

## pCp3M

pCp3Ga

SCF Energy = -8082.52995079 au

C	1.28186700	2.69589500	0.27107900
C	0.78871900	2.91065300	1.55327900
C	-0.56203500	2.76774700	1.83357100
C	-1.47664400	2.40565900	0.84544000
C	-0.98587400	2.22872200	-0.44741500
C	0.36723900	2.36861500	-0.72501000
H	1.47097600	3.18382200	2.35181500
H	-0.91551800	2.92282600	2.84802900
H	-1.66406500	1.97049200	-1.25030800
H	0.72114400	2.20132600	-1.73665000
C	-2.92926500	2.20965400	1.17904200
H	-3.01165400	2.01371700	2.25163300
H	-3.47646400	3.13945600	0.99027300
C	-3.61517300	1.09152700	0.39009900
H	-4.61658600	0.94342700	0.80655700
H	-3.76482100	1.41050900	-0.64413500
C	-2.85225000	-0.20194300	0.40679300
C	-2.45143900	-0.78967400	1.60034200
C	-2.48570200	-0.83507800	-0.77833600
C	-1.67672900	-1.93983000	1.60709300
H	-2.73334500	-0.33676300	2.54471300
C	-1.70445600	-1.98225400	-0.77473500
H	-2.80020300	-0.40990500	-1.72603300
C	-1.26234600	-2.54435300	0.42268800
H	-1.36287200	-2.36546300	2.55473300
H	-1.42729100	-2.44050800	-1.71712500
C	-0.34014800	-3.72797000	0.43384000
H	-0.86226600	-4.60526500	0.03887300
H	-0.07819300	-3.96200200	1.46884200
C	0.92937200	-3.50832000	-0.39519000
H	1.60645800	-4.35182900	-0.22112100
H	0.68039900	-3.54184600	-1.45887500
C	2.75140800	2.74980500	-0.02257000
H	2.90142200	2.70736600	-1.10406800
H	3.17340900	3.70167300	0.31328500
C	3.53063100	1.60725800	0.64672900
H	4.56459500	1.62729100	0.28850200
H	3.56291600	1.77368300	1.72664300
C	2.92822400	0.25904900	0.38437100
C	2.80005300	-0.23947400	-0.91257500
C	2.43227800	-0.52269500	1.42401200
C	2.16517900	-1.45063800	-1.15191300
H	3.19696000	0.32876600	-1.74645900
C	1.80382300	-1.73547000	1.18225300
H	2.52219700	-0.16242100	2.44336900
C	1.64297500	-2.21615600	-0.11120100
H	2.06242000	-1.80397200	-2.17293800

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H	1.42324500	-2.30620800	2.02127700
Cl	-3.14033600	4.90510800	-1.25352500
Cl	-3.36863500	-5.12040400	-1.14598300
Cl	6.37543100	-0.24873900	-0.82670500
Ga	5.10299500	-1.90526000	0.05658500
Ga	-4.20788400	-3.40471200	0.07881200
Ga	-1.06868900	5.20178000	-0.36750400

pCp3In

SCF Energy = -2879.19197765 au

C	-2.34421400	-1.00277300	-0.82673800
C	-1.93027000	-1.38502900	0.44884600
C	-1.06825400	-2.45786600	0.63140900
C	-0.59073400	-3.19631300	-0.44712600
C	-1.02683600	-2.83756300	-1.71827800
C	-1.88402500	-1.76206600	-1.90285800
H	-2.28286800	-0.83951900	1.31357500
H	-0.74525200	-2.71343300	1.63504600
H	-0.68502300	-3.39944900	-2.58188300
H	-2.19343300	-1.49318600	-2.90796300
C	0.41314500	-4.29097100	-0.23908200
H	0.42953800	-4.56141700	0.81993500
H	0.12067200	-5.18955900	-0.79038500
C	1.82982100	-3.88223100	-0.67889500
H	2.52861500	-4.67433000	-0.39279200
H	1.86097700	-3.81122800	-1.76918400
C	2.25584700	-2.56872900	-0.09341800
C	2.49855800	-2.42229500	1.26844100
C	2.35736600	-1.43399900	-0.89195900
C	2.78983600	-1.18004000	1.81335000
H	2.44381900	-3.28849200	1.92026100
C	2.66088700	-0.19222000	-0.34972800
H	2.17496300	-1.51677000	-1.95818800
C	2.86032900	-0.03422700	1.02086300
H	2.94954100	-1.09195000	2.88340700
H	2.73771200	0.66385800	-1.00613900
C	3.14415200	1.30694000	1.63936400
H	4.22603100	1.47820000	1.65118700
H	2.82055300	1.27607500	2.68368700
C	2.49299700	2.49645600	0.92854800
H	2.67308500	3.39106000	1.53259300
H	2.99638600	2.67050700	-0.02543000
C	-3.25139800	0.17574200	-1.05217100
H	-3.06258500	0.57235300	-2.05344000
H	-4.29320900	-0.16248000	-1.04810200
C	-3.12749400	1.29417000	-0.01717800
H	-3.70761100	2.15021300	-0.37672300
H	-3.58480700	0.97608300	0.92295600
C	-1.70937900	1.71818500	0.23276100

## pCp3M

C	-0.84764400	2.01999400	-0.82178200
C	-1.19039100	1.78572100	1.52446500
C	0.48833800	2.31523300	-0.58946600
H	-1.22342700	2.01622300	-1.83807800
C	0.14819000	2.06959500	1.75299600
H	-1.84381600	1.57741400	2.36591100
C	1.02081600	2.31071200	0.69785900
H	1.13896500	2.52753400	-1.43187400
H	0.52023300	2.08257500	2.77214900
Cl	-5.37429600	-1.76091100	1.24003000
Cl	5.96354500	1.17617100	-0.62990600
Cl	-3.13104900	4.67480800	-1.59092600
In	-1.42827300	4.94982600	0.17101600
In	5.61831500	-1.23020800	-0.20080000
In	-4.16404900	-3.54104700	0.03737100

## pCp3Tl

SCF Energy = -2826.32909139 au

C	-2.34564500	-0.98997900	-0.84413500
C	-1.93745600	-1.37314500	0.43316300
C	-1.08994100	-2.45640600	0.62011100
C	-0.62314300	-3.20650700	-0.45539400
C	-1.05209500	-2.84536400	-1.72867600
C	-1.89296300	-1.75744800	-1.91764100
H	-2.28725500	-0.82188200	1.29530700
H	-0.77018700	-2.71209700	1.62487100
H	-0.71507700	-3.41346900	-2.59027400
H	-2.19572500	-1.48578400	-2.92410200
C	0.36703300	-4.31294400	-0.24219500
H	0.37171500	-4.58655900	0.81621500
H	0.07063600	-5.20703100	-0.79888000
C	1.79237100	-3.91911600	-0.66803400
H	2.47866400	-4.72084300	-0.37800800
H	1.83348200	-3.84561500	-1.75788300
C	2.22843500	-2.61178400	-0.07557500
C	2.46045900	-2.47102800	1.28914300
C	2.34532400	-1.47534500	-0.86985100
C	2.75597400	-1.23214000	1.84000600
H	2.38990900	-3.33808000	1.93851300
C	2.65669400	-0.23823400	-0.32184900
H	2.16882400	-1.55323900	-1.93754600
C	2.84533500	-0.08532800	1.05082000
H	2.90451200	-1.14759300	2.91203500
H	2.75091900	0.61845000	-0.97502200
C	3.14126100	1.25075500	1.67407900
H	4.22542400	1.40676700	1.69230800
H	2.80778700	1.22283400	2.71548800
C	2.51454900	2.45097800	0.95897200
H	2.70318200	3.34086600	1.56736700

