667500	0.00029800
C	-0.27462900	1.48582500	0.00005200
C	1.05413600	1.15522500	0.00020400
H	-0.66809900	2.49180400	-0.00000700
H	1.89011700	1.84586800	0.00012300
N	1.31581400	-0.20692300	0.00066100
P	-1.05497100	-0.07114100	-0.00054700
C	2.70825700	-0.65520300	-0.00026300
H	3.22313700	-0.28998500	-0.89408100
H	3.22435900	-0.28966400	0.89271700
H	2.70033200	-1.74366400	-0.00006900
C	-2.82328200	-0.47957300	0.00033000
H	-3.32016400	-0.10346700	0.89587700
H	-3.32142100	-0.10078300	-0.89338500
H	-2.87055100	-1.57212200	-0.00131900

NHC^{Me}

0 1

C	0.00000600	-0.97694800	-0.00005600
C	-0.67572000	1.21040900	0.00007000
N	1.06070100	-0.12166700	-0.00005500
N	-1.06089500	-0.12143000	0.00001300
C	-2.43962500	-0.57077400	0.00003600
H	-2.96468600	-0.21368200	0.88840100
H	-2.96480800	-0.21338400	-0.88813500
H	-2.43213500	-1.65717600	-0.00014400
C	2.43956700	-0.57084400	-0.00002900
H	2.96467300	-0.21308300	-0.88809000
H	2.96439200	-0.21392500	0.88854000
H	2.43222900	-1.65722900	-0.00053600
C	0.67594700	1.21041400	0.00000300
H	-1.37522400	2.02849600	0.00012000
H	1.37587000	2.02812200	-0.00000100

PHC^{Me}

0 1

C	0.00000100	1.23404000	0.00002300
C	-0.66022100	-1.51509300	0.10200900
C	0.66021400	-1.51509400	-0.10201300
C	3.03021800	0.51237300	0.28920400
C	-3.03019200	0.51238200	-0.28926700
H	1.30692000	-2.37270000	-0.19261000
H	-1.30693100	-2.37269900	0.19258000
H	3.79784500	-0.04728700	-0.25990400
H	-3.08718600	0.23288900	-1.34900700
H	3.08727600	0.23286100	1.34893600
H	-3.79785000	-0.04728700	0.25978600
H	-3.26579000	1.58584400	-0.21140800
H	3.26581300	1.58583700	0.21135000
P	1.33276100	0.19436500	-0.42370700
P	-1.33277500	0.19436100	0.42374300

CAAC^{Me}

0 1

C	0.00000600	-0.97694800	-0.00005600
C	-0.67572000	1.21040900	0.00007000
N	1.06070100	-0.12166700	-0.00005500
C	2.43956700	-0.57084400	-0.00002900
H	2.96467300	-0.21308300	-0.88809000
H	2.96439200	-0.21392500	0.88854000
H	2.43222900	-1.65722900	-0.00053600
C	0.67594700	1.21041400	0.00000300
H	-1.37522400	2.02849600	0.00012000
H	1.37587000	2.02812200	-0.00000100
C	-1.06089500	-0.12143000	0.00001300
C	-1.91562040	-0.39074411	-1.25239045
H	-2.14321060	-1.43460617	-1.31116725
H	-2.82504308	0.16966569	-1.19081746
H	-1.37247488	-0.09441261	-2.12536272
C	-1.91555840	-0.39086925	1.25243185
H	-2.79880514	0.21211369	1.21798234
H	-2.19030969	-1.42459511	1.28111234
H	-1.35138464	-0.14733402	2.12838765

Cartesian coordinates of L-E-E-L compounds

NHC^{Me}-E-E- NHC^{Me}

L-E-E-L Group 14(C-Pb)

L-C-C-L

0 1

C	1.69485275	1.40328662	1.55867001
C	-1.72244576	1.41987072	-1.55025438
N	2.79067257	2.18331753	1.51503654
N	-1.76950421	0.65747053	-2.65846794
N	-2.82634529	2.18729117	-1.48971210
N	1.74992884	0.61738040	2.64979772
C	2.98993764	0.91542556	3.37504091
C	-3.65983304	1.89567853	-2.66136352
C	-3.01251397	0.95855969	-3.37719533
C	3.62751485	1.87446471	2.67983292
C	3.09713049	3.17690625	0.47587964
C	-0.74794729	-0.31297706	-3.07783113
C	-3.14346194	3.15414841	-0.42894576
C	0.73831351	-0.37232498	3.04733001
H	4.56521874	2.32560525	2.92873981
H	-3.34120518	0.51728427	-4.29489299

H	-4.60208579	2.34273675	-2.90062611
H	3.32336157	0.45775460	4.28292963
H	3.67580206	3.97050009	0.90065569
H	-0.73758901	-0.38121635	-4.14561257
H	-2.74574455	4.11268814	-0.68948527
H	0.72834021	-0.46394115	4.11331784
H	3.65379364	2.71084001	-0.31015459
H	-0.97499653	-1.27200381	-2.66140153
H	-4.20528866	3.22662522	-0.31827252
H	0.97521834	-1.31981314	2.61015837
H	2.18483228	3.57261300	0.08068361
H	-2.71021429	2.82686997	0.49308416
H	-0.22501217	-0.05361767	2.70774467
H	0.21229483	0.00794630	-2.73169771
C	-0.58333895	1.41434414	-0.51393183
C	0.55578443	1.40882122	0.52238964

L-Si-Si-L

0 1

Si	0.98513600	0.52627500	-0.11097600
Si	-0.98513600	-0.52627500	0.11097600
C	0.19432200	2.29575000	-0.06681400
C	-0.19432200	-2.29575000	0.06681400
N	-0.03626700	3.09214300	1.01684500
N	0.03626700	-3.09214300	-1.01684500
N	0.08968000	-3.09459700	1.13599200
N	-0.08968000	3.09459700	-1.13599200
C	-0.49349900	4.34950700	-0.72392700
C	0.49349900	-4.34950700	0.72392700
C	0.46029200	-4.34785900	-0.62717600
C	-0.46029200	4.34785900	0.62717600
C	0.13169000	2.66656200	2.39564700
C	-0.13169000	-2.66656200	-2.39564700
C	-0.00895100	-2.66252900	2.51868500
C	0.00895100	2.66252900	-2.51868500
H	-0.69945200	5.12132100	1.33449000
H	0.69945200	-5.12132100	-1.33449000
H	0.76667200	-5.12472400	1.41683900
H	-0.76667200	5.12472400	-1.41683900
H	0.20763300	3.55039000	3.02807600
H	-0.20763300	-3.55039000	-3.02807600
H	0.07797900	-3.53463000	3.16501300
H	-0.07797900	3.53463000	-3.16501300
H	-0.70825400	2.05087500	2.71553600
H	0.70825400	-2.05087500	-2.71553600
H	0.77718900	-1.94470900	2.75084900
H	-0.77718900	1.94470900	-2.75084900
H	1.04044000	2.07073000	2.47750600
H	-1.04044000	-2.07073000	-2.47750600
H	-0.97181500	-2.17627200	2.67900200
H	0.97181500	2.17627200	-2.67900200

L-Ge-Ge-L

0 1

Ge	-0.50881200	-0.13648800	1.09043600
Ge	0.49156300	0.09105600	-1.06736800
C	-2.39559400	-0.01479400	0.26318900
C	2.39143300	0.00589700	-0.25230800
N	-3.19447500	-1.03891900	-0.14509200
N	3.23012100	1.06777000	-0.09444100
N	3.15212000	-1.07340700	0.08584100
N	-3.18128800	1.09103600	0.14532200
C	-4.43496100	0.76173400	-0.33447600
C	4.43150500	-0.68769300	0.44091700
C	4.47847000	0.65821200	0.33366100
C	-4.44367800	-0.57772500	-0.51555800
C	-2.77407100	-2.42926300	-0.19126800
C	2.83966000	2.45064800	-0.30879100
C	2.70849100	-2.45568300	0.02328400
C	-2.74138000	2.44092600	0.45430500
H	-5.22023000	-1.23151200	-0.86967400
H	5.27863300	1.34951000	0.52832600
H	5.18544100	-1.39321400	0.74097300
H	-5.20191300	1.49635000	-0.50206100
H	-3.64232000	-3.04958200	-0.40854900
H	3.73779200	3.06364600	-0.37186500
H	3.10875700	-2.94655400	-0.86665900
H	-3.61633700	3.06340800	0.63840900
H	-2.01180200	-2.56836300	-0.95673900
H	2.20607100	2.80143500	0.50596400
H	3.04283500	-2.98784800	0.91365700
H	-2.15715400	2.85498100	-0.36763600
H	-2.34686300	-2.71493900	0.77020000
H	1.62125100	-2.46185500	-0.01621800
H	-2.10975400	2.41441200	1.34141000
H	2.27297700	2.52502600	-1.23685700

L-Sn-Sn-L

0 1

Sn	1.35813100	0.26177200	0.00377100
Sn	-1.35813100	-0.26177200	-0.00377100
C	0.83863400	2.51640000	-0.07621700
C	-0.83863400	-2.51640000	0.07621700
N	0.73900000	3.38797400	0.96283300
N	-0.73900000	-3.38797400	-0.96283300
N	-0.67055000	-3.29379600	1.17894500
N	0.67055000	3.29379600	-1.17894500
C	0.45908200	4.61501600	-0.83293000
C	-0.45908200	-4.61501600	0.83293000
C	-0.50146300	-4.67441100	-0.51673600
C	0.50146300	4.67441100	0.51673600
C	0.82689300	3.01097500	2.36414200
C	-0.82689300	-3.01097500	-2.36414200
C	-0.68138100	-2.79166500	2.54390700
C	0.68138100	2.79166500	-2.54390700
H	0.38885700	5.50852900	1.18577800
H	-0.38885700	-5.50852900	-1.18577800
H	-0.30333100	-5.38772900	1.56413000
H	0.30333100	5.38772900	-1.56413000
H	1.14579900	3.87602200	2.94459500
H	-1.14579900	-3.87602200	-2.94459500
H	-0.76589600	-3.63548200	3.22718600
H	0.76589600	3.63548200	-3.22718600
H	-0.13703800	2.65539000	2.72891600
H	0.13703800	-2.65539000	-2.72891600
H	0.23089700	-2.23303300	2.75066600
H	-0.23089700	2.23303300	-2.75066600
H	1.55315400	2.20713700	2.47295800
H	-1.55315400	-2.20713700	-2.47295800
H	-1.53001900	-2.12208800	2.67940700
H	1.53001900	2.12208800	-2.67940700

L-Pb-Pb-L

0 1

Pb	1.34668900	0.54897200	-0.05663100
Pb	-1.34668900	-0.54897200	0.05663100
C	0.29810800	2.76119200	-0.04964100
C	-0.29810800	-2.76119200	0.04964100
N	0.00045200	3.54406300	1.02032000
N	-0.00045200	-3.54406300	-1.02032000
N	0.06141500	-3.51647300	1.12046600
N	-0.06141500	3.51647300	-1.12046600
C	-0.58143400	4.73545000	-0.72609800
C	0.58143400	-4.73545000	0.72609800
C	0.54252300	-4.75281900	-0.62522400