## pCp3M

H	3.03201900	2.61839200	0.01139000
C	-3.24147500	0.19649700	-1.07256300
H	-3.04911300	0.59081700	-2.07407100
H	-4.28611800	-0.13292000	-1.06670400
C	-3.11073600	1.31426900	-0.03800700
H	-3.67396600	2.17789600	-0.40675600
H	-3.58192900	1.00288900	0.89750100
C	-1.68949900	1.71960000	0.22357100
C	-0.81170000	1.99703800	-0.82454300
C	-1.18485700	1.79613800	1.52051700
C	0.52481200	2.27898900	-0.58030500
H	-1.17732000	1.98790600	-1.84444900
C	0.15403900	2.06921500	1.76143100
H	-1.85045400	1.60343000	2.35625000
C	1.04210300	2.28667000	0.71343300
H	1.18814500	2.47141800	-1.41765600
H	0.51529900	2.08866600	2.78453000
Cl	-5.40608900	-1.62832800	1.28520200
Cl	5.98824500	1.18609100	-0.53632600
Cl	-3.10890100	4.62755400	-1.74187100
Tl	-1.38220700	4.97031500	0.11847300
Tl	5.62919700	-1.32285300	-0.15165900
Tl	-4.22219900	-3.51941200	0.03024200

## pCp3Ge

SCF Energy = -9919.23442478 au

C	1.45227400	1.47743700	-1.30259400
C	1.19725600	1.77383500	0.03935300
C	0.01816700	2.41142400	0.42276800
C	-0.92368200	2.81253800	-0.51648800
C	-0.64736600	2.55521800	-1.85659800
C	0.50916200	1.89379900	-2.23875000
H	1.90000400	1.47178500	0.80524300
H	-0.15640100	2.60718200	1.47388100
H	-1.35666200	2.86592500	-2.61730300
H	0.68447000	1.69079600	-3.29016300
C	-2.21388100	3.44012900	-0.08115500
H	-2.11376500	3.76914300	0.95608200
H	-2.42499600	4.33261100	-0.67692100
C	-3.40725900	2.47659200	-0.20141100
H	-4.28669100	2.94071200	0.25345200
H	-3.64956600	2.31839600	-1.25432300
C	-3.12779000	1.15030900	0.43605100
C	-3.01231400	1.00745500	1.81530700
C	-2.90722400	0.01800200	-0.35042400
C	-2.64974000	-0.20516400	2.38040200
H	-3.19203800	1.86241700	2.45890300
C	-2.54880100	-1.20037300	0.22266000
H	-2.98426300	0.09600100	-1.42935500

## pCp3M

C	-2.40033500	-1.33038600	1.59862700
H	-2.55209900	-0.27944100	3.45881700
H	-2.39208700	-2.05053300	-0.42697400
C	-1.99354100	-2.63080900	2.23525300
H	-2.88873700	-3.21398400	2.47872900
H	-1.51508600	-2.40818800	3.19295400
C	-1.06544300	-3.50401100	1.38545400
H	-0.73733600	-4.34965800	1.99775400
H	-1.61999800	-3.93548300	0.54858100
C	2.69238300	0.75046700	-1.73815200
H	2.47352700	0.22811300	-2.67337600
H	3.47151400	1.48288800	-1.97581500
C	3.26780900	-0.23019800	-0.71550200
H	4.07972500	-0.78407000	-1.19677100
H	3.72686500	0.31496400	0.11188700
C	2.24135600	-1.18314100	-0.17076700
C	1.41100900	-1.92224100	-1.01846400
C	2.02179000	-1.30205100	1.20530700
C	0.37531000	-2.69119400	-0.51188900
H	1.56878000	-1.88176900	-2.08973400
C	0.98492900	-2.07091100	1.70623300
H	2.67384900	-0.76896100	1.88858000
C	0.12474400	-2.75756800	0.85425700
H	-0.26134000	-3.24018000	-1.19775800
H	0.83638000	-2.12100800	2.77946600
Cl	1.84653700	4.93753400	1.86009100
Cl	4.19433900	3.57972200	-0.10752600
Cl	-6.26905000	0.55466800	-1.29545700
Cl	-5.34415800	-2.66759600	-1.11203300
Cl	4.30514700	-3.60252000	-1.98539200
Cl	5.27097700	-2.70316200	1.08526600
Ge	3.55714300	-3.70453900	0.10338300
Ge	-5.48111900	-0.88141500	0.20330500
Ge	2.11955700	4.36534100	-0.26721400

## pCp3Sn

SCF Energy = -4332.0251194 au

C	1.49082900	1.81192100	-0.68292300
C	0.57003400	2.01685000	0.34893800
C	-0.79272100	2.12973500	0.08131600
C	-1.28365300	2.05013900	-1.21875700
C	-0.35698100	1.91275000	-2.24852300
C	0.99909400	1.79784100	-1.98579700
H	0.90975200	2.05565800	1.37790700
H	-1.48019800	2.28086000	0.90596000
H	-0.70107400	1.87312500	-3.27688500
H	1.69382200	1.66880900	-2.80946500
C	-2.76128300	2.04959400	-1.48619900
H	-3.30188300	2.18349700	-0.54655300

## pCp3M

H	-3.03448200	2.90282600	-2.11418200
C	-3.24167500	0.77398200	-2.18477300
H	-4.33627500	0.79971700	-2.21941700
H	-2.89969500	0.76731200	-3.22346900
C	-2.79845300	-0.50853500	-1.53919400
C	-2.61641200	-0.62055200	-0.15830900
C	-2.55171300	-1.64290800	-2.31023700
C	-2.15555100	-1.80600100	0.41257100
H	-2.80843000	0.22810600	0.48557100
C	-2.11865700	-2.82824100	-1.73705300
H	-2.69609200	-1.59177900	-3.38448700
C	-1.89250300	-2.92754000	-0.36649900
H	-2.00675500	-1.85089300	1.48500200
H	-1.93784600	-3.68915500	-2.37297800
C	-1.32229300	-4.16911900	0.25165300
H	-1.91123000	-5.04518900	-0.03585700
H	-1.39030100	-4.08587000	1.33893500
C	0.14304000	-4.40720600	-0.15325500
H	0.53107000	-5.25319000	0.42106600
H	0.18437200	-4.69423500	-1.20708300
C	2.94324500	1.57279600	-0.39127600
H	3.45902500	1.29573800	-1.31389500
H	3.40438900	2.50343100	-0.04550000
C	3.17845900	0.50782000	0.67835900
H	4.25633500	0.33110300	0.75825000
H	2.87706700	0.88888100	1.65747600
C	2.46384400	-0.79653500	0.44311900
C	2.11283500	-1.23756300	-0.83625600
C	2.09841100	-1.61162100	1.52136400
C	1.38790500	-2.40706600	-1.02071300
H	2.39994800	-0.65553800	-1.70136300
C	1.38397200	-2.78477200	1.33104900
H	2.37896100	-1.31157900	2.52501200
C	0.99915300	-3.19418000	0.05607300
H	1.11467500	-2.70640700	-2.02649200
H	1.11390600	-3.38593700	2.19326500
Cl	-0.97395500	5.30393200	1.62318800
Cl	2.55692000	4.93440200	1.11909700
Cl	-6.06342000	0.33555500	0.05075100
Cl	-4.98212400	-2.03888200	2.51943400
Cl	5.55915900	-1.23643300	-1.59003900
Cl	5.71273900	-1.90603700	1.91747900
Sn	4.64552600	-2.81564900	-0.02421900
Sn	-5.22457900	-1.91679800	0.14026000
Sn	0.54203200	4.90700800	-0.18758800