C	-0.54252300	4.75281900	0.62522400
C	0.19491500	3.14203100	2.40436600
C	-0.19491500	-3.14203100	-2.40436600
C	-0.05336600	-3.07800300	2.50220900
C	0.05336600	3.07800300	-2.50220900
H	-0.84430900	5.51094800	1.32548100
H	0.84430900	-5.51094800	-1.32548100
H	0.92362400	-5.47556800	1.42704700
H	-0.92362400	5.47556800	-1.42704700
H	0.15455600	4.02666000	3.03843600
H	-0.15455600	-4.02666000	-3.03843600
H	0.02730100	-3.94513200	3.15624500
H	-0.02730100	3.94513200	-3.15624500
H	-0.57396000	2.43157100	2.70791900
H	0.57396000	-2.43157100	-2.70791900
H	0.72923900	-2.35780700	2.74078600
H	-0.72923900	2.35780700	-2.74078600
H	1.16574300	2.65984100	2.50926900
H	-1.16574300	-2.65984100	-2.50926900
H	-1.01826400	-2.59525600	2.65065800
H	1.01826400	2.59525600	-2.65065800

PNHC^{Me}-E-E- PNHC^{Me}

L-E-E-L Group 14(C-Pb)

L-C-C-L
0 1

C	-4.49134800	0.09491600	-0.29474500
C	-4.03739800	-1.16936800	-0.35093900
H	-5.53347500	0.35662800	-0.38387400
H	-4.64272600	-2.05929400	-0.46553300
N	-2.67160000	-1.35094300	-0.27905600
P	-3.12158700	1.28045600	-0.20432400
C	-1.95333300	-0.15430000	-0.21276600
C	-2.01538700	-2.63709000	-0.35579500
H	-1.35588100	-2.68730200	-1.22694100
H	-1.41051100	-2.81820600	0.53639900
H	-2.76776900	-3.41940000	-0.43461000
C	-3.09169700	1.74967100	1.60232900
H	-2.13815200	2.23398600	1.81936300
H	-3.89004100	2.47223600	1.78336600
H	-3.22480800	0.88922000	2.25750200
C	1.95317500	0.15453600	-0.21244800
N	2.67171600	1.35097000	-0.27853800
P	3.12101400	-1.28056400	-0.20429500
C	4.03745700	1.16903400	-0.35119400
C	2.01578700	2.63723300	-0.35596100
C	4.49107800	-0.09537400	-0.29538600
C	3.09237800	-1.74944500	1.60251300
H	4.64294800	2.05883700	-0.46586400
H	1.35882300	2.68858600	-1.22899300
H	1.40833100	2.81728600	0.53466500
H	2.76846800	3.41957200	-0.43158200
H	5.53311400	-0.35740100	-0.38468400
H	2.13944800	-2.23455800	1.82041200
H	3.89153500	-2.47124300	1.78305800
H	3.22531500	-0.88871200	2.25735000
C	0.62293400	0.07430100	-0.19920400
C	-0.62311800	-0.07391400	-0.19933600

L-Si-Si-L
0 1

C	4.94587600	0.11941800	0.28147300
C	4.42194700	1.25538800	-0.19798100
H	5.98465200	0.00765000	0.54974300
H	4.93530800	2.19503700	-0.35202300
N	3.07110400	1.20213400	-0.55593700
P	3.72128100	-1.20797600	0.18553800
C	2.45984200	-0.00196100	-0.39630900
C	2.39282700	2.37611500	-1.09307900
H	1.74732500	2.06803500	-1.91862200
H	1.76994500	2.85259100	-0.33810800
H	3.13558600	3.08633000	-1.45291100
C	3.19051000	-1.46900900	1.95148800
H	2.26887000	-2.05097500	1.94088700
H	3.96389600	-2.04492000	2.46206200
H	3.02099700	-0.52943900	2.47477300
C	-2.35748200	-0.05761000	-0.07572900
N	-2.94803500	-1.25134200	-0.36764600
P	-3.68176300	1.21944700	-0.01553600
C	-4.34139300	-1.23466500	-0.47601300
C	-2.21827000	-2.48165800	-0.63979000
C	-4.93671200	-0.05329200	-0.26303600
C	-3.83592300	1.65955100	1.78496000
H	-4.82299700	-2.16511600	-0.74522800
H	-1.93026000	-2.54348100	-1.68996100
H	-1.30829400	-2.50229300	-0.04054900
H	-2.84842800	-3.33473400	-0.38853400
H	-6.00011800	0.10572400	-0.34780700
H	-2.95892900	2.24440700	2.06114100
H	-4.72758100	2.27569100	1.91640000
H	-3.89958800	0.77442700	2.41625000
Si	0.79863700	-0.56905200	-0.97215000
Si	-0.66377800	0.50189400	0.40869500

L-Ge-Ge-L
0 1

C	-4.36791500	-1.10230800	-0.77764400
C	-4.67907600	0.11122000	-0.28640800
H	-5.08810900	-1.75562700	-1.24510100
H	-5.65155800	0.58497100	-0.28313500
N	-3.61457000	0.83277100	0.25053700
P	-2.57677800	-1.31482800	-0.73330500
C	-2.38563400	0.25210000	0.15157600
C	-3.79673800	2.17142400	0.78873200
H	-3.38847800	2.92294400	0.10833100
H	-4.85748800	2.36144300	0.94196200
H	-3.27351700	2.25397800	1.74309400
C	-2.31252700	-2.68175700	0.49306000
H	-2.86912700	-2.51817000	1.41512500
H	-2.62650300	-3.62136400	0.03401700
H	-1.24499300	-2.73217300	0.70368500
Ge	-0.70541900	0.94329800	0.89452100
Ge	0.50118600	-0.12127500	-0.95019100
C	2.37463700	0.03338900	-0.35831800
N	3.18425700	1.11587600	-0.44374900
P	3.41613100	-1.41753400	0.04365700
C	4.53445300	0.90647600	-0.13290800
C	2.69656500	2.43200900	-0.83805700
C	4.85854600	-0.34255800	0.22776900
C	2.88681900	-1.80364600	1.78483300
H	5.20029800	1.75405200	-0.22431700
H	2.04860400	2.32627200	-1.71202400
H	2.11628500	2.88852000	-0.03697700
H	3.54110500	3.07262200	-1.08509600
H	5.86663400	-0.65782500	0.44679000
H	1.87929300	-2.21710500	1.74321600
H	3.56010000	-2.55969700	2.19151700
H	2.89001600	-0.92079500	2.42176000