## pCp3Pb

SCF Energy = -4267.73338662 au

C	1.90619300	1.21150400	-1.26445100
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## pCp3M

C	1.60554000	1.55011800	0.05721800
C	0.61394200	2.48169400	0.35313000
C	-0.10231500	3.12210600	-0.65730500
C	0.20590300	2.79280000	-1.97444200
C	1.18478400	1.85324200	-2.26949800
H	2.14793400	1.08782400	0.87115800
H	0.40695000	2.72282300	1.38894300
H	-0.33140500	3.27318500	-2.78609300
H	1.39499100	1.61125000	-3.30628300
C	-1.20158700	4.08002100	-0.30765700
H	-1.05539800	4.41919900	0.72074800
H	-1.15214100	4.96885500	-0.94261600
C	-2.60028500	3.45215100	-0.45192700
H	-3.33677600	4.14192900	-0.02991400
H	-2.84162500	3.33938500	-1.51163000
C	-2.69374700	2.10960300	0.20888100
C	-2.69201800	1.96674900	1.59462400
C	-2.70961300	0.94895900	-0.55905100
C	-2.67242200	0.71286200	2.18746800
H	-2.68581000	2.85110300	2.22391300
C	-2.71201600	-0.31160100	0.03548500
H	-2.72814800	1.02165300	-1.64009200
C	-2.67158200	-0.45433200	1.42483800
H	-2.64791400	0.63632200	3.26960600
H	-2.73021800	-1.18711400	-0.59997100
C	-2.63624900	-1.80289600	2.08772600
H	-3.66242800	-2.13060800	2.28692200
H	-2.15103300	-1.69144200	3.06134100
C	-1.94287600	-2.90490200	1.28155300
H	-1.88892500	-3.79794800	1.91137600
H	-2.56288300	-3.17690600	0.42423200
C	2.97374800	0.20758600	-1.60061300
H	2.73046400	-0.25121700	-2.56271100
H	3.92438700	0.73179800	-1.74851000
C	3.20325200	-0.87415300	-0.54490600
H	3.87782800	-1.62439600	-0.96913400
H	3.72614000	-0.45364800	0.31648200
C	1.93153300	-1.52616700	-0.07980500
C	0.96232800	-1.97110900	-0.98457600
C	1.64484600	-1.65711000	1.28309100
C	-0.26142600	-2.45470000	-0.54191600
H	1.16210600	-1.92434500	-2.04843500
C	0.41905500	-2.13657300	1.71892200
H	2.39582300	-1.36082300	2.00729300
C	-0.57082100	-2.51283000	0.81362400
H	-0.99823500	-2.77525800	-1.27105800
H	0.22586000	-2.19745000	2.78475500
Cl	2.34448300	5.12065900	1.94198600
Cl	4.90593700	2.61787100	0.67802900

## pCp3M

Cl	-5.72696300	0.41068500	-2.36547000
Cl	-5.69747300	-2.32392900	0.22588500
Cl	3.40745900	-4.23024200	-2.25744000
Cl	4.53204800	-3.87124400	1.29023600
Pb	2.46866900	-4.48799200	0.04393200
Pb	3.10643700	4.10579700	-0.20936500
Pb	-5.60361700	0.17686700	0.11131600

## pCp3As

SCF Energy = -11776.0187045 au

C	2.29672900	-1.61636200	0.89427100
C	1.78329900	-1.77544100	-0.39040100
C	0.57152000	-2.41496500	-0.60114800
C	-0.16634800	-2.93442200	0.45821000
C	0.35963100	-2.79993100	1.73887800
C	1.56420500	-2.14669200	1.95137400
H	2.32766200	-1.38491000	-1.24212200
H	0.18900300	-2.51133900	-1.61122600
H	-0.18658700	-3.19654600	2.58876600
H	1.94127400	-2.03860900	2.96335100
C	-1.50955300	-3.56063600	0.22128100
H	-1.68354500	-3.62282100	-0.85551500
H	-1.52380300	-4.58970900	0.59383000
C	-2.65539000	-2.78349700	0.88702500
H	-3.60737300	-3.20469200	0.54703500
H	-2.61793400	-2.93319600	1.96904600
C	-2.61249700	-1.31018100	0.60374800
C	-2.63178900	-0.82312300	-0.70112900
C	-2.51171400	-0.38500300	1.63620600
C	-2.52843700	0.53558000	-0.95696500
H	-2.72086200	-1.51383000	-1.53262000
C	-2.42445900	0.97499400	1.38062200
H	-2.49150500	-0.73723300	2.66225000
C	-2.41858600	1.46123200	0.07796600
H	-2.53281400	0.88682300	-1.98329500
H	-2.34131300	1.66401700	2.21389300
C	-2.27049600	2.92677600	-0.21977700
H	-3.20685600	3.45228600	-0.00315400
H	-2.10462700	3.04670300	-1.29311000
C	-1.13521000	3.60502700	0.55732200
H	-0.99322300	4.61303000	0.15382100
H	-1.42325100	3.73324300	1.60374800
C	3.58622700	-0.88493000	1.14021600
H	3.66195400	-0.66662700	2.20865600
H	4.43386500	-1.53732300	0.90299600
C	3.73254000	0.41062800	0.33385600
H	4.61310800	0.94896500	0.69930600
H	3.94095600	0.17717300	-0.71287800
C	2.51827500	1.29248200	0.39964900



## pCp3M

C	1.96119200	1.67440200	1.61507100
C	1.88520900	1.72060300	-0.76434000
C	0.80035700	2.43089300	1.66252000
H	2.42754000	1.36169600	2.54331400
C	0.72891900	2.48357600	-0.71715700
H	2.30441400	1.44744500	-1.72681700
C	0.15608400	2.84133400	0.50082700
H	0.37770600	2.69873100	2.62544100
H	0.26157700	2.79530600	-1.64474200
Cl	1.65609400	-5.64060700	-1.80419100
Cl	3.41934100	-6.72469200	0.76214300
Cl	4.46927900	-4.11871400	-0.96317300
Cl	-6.13987400	-1.60730200	-0.99233400
Cl	-5.93385800	1.64697100	-1.55844400
Cl	-7.44855200	0.53096100	1.14980300
Cl	4.07431600	6.24457800	1.07021800
Cl	1.71959300	5.91436200	-1.21423200
Cl	4.50093200	4.13415400	-1.42700500
As	-5.58124600	0.22410200	0.05813500
As	2.98004800	4.65402500	0.04817800
As	2.63400900	-4.84412000	-0.02467900

## pCp3Sb

SCF Energy = -5790.10475089 au

C	1.58637300	1.95624600	-0.40281600
C	0.72597300	2.11026700	0.68295600
C	-0.63782200	2.27928500	0.49477800
C	-1.19541900	2.30455900	-0.78129500
C	-0.32946600	2.20161400	-1.86525800
C	1.03390900	2.03058000	-1.67776500
H	1.12085800	2.08147600	1.69210400
H	-1.28364600	2.38692500	1.35926700
H	-0.72566200	2.23140700	-2.87497000
H	1.68262800	1.93111100	-2.54224400
C	-2.68402700	2.37382800	-0.96926700
H	-3.16523300	2.43715100	0.00943700
H	-2.96063200	3.29105000	-1.49831500
C	-3.24504600	1.18286300	-1.75361000
H	-4.33889100	1.23516700	-1.71753600
H	-2.97188100	1.27432700	-2.80841700
C	-2.79016300	-0.16446000	-1.26478900
C	-2.57794100	-0.42428900	0.08764500
C	-2.56583200	-1.20590600	-2.16192100
C	-2.12577100	-1.66411600	0.51713500
H	-2.75687000	0.35060300	0.82193800
C	-2.13568100	-2.45177300	-1.73034100
H	-2.72664700	-1.03519900	-3.22164700
C	-1.89266800	-2.70002400	-0.38229600
H	-1.95380900	-1.82963400	1.57447000