L-Sn-Sn-L
0 1

C	4.73045300	0.91519300	0.53802700
C	4.76451500	-0.42171900	0.67066400
H	5.55268800	1.56131100	0.80325400
H	5.58636100	-1.02312900	1.03467400
N	3.58507600	-1.08658500	0.31611300
P	3.04518100	1.41255200	0.13525000
C	2.54592500	-0.31432000	-0.08196900
C	3.47596000	-2.53443900	0.42355400
H	2.82114000	-2.80869900	1.25410400

H	3.05142800	-2.93697200	-0.49793700
H	4.46224400	-2.96641500	0.58250200
C	3.11056000	2.15309000	-1.56401900
H	2.08435900	2.27249700	-1.91085300
H	3.57196300	3.13958800	-1.49328800
H	3.66844900	1.53107400	-2.26249600
C	-2.54596300	0.31441500	0.08177100
N	-3.58525300	1.08651400	-0.31622300
P	-3.04512900	-1.41254500	-0.13493900
C	-4.76474400	0.42149600	-0.67029500
C	-3.47632300	2.53442400	-0.42322400
C	-4.73053800	-0.91539300	-0.53743200
C	-3.11005400	-2.15266100	1.56454200
H	-5.58673200	1.02277500	-1.03419600
H	-3.05491100	2.93719900	0.49961400
H	-2.81888300	2.80883700	-1.25164000
H	-4.46222100	2.96603100	-0.58544300
H	-5.55273200	-1.56164400	-0.80246900
H	-3.66827600	-1.53074500	2.26284700
H	-3.57083800	-3.13946500	1.49415600
H	-2.08375700	-2.27129800	1.91137000
Sn	0.57631500	-0.97478100	-0.83856200
Sn	-0.57628600	0.97476000	0.83820500

L-Pb-Pb-L

0 1

C	-5.11935700	-0.45823000	-0.46191600
C	-4.57074600	-1.42010700	0.29310000
H	-6.12658000	-0.50089200	-0.84606600
H	-5.02503900	-2.35118200	0.60475100
N	-3.26105600	-1.16137900	0.73898000
P	-4.00673900	0.96205000	-0.47852400
C	-2.71232800	0.01244500	0.37340700
C	-2.61211500	-2.14023600	1.60924400
H	-1.57437700	-1.85344800	1.74901300
H	-3.11687600	-2.17316900	2.57810000
H	-2.64991300	-3.12930600	1.15161700
C	-3.39058500	1.11912600	-2.22213100
H	-3.04844700	0.16492300	-2.61950300
H	-4.19444900	1.52054400	-2.84155000
H	-2.56141300	1.82579600	-2.21743200
C	2.71232800	-0.01235200	-0.37330500
N	3.26077700	1.16188100	-0.73795700
P	4.00695500	-0.96227000	0.47798000
C	4.57034000	1.42066000	-0.29170900
C	2.61161100	2.14147600	-1.60723700
C	5.11915000	0.45836100	0.46261800
C	3.39068300	-1.12085900	2.22141300
H	5.02438600	2.35211000	-0.60260200
H	1.57487000	1.85262600	-1.75016500
H	2.64596300	3.12949500	-1.14705700
H	3.11863000	2.17803500	-2.57476900
H	6.12635000	0.50098300	0.84683500
H	2.56199400	-1.82809100	2.21618000
H	4.19474400	-1.52213000	2.84067400
H	3.04785600	-0.16713000	2.61932700
Pb	0.64569400	-1.01210400	-0.86694000
Pb	-0.64560800	1.01209100	0.86660800

PHC^{Me}-E-E- PHC^{Me}

L-E-E-L Group 14(C-Pb)L-C-C-L

0 1

C	4.53363800	0.66420400	-0.05716500
P	2.94302200	-1.54980500	-0.00132300
P	2.94219100	1.54611200	0.00139000
C	2.74640900	-2.13960200	1.75155300
H	2.94216100	-1.35440100	2.48130600
H	1.72727400	-2.50726000	1.87533900
H	3.42999300	-2.97377200	1.91902300
C	2.74645700	2.13845400	-1.75066700
H	2.93923800	1.35347200	-2.48166900
H	1.72865000	2.51008400	-1.87384800
H	3.43303700	2.97029000	-1.91724000
P	-2.94240100	-1.54980800	-0.00066400
P	-2.94289900	1.54604500	-0.00326800
C	-2.76009000	-2.12912500	-1.75866200
C	-4.53325000	0.66387700	0.07206300
C	-2.73263300	2.14919700	1.74330400
H	-2.96081100	-1.33940900	-2.48206900
H	-1.74243200	-2.49727800	-1.89276200
H	-3.44615500	-2.96140400	-1.92556500
H	-2.91977400	1.36891000	2.48056700
H	-1.71362200	2.52078100	1.85566200
H	-3.41725700	2.98252900	1.91039800
C	1.95167700	-0.00223800	-0.00064200
C	-1.95169900	-0.00103000	-0.00182700
C	4.53399800	-0.66675100	0.05682000
C	-4.53426000	-0.66712400	-0.04206000
H	5.45562500	1.23646900	-0.10133400
H	5.45635900	-1.23847000	0.10085800
H	-5.45482000	1.23605200	0.12484800
H	-5.45684900	-1.23897200	-0.07750500
C	0.63023900	-0.00156200	-0.00101600
C	-0.63037200	-0.00092900	-0.00137600

CAAC^{Me}-E-E- CAAC^{Me}

L-E-E-L Group 14(C-Pb)

L-C-C-L

0 1

C	1.94529800	0.22252800	0.02421300
C	-1.94529600	-0.22248800	-0.02414500
N	2.63636300	1.43491500	0.07106200
N	-2.63629000	-1.43493200	-0.07096200
C	4.27817200	-0.11626200	-0.04921100
C	-4.27816000	0.11617200	0.04959500
C	-4.00249800	-1.18991800	0.00593700
C	4.00257400	1.18984100	-0.00547300
C	2.00428600	2.72341200	-0.03247500
C	-2.00409700	-2.72332100	0.03325100
H	4.68399100	2.02779800	-0.00580100
H	-4.68386900	-2.02791200	0.00651100
H	-5.26032500	0.55990600	0.07766900
H	5.26031700	-0.56005800	-0.07696200
H	2.75129900	3.50194200	0.11567400
H	-2.75117400	-3.50199100	-0.11382000
H	1.53292600	2.86877200	-1.01172700
H	-1.53218400	-2.86783100	1.01236200
H	1.23192200	2.83283800	0.73251900
H	-1.23215200	-2.83339200	-0.73207800
C	2.98589800	-0.91358500	-0.00977800
C	-2.98596500	0.91356600	0.00957300
C	2.89543300	-1.78328300	1.25884800
H	1.92609700	-2.28380700	1.31127300
H	3.67728400	-2.54679700	1.25300600
H	3.01686200	-1.17653800	2.15657400
C	2.81208900	-1.79569300	-1.25863800
H	1.83909500	-2.29154000	-1.24597000
H	2.88078200	-1.20039200	-2.16932000
H	3.58844100	-2.56408600	-1.29187100
C	-2.81198300	1.79642800	1.25784300
H	-2.88046600	1.20169200	2.16891100

H	-1.83903100	2.29234100	1.24469500
H	-3.58837800	2.56479100	1.29073900
C	-2.89580600	1.78252600	-1.25961700
H	-3.01733300	1.17521200	-2.15694500
H	-3.67773200	2.54596800	-1.25411400
H	-1.92651900	2.28310000	-1.31250600
C	0.62279300	0.09157100	0.00797600
C	-0.62279900	-0.09147800	-0.00781800

L-Si-Si-L

0 1

C	-2.35689700	-0.16571200	0.18876800
C	2.35692200	0.16568600	-0.18882000
N	-2.85836800	-1.41151500	0.05839400
N	2.85842800	1.41151600	-0.05889600
C	-4.69197900	-0.15487800	-0.29689100
C	4.69191500	0.15493000	0.29721400
C	4.24015400	1.40341800	0.22617500
C	-4.24012700	-1.40337000	-0.22648400
C	-2.12912000	-2.65957500	0.20305900
C	2.12930900	2.65956300	-0.20437200
H	-4.75729200	-2.34200100	-0.35396900
H	4.75734500	2.34207300	0.35337800
H	5.70666600	-0.15141300	0.49695800
H	-5.70676400	0.15147900	-0.49644500
H	-2.75462900	-3.38199900	0.73073300
H	2.75500900	3.38166600	-0.73225900
H	-1.85176400	-3.06813000	-0.76921500
H	1.85174500	3.06863000	0.76762200
H	-1.21587500	-2.47391500	0.76495400
H	1.21618800	2.47369500	-0.76640500
C	-3.54389200	0.79223500	-0.04238900
C	3.54380900	-0.79222500	0.04288300
C	-3.81901400	1.67760900	1.19047700
H	-2.95884000	2.31663000	1.39618100
H	-4.69258200	2.30896700	1.00982700
H	-4.00771600	1.07054100	2.07593600
C	-3.27618500	1.68235400	-1.27601600
H	-2.40939700	2.32020000	-1.09917200
H	-3.07510100	1.07742500	-2.16020900
H	-4.14506800	2.31367100	-1.47692300
C	3.27590200	-1.68198900	1.27670300
H	3.07470600	-1.07681500	2.16070400
H	2.40912800	-2.31986800	1.09991800
H	4.14473900	-2.31327400	1.47790600
C	3.81908700	-1.67796900	-1.18970900
H	4.00795100	-1.07115700	-2.07530600
H	4.69259500	-2.30931700	-1.00873900
H	2.95891000	-2.31700400	-1.39535400
Si	0.68724100	-0.42425400	-0.79248800
Si	-0.68721800	0.42421400	0.79247500