## pCp3M

H	-1.97130100	-3.23901100	-2.45944500
C	-1.33607800	-4.01039200	0.09073300
H	-1.95313700	-4.84086700	-0.26563500
H	-1.37659400	-4.03671400	1.18228000
C	0.11212700	-4.24081200	-0.37464200
H	0.49481800	-5.14264800	0.11242000
H	0.11953200	-4.43627100	-1.44998800
C	3.04712600	1.67390300	-0.19955000
H	3.51346000	1.47849200	-1.16848400
H	3.54472700	2.56096400	0.20522500
C	3.30834300	0.50524400	0.75290400
H	4.38081100	0.28270000	0.74065400
H	3.08424000	0.80580600	1.77954400
C	2.52688500	-0.74322100	0.44552000
C	2.19242800	-1.10567700	-0.85785300
C	2.10037500	-1.58348000	1.47499700
C	1.44000600	-2.24138900	-1.11591400
H	2.51542500	-0.49041600	-1.68756700
C	1.35924600	-2.72623700	1.21456700
H	2.35632000	-1.33442400	2.49928700
C	1.00196600	-3.06787500	-0.08742300
H	1.17636600	-2.48254900	-2.14004700
H	1.04064700	-3.35258000	2.04184700
Cl	-1.03694700	5.70378800	1.47569400
Cl	0.93528000	7.48265400	-0.80489300
Cl	2.44410100	5.20315300	1.38024000
Cl	-6.09590000	0.06104100	0.54621500
Cl	-5.05757500	-2.88145700	2.17354400
Cl	-7.47001900	-3.02695300	-0.35690400
Cl	5.67841600	-1.52861100	-1.44584000
Cl	6.28604800	-4.80972500	-0.39263700
Cl	5.63843400	-2.30539400	1.96861200
Sb	4.68801300	-3.12084200	-0.02057400
Sb	0.62951500	5.25121200	-0.11802500
Sb	-5.33379900	-2.09377700	-0.02319800

## pCp3Bi

SCF Energy = -5713.26773151 au

C	-2.24957100	-1.64035800	-1.00957100
C	-1.73600500	-1.76352800	0.28114500
C	-0.52754800	-2.40552000	0.51323600
C	0.20797200	-2.96498500	-0.52966400
C	-0.31797900	-2.86695000	-1.81573700
C	-1.51924000	-2.21117900	-2.04990900
H	-2.28209300	-1.35264000	1.12139300
H	-0.15253900	-2.48143900	1.52742900
H	0.22463600	-3.29610400	-2.65209700
H	-1.89561700	-2.13471800	-3.06499600
C	1.54719000	-3.59034600	-0.27066100

## pCp3M

H	1.69432800	-3.67643900	0.80801300
H	1.58017000	-4.60919600	-0.66768400
C	2.70246900	-2.78847600	-0.89106900
H	3.64885700	-3.20523600	-0.53185900
H	2.69347300	-2.91471200	-1.97662000
C	2.63361700	-1.32345000	-0.57408800
C	2.66422500	-0.86636500	0.74382900
C	2.49932200	-0.37424700	-1.58281700
C	2.53934200	0.48489900	1.03470000
H	2.78885600	-1.57415900	1.55586500
C	2.39065600	0.97916900	-1.29194700
H	2.47139100	-0.70093500	-2.61704100
C	2.39537600	1.43515800	0.02346000
H	2.56202100	0.81146100	2.06856300
H	2.28379700	1.68567600	-2.10737500
C	2.22992800	2.89048000	0.36199300
H	3.17162100	3.42501000	0.19839800
H	2.02880600	2.97538900	1.43214600
C	1.12063000	3.59172200	-0.43089500
H	0.95870800	4.58248800	0.00541800
H	1.44096600	3.75852300	-1.46230800
C	-3.53937400	-0.91698500	-1.27885000
H	-3.58607900	-0.67819900	-2.34456800
H	-4.38365300	-1.58521700	-1.07763600
C	-3.73049800	0.35611300	-0.44778800
H	-4.60523900	0.88996100	-0.83202200
H	-3.97459200	0.09664300	0.58446900
C	-2.52550100	1.25331200	-0.45299000
C	-1.93212600	1.67170300	-1.64094500
C	-1.93396000	1.65993200	0.74251000
C	-0.77466200	2.43819800	-1.63217700
H	-2.36626400	1.38044600	-2.59152000
C	-0.78018000	2.43072700	0.75170500
H	-2.38761400	1.37027100	1.68397200
C	-0.16767200	2.82113500	-0.43917800
H	-0.32577400	2.73530000	-2.57441900
H	-0.35039800	2.72941900	1.70117000
Bi	-2.61798300	-4.85947300	-0.02376400
Cl	-1.57302300	-5.53743800	2.07736300
Cl	-3.57452600	-7.03251100	-0.61341200
Cl	-4.65257600	-3.87759100	0.92323300
Bi	5.59850600	0.24801300	-0.10251000
Cl	6.16083400	-1.84635700	1.03211500
Cl	5.91541800	1.76227100	1.79006000
Cl	7.77095300	0.61408400	-1.16715100
Bi	-3.00689100	4.63981900	-0.09015500
Cl	-4.27443200	6.50094000	-1.04720000
Cl	-1.51723100	5.97466400	1.32127100
Cl	-4.62175100	4.00745000	1.63025800

## pCp2M

pCp2Ga

SCF Energy = -5697.78524848 au

C	-3.04746600	1.53569800	0.15454500
C	-3.18595800	1.07386400	1.45864400
C	-2.65649200	-0.14876300	1.84480100
C	-1.96824100	-0.96153300	0.94444500
C	-1.86224300	-0.51208700	-0.37104900
C	-2.38933400	0.71334300	-0.75426500
H	-3.70643800	1.68288800	2.19082900
H	-2.76352700	-0.47473600	2.87464100
H	-1.35462400	-1.11871500	-1.10859300
H	-2.26503200	1.04635200	-1.77869600
C	-1.36472900	-2.26376100	1.39493100
H	-1.13941600	-2.18478400	2.46226100
H	-2.10657600	-3.06341100	1.29558700
C	-0.11249500	-2.68917200	0.62672300
H	0.30740600	-3.57163000	1.12013500
H	-0.39320700	-3.01307600	-0.37844100
C	0.92499700	-1.60677700	0.53126200
C	1.36393600	-0.92245400	1.65774300
C	1.44781400	-1.22161300	-0.70114600
C	2.25018800	0.13854600	1.55005200
H	0.99538900	-1.20524900	2.63782600
C	2.32553500	-0.15242300	-0.81302100
H	1.13978600	-1.75191400	-1.59678300
C	2.72230600	0.56944900	0.31269800
H	2.55845500	0.66798100	2.44567300
H	2.69677800	0.13304600	-1.79056400
C	3.58219400	1.79214000	0.18720900
H	4.56678000	1.51080500	-0.19988700
H	3.74829200	2.21226500	1.18257300
C	2.98137400	2.85314700	-0.74070700
H	3.60465700	3.75248600	-0.68087000
H	3.05562000	2.51109200	-1.77646800
C	-3.52399500	2.89682800	-0.25399200
H	-3.54271800	2.95244800	-1.34540400
H	-4.55067300	3.05949000	0.08744900
C	-2.63300900	4.02262400	0.29842100
H	-2.96468400	4.97141600	-0.13571000
H	-2.78437600	4.10267400	1.37823500
C	-1.17235200	3.80100700	0.02972300
C	-0.67179300	3.74402900	-1.26728700
C	-0.28486000	3.57820100	1.07485000
C	0.65887600	3.44189500	-1.50422800
H	-1.33598700	3.91779000	-2.10855500
C	1.05034400	3.29425500	0.83777800
H	-0.65038800	3.61156000	2.09609300
C	1.54567600	3.20482300	-0.45780400
H	1.01870200	3.38012500	-2.52666000

## pCp2M

H	1.70853100	3.11957100	1.68108900
Cl	-3.65701400	-3.42581400	-1.17081000
Cl	5.80265600	-0.90072900	-1.06759400
Ga	4.37590800	-2.02703000	0.29138300
Ga	-4.64043300	-1.51441600	-0.42734600

## pCp2In

SCF Energy = -2228.89299523 au

C	-1.37536600	-0.87440600	0.55566700
C	-1.72261300	-0.20698200	-0.61868100
C	-2.44179000	0.97904400	-0.58099800
C	-2.84011300	1.54964800	0.62517700
C	-2.52341800	0.86870600	1.79513100
C	-1.80842100	-0.32065500	1.75982100
H	-1.42268900	-0.61445600	-1.57580800
H	-2.67841200	1.48422300	-1.51117900
H	-2.82956300	1.27620000	2.75337400
H	-1.55884900	-0.82157000	2.68988000
C	-3.53224000	2.88028900	0.65272500
H	-3.84891200	3.13593700	-0.36159200
H	-4.44404400	2.82194900	1.25499500
C	-2.64825700	4.00286500	1.21696300
H	-3.18093900	4.95313200	1.09997700
H	-2.52130600	3.85307900	2.29252100
C	-1.28770200	4.08480400	0.58324900
C	-1.12470500	4.11108200	-0.79739000
C	-0.14017500	4.09622900	1.36802700
C	0.13763900	4.09787400	-1.36739200
H	-1.99573700	4.11581400	-1.44419400
C	1.12216500	4.11020600	0.79803900
H	-0.23759100	4.07932200	2.44885400
C	1.28517500	4.08558700	-0.58262600
H	0.23505300	4.08227300	-2.44824100
H	1.99317900	4.11425200	1.44486200
C	2.64574100	4.00458500	-1.21645900
H	3.17781400	4.95518900	-1.09940200
H	2.51877100	3.85490800	-2.29203200
C	3.53055700	2.88250900	-0.65254800
H	4.44232000	2.82492800	-1.25495300
H	3.84721200	3.13815200	0.36177500
C	-0.54956200	-2.12961700	0.53024800
H	-0.11214400	-2.28911500	1.51916300
H	-1.19777800	-2.99017400	0.33464000
C	0.55106900	-2.12929100	-0.53079600
H	1.19974700	-2.98950800	-0.33523000
H	0.11373900	-2.28896600	-1.51972100
C	1.37615800	-0.87360100	-0.55610300
C	1.72352000	-0.20647800	0.61839000
C	1.80833100	-0.31907900	-1.76021100

pCp2M

C	2.44194200	0.98001600	0.58089300
H	1.42427600	-0.61457300	1.57547000
C	2.52257600	0.87073400	-1.79531800
H	1.55862400	-0.81973300	-2.69037200
C	2.83934800	1.55138000	-0.62521200
H	2.67872800	1.48490800	1.51118900
H	2.82800100	1.27886400	-2.75352100
Cl	-3.39320600	-3.22742000	-1.56066800
Cl	3.39499100	-3.22735600	1.55994400
In	4.46397300	-1.59995700	0.04198300
In	-4.46313700	-1.60140100	-0.04181400

pCp2Tl

SCF Energy = -2193.65090942 au

C	-1.37001400	-0.57913200	0.56206200
C	-1.72074300	0.09070900	-0.60994400
C	-2.44089300	1.27562900	-0.56783800
C	-2.83890100	1.84205600	0.64064300
C	-2.51738300	1.15942800	1.80876200
C	-1.79864800	-0.02780900	1.76891800
H	-1.42594700	-0.31746200	-1.56831800
H	-2.67955600	1.78326600	-1.49626200
H	-2.81947200	1.56599300	2.76883400
H	-1.54309100	-0.52915400	2.69720400
C	-3.52918400	3.17386400	0.67265200
H	-3.85188300	3.43012200	-0.33969800
H	-4.43708500	3.11838200	1.28122200
C	-2.63998000	4.29536700	1.23110500
H	-3.17193000	5.24646600	1.11716500
H	-2.50705300	4.14536400	2.30591300
C	-1.28280300	4.37587400	0.58994000
C	-1.12689200	4.40043300	-0.79152600
C	-0.13124400	4.38888800	1.36879700
C	0.13251300	4.38714100	-1.36796200
H	-2.00114000	4.40389200	-1.43394400
C	1.12813900	4.40317300	0.79235200
H	-0.22307300	4.37307300	2.45012100
C	1.28406600	4.37688900	-0.58910000
H	0.22435800	4.36989700	-2.44926000
H	2.00243300	4.40873000	1.43472000
C	2.64136300	4.29713300	-1.23004400
H	3.17326800	5.24811900	-1.11504100
H	2.50877000	4.14803900	-2.30501600
C	3.53034200	3.17514100	-0.67216000
H	4.43849800	3.12007900	-1.28038700
H	3.85256400	3.43065700	0.34052900
C	-0.54815800	-1.83647400	0.52977800
H	-0.10857900	-2.00338200	1.51649000
H	-1.20018300	-2.69286100	0.32795600

## pCp2M

C	0.54984500	-1.83572700	-0.53401900
H	1.20202400	-2.69222200	-0.33314500
H	0.11035900	-2.00163200	-1.52094400
C	1.37140000	-0.57811500	-0.56501600
C	1.72079300	0.09147600	0.60754800
C	1.80118000	-0.02634100	-1.77125700
C	2.44076800	1.27654800	0.56651600
H	1.42509800	-0.31703300	1.56550700
C	2.51980400	1.16100700	-1.81001900
H	1.54671200	-0.52747800	-2.69995500
C	2.84002600	1.84333700	-0.64137100
H	2.67830100	1.78403600	1.49531100
H	2.82288400	1.56783300	-2.76966900
Cl	-3.34317100	-2.96209300	-1.63289600
Cl	3.34086500	-2.96509000	1.63127400
Tl	4.48133800	-1.32828300	0.02304400
Tl	-4.48219500	-1.32707000	-0.02174300

## pCp2Ge

SCF Energy = -6922.25547578 au

C	-1.01876500	-0.97790000	1.26986500
C	-1.44633200	-0.61014500	-0.00956500
C	-2.50009700	0.28524000	-0.18470200
C	-3.18720200	0.81316100	0.90187500
C	-2.78563000	0.41354500	2.17294900
C	-1.71951600	-0.45442000	2.35246700
H	-0.93075500	-0.98738200	-0.88355000
H	-2.79056500	0.56598800	-1.18945700
H	-3.30822700	0.79853800	3.04300100
H	-1.41934400	-0.73011300	3.35817600
C	-4.27659100	1.82196700	0.69622100
H	-4.60012200	1.78285500	-0.34667600
H	-5.14956000	1.56774400	1.30459200
C	-3.83020200	3.25188500	1.04372400
H	-4.62649900	3.94378500	0.75088900
H	-3.72138200	3.34178400	2.12797900
C	-2.53179800	3.63518500	0.39373000
C	-2.38964600	3.65072300	-0.99031000
C	-1.41011100	3.92106300	1.16199300
C	-1.16075400	3.90323400	-1.57678500
H	-3.24622400	3.43819100	-1.62251400
C	-0.18565700	4.19441100	0.57428800
H	-1.49287300	3.91411200	2.24397700
C	-0.03293700	4.17079300	-0.80692800
H	-1.07090700	3.88120700	-2.65838100
H	0.66633600	4.40669600	1.21035900
C	1.29968700	4.40273200	-1.46529100
H	1.50363300	5.47721900	-1.53425300
H	1.24090900	4.04338900	-2.49639000