L-Ge-Ge-L

0 1

Ge	-0.68869200	0.53394600	0.83189800
Ge	0.68860300	-0.53394400	-0.83162900
C	-2.43298000	-0.17186900	0.18676200
C	2.43301900	0.17183300	-0.18682300
N	-2.91124700	-1.42570700	0.12601500
N	2.91136200	1.42566300	-0.12653400
C	-4.74595600	-0.22769700	-0.38931100
C	4.74620700	0.22769700	0.38842300
C	4.28390900	1.46165200	0.21349400
C	-4.28366100	-1.46167700	-0.21455200
C	-2.18174400	-2.65280900	0.40078500
C	2.18179400	2.65274700	-0.40123700
H	-4.78235800	-2.41535500	-0.29630600
H	4.78270200	2.41532100	0.29476000
H	5.75508900	-0.04946800	0.65118900
H	-5.75470300	0.04947400	-0.65258700
H	-2.77513700	-3.28599800	1.06411200
H	2.77499100	3.28583100	-1.06483700
H	-1.97628000	-3.19665100	-0.52198600
H	1.97664800	3.19671000	0.52153000
H	-1.23341900	-2.40298100	0.87055600
H	1.23331300	2.40288500	-0.87067600
C	-3.61743400	0.74828000	-0.15632200
C	3.61748000	-0.74828000	0.15631000
C	-3.94313600	1.71024000	1.00514000
H	-3.09498500	2.36824300	1.19970100
H	-4.81222000	2.32201000	0.75101100
H	-4.16247000	1.16120300	1.92101000
C	-3.31352400	1.55715700	-1.43662300
H	-2.46215800	2.21800000	-1.27007800
H	-3.06940000	0.89699300	-2.26892800
H	-4.18254000	2.15927900	-1.71286500
C	3.31376300	-1.55608000	1.43738300
H	3.07014900	-0.89518300	2.26925500
H	2.46212600	-2.21677800	1.27164900
H	4.18269000	-2.15825400	1.71379300
C	3.94263600	-1.71119000	-1.00444700
H	4.16198900	-1.16293200	-1.92078100
H	4.81155700	-2.32307500	-0.75003000
H	3.09424400	-2.36906800	-1.19838000

L-Sn-Sn-L

0 1

C	-2.66456200	-0.16046200	0.21711200
C	2.66470200	0.16040900	-0.21742100
N	-3.11970400	-1.41143700	0.32723200
N	3.12032900	1.41110800	-0.32861200
C	-4.91894500	-0.37201000	-0.53204000
C	4.91937300	0.37159700	0.53095700
C	4.46043600	1.54764800	0.11579100
C	-4.45960500	-1.54820700	-0.11774800
C	-2.40416000	-2.55457700	0.87314400
C	2.40495400	2.55411600	-0.87499900
H	-4.93492400	-2.51640100	-0.08002500
H	4.93619700	2.51558600	0.07705700
H	5.90454000	0.16768700	0.92063300
H	-5.90405700	-0.16821600	-0.92191700
H	-3.01434800	-3.03185800	1.64332300
H	3.01477400	3.03044500	-1.64606000
H	-2.18743200	-3.28013700	0.08825400
H	2.18916300	3.28045200	-0.09056400
H	-1.46477600	-2.21374400	1.30059600
H	1.46509600	2.21335600	-1.30146300
C	-3.82520700	0.65615500	-0.36790700
C	3.82501900	-0.65616100	0.36832700
C	-4.25780700	1.77892200	0.59974400
H	-3.43977600	2.48461300	0.75090300
H	-5.11290100	2.31779600	0.18515200
H	-4.54199800	1.37471100	1.57151200
C	-3.42850900	1.26474600	-1.73085500
H	-2.60497100	1.96821900	-1.60312200
H	-3.10337400	0.49193900	-2.42734700
H	-4.28176900	1.79072600	-2.16620200
C	3.42802500	-1.26228900	1.73234000
H	3.10349200	-0.48813800	2.42762200
H	2.60395700	-1.96535800	1.60577700
H	4.28095800	-1.78815700	2.16845500
C	4.25668400	-1.78076800	-0.59751500
H	4.54103500	-1.37836100	-1.56998400
H	5.11143600	-2.31959600	-0.18215800
H	3.43812900	-2.48612000	-0.74740200
Sn	-0.74044000	0.76008600	0.90376000
Sn	0.74033600	-0.75992300	-0.90349900

L-Pb-Pb-L

0 1

C	-2.76491300	0.17215900	-0.21408300
C	2.76477400	-0.17219500	0.21369300
N	-3.18856700	1.33713300	-0.70131600
N	3.18852200	-1.33750200	0.70007900
C	-4.97432400	0.71020200	0.51206000
C	4.97379900	-0.71013300	-0.51377800
C	4.50266600	-1.67089400	0.27409300
C	-4.50298200	1.67057400	-0.27616200
C	-2.47232900	2.20234300	-1.62642500
C	2.47270400	-2.20303100	1.62522600
H	-4.95057600	2.59541000	-0.60673100

H	4.95026700	-2.59599400	0.60391400
H	5.94202900	-0.68709900	-0.98951600
H	-5.94277500	0.68731000	0.98735800
H	-3.04092200	2.30111500	-2.55453500
H	3.04184900	-2.30230900	2.55294700
H	-2.33410800	3.19106800	-1.18692000
H	2.33405800	-3.19153600	1.18536900
H	-1.49843600	1.76680000	-1.83377700
H	1.49900900	-1.76742100	1.83336600
C	-3.91739700	-0.36107900	0.64623700
C	3.91703400	0.36149900	-0.64666500
C	-4.42126600	-1.71508100	0.10157100
H	-3.62883800	-2.46279400	0.15725800
H	-5.27107900	-2.06196800	0.69403900
H	-4.73723100	-1.63003600	-0.93838200
C	-3.47633500	-0.52247700	2.11707800
H	-2.67605000	-1.25971900	2.19067400
H	-3.10432400	0.41814000	2.52331800
H	-4.32251000	-0.85308400	2.72455400
C	3.47562900	0.52456700	-2.11718100
H	3.10303300	-0.41545100	-2.52426300
H	2.67570800	1.26230100	-2.18984900
H	4.32179100	0.85538400	-2.72456900
C	4.42146800	1.71481900	-0.10074100
H	4.73779600	1.62859900	0.93900300
H	5.27114300	2.06210700	-0.69316900
H	3.62918600	2.46276700	-0.15534800
Pb	0.78042600	1.05547000	0.64786200
Pb	-0.78030200	-1.05557500	-0.64732100