## pCp2M

C	2.48607600	3.73423100	-0.76024600
H	3.37372600	3.85686400	-1.38894000
H	2.70503000	4.25175300	0.17687000
C	0.14441700	-1.90344400	1.48324600
H	0.57627800	-1.69448300	2.46569400
H	-0.22041100	-2.93535400	1.52656600
C	1.23000100	-1.83470600	0.40921400
H	2.08085200	-2.43431600	0.74723100
H	0.87963600	-2.30751000	-0.51075300
C	1.67267700	-0.43112100	0.10244700
C	1.97744100	0.47689900	1.12101200
C	1.71455300	0.04409400	-1.21281000
C	2.26119400	1.80279700	0.83576100
H	1.97894500	0.14282100	2.15158200
C	2.00060700	1.36995100	-1.49203400
H	1.50806500	-0.64370400	-2.02554500
C	2.25915300	2.27920100	-0.47017600
H	2.47944700	2.48450200	1.65055100
H	2.00894400	1.70276700	-2.52438000
Cl	-4.25524800	-2.05139800	-1.98821600
Cl	-1.98208100	-4.02250900	-0.51222500
Cl	4.68527300	-1.59555500	1.80907500
Cl	4.34572500	-2.31146500	-1.43918700
Ge	4.49888300	-0.52631100	-0.13319300
Ge	-3.47828100	-2.47205800	0.05016500

## pCp2Sn

SCF Energy = -3197.44977347 au

C	1.07638800	-0.78906900	-1.16898600
C	1.54136800	-0.30850300	0.05886700
C	2.50386100	0.69691500	0.11898700
C	3.04515600	1.25063700	-1.03795600
C	2.59983800	0.75203600	-2.25875600
C	1.63566400	-0.24375000	-2.32212700
H	1.13353100	-0.69749700	0.98366000
H	2.83656700	1.04769700	1.08784500
H	3.00798500	1.15486200	-3.18040000
H	1.30018300	-0.60114000	-3.29033200
C	4.02252900	2.38433000	-0.95041700
H	4.44914000	2.40368400	0.05528400
H	4.85640700	2.22060300	-1.63907500
C	3.38396700	3.74652800	-1.27053000
H	4.12090400	4.52872200	-1.05937600
H	3.17370500	3.80058900	-2.34214000
C	2.10942200	4.00846100	-0.51933900
C	2.04388000	3.91100200	0.86675600
C	0.93678800	4.31257200	-1.20092100
C	0.83941700	4.05639000	1.53514200
H	2.94132200	3.69147900	1.43595700



## pCp2M

C	-0.26200800	4.48707700	-0.52925300
H	0.96049300	4.40154100	-2.28228600
C	-0.33876900	4.33491700	0.85055600
H	0.81097900	3.94031900	2.61388600
H	-1.15475900	4.72388900	-1.09803300
C	-1.64524800	4.43596300	1.58835800
H	-1.95389200	5.48401000	1.67097800
H	-1.49317400	4.08157400	2.61148400
C	-2.79549200	3.64555600	0.94751900
H	-3.66185100	3.69618900	1.61389900
H	-3.09787700	4.12313700	0.01244900
C	0.00931300	-1.84441500	-1.24700100
H	-0.50183400	-1.75979400	-2.20970300
H	0.47874800	-2.83389900	-1.23850900
C	-1.00432100	-1.80313000	-0.10665300
H	-1.80733300	-2.51026900	-0.33714200
H	-0.54640500	-2.17251900	0.81395600
C	-1.57336100	-0.43406200	0.15111300
C	-1.82474100	0.46764800	-0.88800300
C	-1.81769500	0.00961600	1.45572200
C	-2.24410000	1.76416000	-0.62741500
H	-1.67196900	0.15762600	-1.91408600
C	-2.23869600	1.30631300	1.70946200
H	-1.66052400	-0.67624700	2.28097400
C	-2.43713600	2.21539600	0.67308800
H	-2.41058400	2.44175600	-1.45706400
H	-2.40249100	1.61761000	2.73598500
Cl	4.77295300	-1.22008300	1.99860900
Cl	2.43543500	-3.67296300	0.80913500
Cl	-4.16174500	-1.90877500	-2.09395000
Cl	-4.30736300	-2.62777700	1.40181800
Sn	-4.53885400	-0.72314800	-0.03542400
Sn	3.90543100	-1.99957800	-0.10063400

## pCp2Pb

SCF Energy = -3154.5879396 au

C	1.10323000	-0.59962400	-1.07814700
C	1.56213300	-0.02939700	0.11298900
C	2.45785600	1.03628900	0.10215600
C	2.93440700	1.56973400	-1.09383400
C	2.49649100	0.98393100	-2.27853900
C	1.59930000	-0.07588000	-2.27014300
H	1.20833100	-0.40484300	1.06511100
H	2.79356800	1.44950200	1.04476400
H	2.85466400	1.36832800	-3.22846500
H	1.26536400	-0.50044400	-3.21145700
C	3.83485200	2.76857000	-1.08046100
H	4.29876800	2.84808600	-0.09448900
H	4.65010200	2.63990600	-1.79827100

## pCp2M

C	3.09430400	4.07431400	-1.41443200
H	3.78745600	4.90863600	-1.26256700
H	2.83443900	4.07782700	-2.47652900
C	1.83872900	4.28348500	-0.61505300
C	1.83389800	4.20399400	0.77385100
C	0.62616500	4.52152200	-1.25160100
C	0.65131000	4.29611900	1.48923200
H	2.76328000	4.03907900	1.30896900
C	-0.55143300	4.64743400	-0.53307900
H	0.60170500	4.59742200	-2.33398300
C	-0.56588300	4.50570100	0.85009200
H	0.67231200	4.19170700	2.56932100
H	-1.47680900	4.83526500	-1.06685600
C	-1.84647800	4.54283800	1.63769600
H	-2.21726900	5.57117300	1.71144100
H	-1.63357200	4.21983800	2.66034700
C	-2.97044900	3.66847700	1.05952000
H	-3.81287100	3.68586000	1.75725300
H	-3.33274600	4.10350900	0.12480400
C	0.10320300	-1.72183700	-1.07428100
H	-0.44492400	-1.71557600	-2.02031600
H	0.63561200	-2.67810700	-1.03436100
C	-0.87204100	-1.68937400	0.09847900
H	-1.64351700	-2.44713000	-0.07260500
H	-0.36427900	-1.99844900	1.01543900
C	-1.51058700	-0.34632700	0.32891000
C	-1.76093400	0.54207100	-0.72218900
C	-1.83788300	0.08276700	1.62025500
C	-2.26080500	1.81483500	-0.48344800
H	-1.55104000	0.23998500	-1.74001800
C	-2.33694300	1.35628400	1.85244700
H	-1.68416200	-0.59480700	2.45295800
C	-2.53556600	2.25573100	0.80642700
H	-2.42299800	2.48210600	-1.32182500
H	-2.56256800	1.65855000	2.87004400
Cl	5.06359700	-0.48344800	1.95527300
Cl	2.72671800	-3.30212200	1.01138600
Cl	-3.86743100	-1.83720200	-2.23806200
Cl	-4.21023100	-2.74368100	1.37851800
Pb	-4.46131700	-0.73292700	-0.07101800
Pb	4.08503400	-1.51704500	-0.09679600