CPACMe-E-E- CPACMe

L-E-E-L Group 14(C-Pb)

L-C-C-L

0 1

C	1.94935500	0.00441400	-0.21088500
C	4.44674900	-0.60255500	-0.21615900
C	4.25969800	0.68441100	0.06822800
H	5.42674900	-1.05980300	-0.27796200
H	5.07690900	1.37200900	0.26725200
P	2.92329900	-1.49259500	-0.66085700
C	2.84519400	1.21864800	0.09544500
C	2.52505300	1.81247700	1.48094700
H	3.19470000	2.64722300	1.70234500
H	1.49870100	2.18197000	1.50945100
H	2.64096900	1.06345500	2.26489100
C	2.66602600	2.30758200	-0.98323500
H	1.63954800	2.67775000	-0.98041000
H	3.33499300	3.15013500	-0.79119000
H	2.88580200	1.91544300	-1.97681000
C	2.65150300	-2.61234000	0.80050800
H	2.78016200	-2.10055700	1.75386100
H	1.64220300	-3.02113100	0.73920700
H	3.35456100	-3.44505400	0.73517500
C	-1.94897500	0.00538300	-0.20940800
P	-2.91852400	-1.49398900	-0.66106700
C	-2.84836800	1.21714200	0.09594200
C	-4.44488700	-0.60796400	-0.21843900
C	-2.64631300	-2.61394100	0.79998900
C	-4.26151700	0.67941400	0.06648400
C	-2.67035900	2.30666800	-0.98234700
C	-2.53181900	1.81158900	1.48199600
H	-5.42360900	-1.06771900	-0.28190700
H	-2.77748400	-2.10307700	1.75348800
H	-3.34752700	-3.44809600	0.73303400
H	-1.63608800	-3.02060500	0.73990300
H	-5.08075600	1.36493400	0.26431100
H	-3.34175000	3.14746700	-0.79113300
H	-1.64483800	2.67952100	-0.97805500
H	-2.88772900	1.91411000	-1.97628800
H	-1.50653700	2.18394700	1.51201600
H	-3.20409100	2.64442400	1.70266700
H	-2.64673000	1.06208200	2.26562100
C	-0.63174300	0.03453300	-0.20348500
C	0.63210400	0.03126500	-0.20901300

L-Si-Si-L

0 1

C	2.60978600	0.05108000	0.15236800
C	5.15666900	0.07666600	0.57683900
C	4.72829600	-1.13310300	0.23278000
H	6.18416000	0.29911800	0.83703900
H	5.38110800	-2.00026300	0.17867800
P	3.84084500	1.33924100	0.60711800
C	3.26280200	-1.31662700	-0.11136200
C	3.12956700	-1.73858800	-1.59234700
H	3.66587700	-2.67397700	-1.77319000
H	2.08008400	-1.89308000	-1.84960900
H	3.53690700	-0.97639900	-2.25629200
C	2.65586100	-2.41953900	0.77954400
H	1.60073200	-2.56666700	0.54307800
H	3.17255700	-3.36897900	0.61747900
H	2.73893700	-2.15695300	1.83430000
C	4.20247600	2.24194700	-0.98759200
H	4.33120600	1.56556700	-1.83251700
H	3.38562700	2.93427100	-1.19431900
H	5.11445700	2.82821800	-0.85129600
C	-2.60991100	-0.05130800	-0.15232900
P	-3.84134600	-1.33881100	-0.60787400
C	-3.26248200	1.31663100	0.11165500
C	-5.15682100	-0.07592700	-0.57662800
C	-4.20293100	-2.24269900	0.98617100
C	-4.72808500	1.13360300	-0.23220300
C	-2.65539100	2.41936200	-0.77936200
C	-3.12883900	1.73852100	1.59261800
H	-6.18440200	-0.29802600	-0.83677700
H	-4.33137200	-1.56690700	1.83160800
H	-5.11504800	-2.82867600	0.84955200
H	-3.38620500	-2.93536000	1.19223900
H	-5.38065600	2.00092000	-0.17771400
H	-3.17172600	3.36897700	-0.61715100
H	-1.60015500	2.56612000	-0.54314300
H	-2.73880200	2.15684600	-1.83411200
H	-2.07926000	1.89263400	1.84971700
H	-3.66476700	2.67411600	1.77354500
H	-3.53636700	0.97647800	2.25661500
Si	-0.96840300	-0.58197000	-0.24938800
Si	0.96830600	0.58164600	0.25029500

L-Ge-Ge-L

0 1

C	2.69755600	-0.04878500	0.17683600
C	5.27513800	-0.01920800	0.35391500
C	4.78908300	1.19202100	0.10288200
H	6.32872800	-0.22590400	0.49620200
H	5.41399900	2.07673700	0.01338400
P	3.98937400	-1.30189500	0.50777000
C	3.29121900	1.34712100	-0.07661200
C	2.75730300	2.40230700	0.91584800
H	3.24739700	3.36503300	0.74927500
H	1.68306500	2.54340700	0.78324500
H	2.93955200	2.09519000	1.94584000
C	2.99368400	1.82143300	-1.51798400
H	1.91929800	1.94175600	-1.66862500
H	3.47280400	2.78568000	-1.70754000
H	3.36504000	1.10465200	-2.24998000
C	4.17704800	-2.20031000	-1.11929700
H	4.20556600	-1.52328700	-1.97281300
H	5.10199100	-2.78073300	-1.08478100
H	3.34643600	-2.89755700	-1.23418800
C	-2.69745200	0.04853000	-0.17672800
P	-3.98819200	1.30337900	-0.50564200
C	-3.29243100	-1.34681300	0.07646100
C	-5.27521000	0.02185200	-0.35196500
C	-4.17380800	2.20026500	1.12255500

C	-4.79027500	-1.19001400	-0.10186000
C	-2.99425300	-1.82213800	1.51737200
C	-2.76040200	-2.40204600	-0.91693400
H	-6.32867100	0.22976500	-0.49343900
H	-3.34227900	2.89634400	1.23782400
H	-5.09808300	2.78181700	1.08924200
H	-4.20271900	1.52222200	1.97523900
H	-5.41607100	-2.07410200	-0.01230500
H	-3.47438700	-2.78589100	1.70687700
H	-1.91989300	-1.94385300	1.66705500
H	-3.36409500	-1.10524600	2.25001900
H	-1.68624700	-2.54454800	-0.78512100
H	-3.25156000	-3.36427100	-0.75061700
H	-2.94293500	-2.09411300	-1.94663700
Ge	0.97011500	-0.54350800	0.52699200
Ge	-0.97004900	0.54192500	-0.52908600

L-Sn-Sn-L
E0 = -1658.34164836 (Hartrees)
0 1

C	2.87582900	0.01853100	0.09938700
C	5.46186300	0.31481800	0.21335300
C	4.86099200	1.43228000	-0.18819600
H	6.53387700	0.20408200	0.31782400
H	5.39883900	2.33572400	-0.46178800
P	4.25381600	-0.90926400	0.79218700
C	3.34256100	1.45031100	-0.20243500
C	2.84688600	2.41850200	0.90348400
H	3.21802200	3.42907400	0.71387600
H	1.75720200	2.45271900	0.92342100
H	3.19972400	2.10071300	1.88452600
C	2.83823700	1.95941200	-1.56964600
H	1.74833900	2.01763200	-1.58004400
H	3.23250000	2.95961500	-1.76855100
H	3.15549100	1.29711200	-2.37547800
C	4.50130200	-2.40919400	-0.27632400
H	4.48164400	-2.15895900	-1.33709500
H	5.45928100	-2.86470000	-0.01790600
H	3.71785600	-3.13499100	-0.05726700
C	-2.87582900	-0.01853500	-0.09947400
P	-4.25387800	0.90917100	-0.79226100
C	-3.34251800	-1.45032100	0.20234700
C	-5.46187000	-0.31483000	-0.21317700
C	-4.50110900	2.40935800	0.27588400
C	-4.86094100	-1.43230900	0.18826000
C	-2.83808400	-1.95944700	1.56953000
C	-2.84686400	-2.41845200	-0.90360600
H	-6.53389300	-0.20410500	-0.31753400
H	-3.71768800	3.13506900	0.05649400
H	-5.45911100	2.86482700	0.01746500
H	-4.48134700	2.15940200	1.33672200
H	-5.39874400	-2.33578900	0.46181700
H	-3.23238100	-2.95962900	1.76845700
H	-1.74818800	-2.01773500	1.57981300
H	-3.15523800	-1.29711900	2.37537500
H	-1.75717800	-2.45268600	-0.92353900
H	-3.21801200	-3.42903800	-0.71408300
H	-3.19966600	-2.10060800	-1.88464700
Sn	1.06464000	-0.92644600	-0.34207800
Sn	-1.06470300	0.92644800	0.34221700

L-Pb-Pb-L
0 1

C	-2.93695700	-0.13543800	0.11431900
C	-5.50197200	-0.57383100	0.23866300
C	-4.85390700	-1.61872000	-0.27229500
H	-6.57642600	-0.52554400	0.36377000
H	-5.35189900	-2.51775800	-0.62477700
P	-4.33414600	0.63135000	0.93110200
C	-3.33501200	-1.55893900	-0.29466400
C	-2.78496100	-2.58567900	0.73104300
H	-3.11045600	-3.59529800	0.46684600
H	-1.69491400	-2.56828400	0.74173100
H	-3.14251400	-2.36031300	1.73559600
C	-2.81315300	-1.93326800	-1.69783000
H	-1.72157900	-1.93263500	-1.71520300
H	-3.15469300	-2.93441900	-1.97503100
H	-3.16931000	-1.22789400	-2.44909400
C	-4.66007700	2.24325800	0.06928900
H	-4.64156300	2.13412900	-1.01521000
H	-5.63313900	2.61956500	0.39056800
H	-3.90654200	2.96904000	0.37667200
C	2.93723100	0.13510900	-0.11413100
P	4.33441500	-0.63274600	-0.92990100
C	3.33559800	1.55874400	0.29401000
C	5.50240800	0.57276000	-0.23833300
C	4.65976300	-2.24404800	-0.06676100
C	4.85448700	1.61821100	0.27166700
C	2.81385300	1.93395000	1.69700200
C	2.78570300	2.58504000	-0.73222500
H	6.57686500	0.52415900	-0.36327400
H	3.90616200	-2.96988600	-0.37385400
H	5.63284200	-2.62080200	-0.38745200
H	4.64089800	-2.13411900	1.01765100
H	5.35262800	2.51744500	0.62344200
H	3.15555000	2.93522100	1.97357400
H	1.72228300	1.93345600	1.71443800
H	3.16996400	1.22896700	2.44865100
H	1.69565300	2.56774500	-0.74292800
H	3.11130200	3.59475500	-0.46851200
H	3.14325200	2.35913000	-1.73665600
Pb	-1.11122200	1.00748300	-0.34323500
Pb	1.11089900	-1.00697800	0.34302200