## pCp2As

SCF Energy = -8160.11118171 au

C	-1.21290500	4.04283500	-0.13977600
C	-0.45356900	3.90306600	-1.29586200
C	0.92817200	3.83345200	-1.23563600
C	1.60318400	3.90185100	-0.02192300
C	0.84597900	4.08652900	1.12936700

## pCp2M

C	-0.53563300	4.15480800	1.06929800
H	-0.94772100	3.81973100	-2.25839600
H	1.49563800	3.69980200	-2.15134000
H	1.33847000	4.15230200	2.09402200
H	-1.10397300	4.27472100	1.98643600
C	3.09370000	3.71865700	0.04352100
H	3.46949500	3.50588200	-0.96081200
H	3.57965500	4.64963200	0.35348500
C	3.53063400	2.61021600	1.00686000
H	4.60696600	2.44669400	0.87932300
H	3.39849400	2.94526000	2.03921700
C	2.80181800	1.30630800	0.83741600
C	2.42605500	0.83247100	-0.41688100
C	2.47843300	0.52524500	1.94311400
C	1.72926100	-0.35855500	-0.55244700
H	2.66484600	1.40462300	-1.30462000
C	1.79662300	-0.67442700	1.80628100
H	2.76007300	0.86854000	2.93360100
C	1.39622400	-1.13214300	0.55484100
H	1.43439500	-0.69266000	-1.54096700
H	1.55752300	-1.25455000	2.69216400
C	0.56910400	-2.37419600	0.39925100
H	1.05859300	-3.22603900	0.88125900
H	0.49533400	-2.61806200	-0.66328100
C	-0.84176600	-2.21823900	0.98958300
H	-1.43594900	-3.09768600	0.72133700
H	-0.77796000	-2.20189000	2.08059200
C	-2.71493100	4.00500400	-0.18296900
H	-3.09965900	4.07779300	0.83777600
H	-3.10502900	4.87948800	-0.71391200
C	-3.26786900	2.74795900	-0.86355200
H	-4.35699200	2.73011900	-0.74137300
H	-3.09463900	2.80841300	-1.94115800
C	-2.67968200	1.45707800	-0.36510100
C	-2.39612500	1.24579300	0.97930100
C	-2.39062200	0.42417400	-1.25487400
C	-1.82341000	0.05967100	1.41299800
H	-2.60312700	2.02496200	1.70321600
C	-1.83323600	-0.76825700	-0.81951800
H	-2.60678300	0.55802100	-2.30958400
C	-1.52713500	-0.96720900	0.52527400
H	-1.58713400	-0.06466100	2.46446400
H	-1.62488900	-1.55223900	-1.54009400
Cl	5.93251400	0.25029200	-1.01161200
Cl	4.34562700	-2.56674000	-1.70521600
Cl	6.43503200	-2.42943800	0.84178000
Cl	-6.61316500	-1.42408500	1.42334900
Cl	-4.57870400	-3.11504500	-0.54681200
Cl	-5.93377800	-0.28383100	-1.59590600

## pCp2M

As	4.76404700	-1.28803100	0.01275900
As	-4.87427100	-1.06470700	0.14700900

## pCp2Sb

SCF Energy = -4169.50234524 au

C	1.25720900	-0.53256800	-0.91000400
C	1.59735400	0.00907500	0.32857400
C	2.42460600	1.11838400	0.42156600
C	2.95523700	1.72355100	-0.71466600
C	2.63965900	1.16536100	-1.94969100
C	1.80305200	0.06264300	-2.04411300
H	1.20288900	-0.42830600	1.23730500
H	2.66154200	1.52247400	1.39847000
H	3.04081200	1.60820700	-2.85593500
H	1.55917900	-0.34025500	-3.02206200
C	3.77974800	2.97099600	-0.60041100
H	4.08974700	3.09512300	0.43989900
H	4.69837300	2.87709900	-1.18743300
C	3.02543900	4.22433800	-1.07305800
H	3.63910300	5.10239100	-0.84498600
H	2.92368500	4.19291600	-2.16120400
C	1.65733500	4.36883000	-0.46924400
C	1.46125600	4.34680600	0.90744800
C	0.53383500	4.48528500	-1.27925200
C	0.18639800	4.39300000	1.44689100
H	2.31464500	4.26980700	1.57328900
C	-0.73946900	4.55682500	-0.73856900
H	0.65798200	4.50736800	-2.35719000
C	-0.93919300	4.48857700	0.63551100
H	0.06064700	4.34241700	2.52381200
H	-1.59062100	4.64530000	-1.40529300
C	-2.31764100	4.48493100	1.23613800
H	-2.75026900	5.49093100	1.20024000
H	-2.23218600	4.22890200	2.29564200
C	-3.29711600	3.51524000	0.55878500
H	-4.22170400	3.49460700	1.14411900
H	-3.56892800	3.89285600	-0.42990500
C	0.32821600	-1.70879000	-1.02607600
H	-0.08818100	-1.72671200	-2.03674200
H	0.89610700	-2.63931700	-0.91942200
C	-0.80127300	-1.72330700	0.00565500
H	-1.51112300	-2.50916600	-0.27274200
H	-0.41143400	-2.01251700	0.98455800
C	-1.51591200	-0.40729400	0.13981500
C	-1.83374000	0.36602600	-0.97514400
C	-1.85420800	0.10197300	1.39355300
C	-2.43282300	1.60825500	-0.83732800
H	-1.59774500	0.00094000	-1.96737300
C	-2.45711000	1.34359300	1.52907100

pCp2M

H	-1.63250900	-0.48481400	2.27866800
C	-2.74082400	2.12913000	0.41527500
H	-2.64907500	2.19366200	-1.72423400
H	-2.69232300	1.71340300	2.52189900
Cl	5.35636400	-0.35511000	1.82413500
Cl	6.34026300	-2.70208400	-0.57570700
Cl	3.25841500	-3.06691200	1.03533400
Cl	-4.14379000	-2.16905600	-1.94572100
Cl	-7.01227900	-1.38947700	-0.09818000
Cl	-4.19053700	-2.69060400	1.51332900
Sb	-4.69552600	-0.96298400	0.00091500
Sb	4.45116800	-1.37500300	-0.09154200

pCp2Bi

SCF Energy = -4118.2788967 au

C	-2.78501500	1.57634000	-0.93244300
C	-2.40166900	1.13405800	0.33344500
C	-1.72664200	-0.06748700	0.49991900
C	-1.42343700	-0.88543500	-0.58661100
C	-1.82951200	-0.45828100	-1.84912100
C	-2.48958400	0.75177200	-2.01700600
H	-2.62498100	1.73461500	1.20539700
H	-1.43637900	-0.37958500	1.49658000
H	-1.61400600	-1.07174500	-2.71844000
H	-2.77651700	1.06786900	-3.01491900
C	-0.62254300	-2.13963900	-0.39718800
H	-0.58877700	-2.38052700	0.66762900
H	-1.10583700	-2.98606600	-0.89361200
C	0.80948700	-2.00401500	-0.94171600
H	1.38352300	-2.88637400	-0.64242600
H	0.78300500	-1.99724800	-2.03433500
C	1.48883300	-0.75504200	-0.46319600
C	1.79407000	-0.57032400	0.88569600
C	1.78316400	0.28499100	-1.33926400
C	2.35075600	0.61901900	1.33525700
H	1.59684700	-1.36641200	1.59549200
C	2.35198000	1.46969500	-0.89062900
H	1.55012900	0.17278600	-2.39282000
C	2.63489700	1.66747200	0.45819800
H	2.57174200	0.73796800	2.39055800
H	2.55596500	2.25748600	-1.60542000
C	3.21804100	2.95306900	0.97572300
H	4.31075100	2.91565900	0.90268100
H	3.00196500	3.01623300	2.04506500
C	2.70966200	4.21510400	0.27185300
H	3.09293100	5.08325100	0.81725100
H	3.13486800	4.28277200	-0.73320600
C	-3.49667900	2.88534100	-1.13423200
H	-3.32500900	3.21241600	-2.16327200

pCp2M

H	-4.57740000	2.72780500	-1.04229700
C	-3.08923600	3.99409100	-0.15947000
H	-3.55810900	4.92552500	-0.49218700
H	-3.50634700	3.78721700	0.82946500
C	-1.60062000	4.16716200	-0.04133700
C	-0.80172200	4.34089600	-1.16595300
C	-0.96969000	4.09728700	1.19609900
C	0.57776700	4.39354400	-1.05762900
H	-1.25932900	4.41379100	-2.14715000
C	0.40978100	4.14922000	1.30433700
H	-1.57066900	3.97836000	2.09228900
C	1.21074400	4.27434100	0.17461800
H	1.17881600	4.50976900	-1.95421600
H	0.86805000	4.06697100	2.28452100
Bi	-4.78512200	-0.97701500	-0.05346000
Cl	-4.25157400	-2.29797100	1.93478000
Cl	-6.75977400	-2.25165100	-0.75054500
Cl	-5.98041100	0.84334300	1.07256900
Bi	4.85246500	-0.81073500	-0.15708700
Cl	4.56235900	-2.94045300	1.01188000
Cl	6.12059100	0.35708700	1.58234600
Cl	6.76224000	-1.47496200	-1.54357900

## pCp1M

pCp1Ga

SCF Energy = -3313.04137362 au

C	-1.85839200	-1.44280500	-1.65148900
C	-2.00303700	-1.96325400	-0.36861200
C	-0.96468200	-2.65981200	0.23797900
C	0.24599400	-2.87874400	-0.41619500
C	0.35655100	-2.42003800	-1.72258400
C	-0.67320700	-1.71509900	-2.32441100
H	-2.92235600	-1.79805600	0.18231100
H	-1.10134100	-3.04194000	1.24587600
H	1.27137900	-2.58819800	-2.27838500
H	-0.54091800	-1.34891300	-3.33704500
C	1.38337500	-3.57010100	0.28538000
H	1.20336600	-3.51556100	1.36283200
H	1.38264700	-4.63755200	0.03540800
C	2.77592500	-3.00331500	-0.02335300
H	3.49931900	-3.52161900	0.61438600
H	3.05555900	-3.24354600	-1.05251700
C	2.87728800	-1.51729600	0.17715300
C	2.65085300	-0.93981500	1.42070500
C	3.14364300	-0.66472900	-0.88882000
C	2.62564300	0.43702500	1.57357400
H	2.45346300	-1.57210100	2.28068500
C	3.12895600	0.71146600	-0.73296800
H	3.34458600	-1.08636700	-1.86843400
C	2.83575000	1.29098100	0.49665000
H	2.40693700	0.85966200	2.54889600
H	3.32377600	1.34041600	-1.59425700
C	2.70710200	2.78001900	0.67032500
H	3.69917300	3.23758100	0.76070100
H	2.19972400	2.96910800	1.62069800
C	1.94878000	3.50022400	-0.45474100
H	1.82872800	4.54858300	-0.16390600
H	2.55526200	3.50484500	-1.36420100
C	-2.91398400	-0.56295600	-2.25890100
H	-2.66551100	-0.37936800	-3.30770600
H	-3.87930800	-1.07825800	-2.26028400
C	-3.09420700	0.76964700	-1.51647500
H	-3.81276300	1.38077200	-2.07486500
H	-3.55132300	0.58019200	-0.54114200
C	-1.82549800	1.54827400	-1.29428300
C	-0.79034600	1.55714600	-2.22149100
C	-1.64108100	2.28163000	-0.12178600
C	0.40121800	2.21204100	-1.96063700
H	-0.90230900	1.02848900	-3.15994000
C	-0.44560800	2.94306500	0.13580600
H	-2.44811500	2.32972100	0.60234500
C	0.61131400	2.89236500	-0.76665300
H	1.19674300	2.17680200	-2.69721200

	pCp1M		
H	-0.33389000	3.49246000	1.06586100
Cl	-3.11095200	0.06587600	2.36044600
Ga	-0.87970200	0.05572400	1.79378300

pCp1In

SCF Energy = -1578.58868655 au

C	2.21610300	1.97942000	-0.85021000
C	1.81898700	2.58261100	0.34222300
C	0.51751900	3.03869300	0.51519600
C	-0.43711900	2.91525800	-0.49570100
C	0.00000000	2.43112700	-1.72289500
C	1.29462100	1.96981800	-1.89229200
H	2.51548700	2.65040000	1.17202400
H	0.22331000	3.43939700	1.48019300
H	-0.68972500	2.36602100	-2.55467500
H	1.58439600	1.56067800	-2.85389800
C	-1.88458200	3.24239300	-0.22748700
H	-2.06380600	3.11658700	0.84465700
H	-2.07041300	4.30225000	-0.43764000
C	-2.92940100	2.42307200	-1.00713000
H	-3.91594200	2.75876700	-0.67315900
H	-2.87149800	2.67121400	-2.07043300
C	-2.82228000	0.92949200	-0.85021000
C	-3.14610100	0.28398300	0.34222300
C	-2.35322300	0.13626600	-1.89229200
C	-2.89034500	-1.07116200	0.51519600
H	-3.55305700	0.85327500	1.17202400
C	-2.10541800	-1.21556400	-1.72289500
H	-2.14378500	0.59178800	-2.85389800
C	-2.30612800	-1.83618500	-0.49570100
H	-3.09026000	-1.52630700	1.48019300
H	-1.70417200	-1.78033000	-2.55467500
C	-1.86570400	-3.25329200	-0.22748700
H	-2.69065100	-3.94415500	-0.43764000
H	-1.66714000	-3.34560200	0.84465700
C	-0.63374100	-3.74847200	-1.00713000
H	-0.43119200	-4.77068900	-0.67315900
H	-0.87759000	-3.82239700	-2.07043300
C	3.56314200	1.32540000	-1.00713000
H	3.74908800	1.15118300	-2.07043300
H	4.34713400	2.01192100	-0.67315900
C	3.75028600	0.01089900	-0.22748700
H	4.76106400	-0.35809500	-0.43764000
H	3.73094700	0.22901500	0.84465700
C	2.74324700	-1.07907300	-0.49570100
C	2.10541800	-1.21556400	-1.72289500
C	2.37282600	-1.96753100	0.51519600
C	1.05860200	-2.10608400	-1.89229200
H	2.39389700	-0.58569100	-2.55467500



			pCp1M
C	1.32711400	-2.86659500	0.34222300
H	2.86695000	-1.91309000	1.48019300
C	0.60617600	-2.90891200	-0.85021000
H	0.55938800	-2.15246600	-2.85389800
H	1.03757100	-3.50367600	1.17202400
Cl	0.00000000	0.00000000	3.56126700
In	0.00000000	0.00000000	1.03727700

pCp1Tl

SCF Energy = -1560.97740491 au

C	-0.84845200	-2.87723200	-1.13084600
C	0.38312400	-2.90188400	-0.48271400
C	1.45565100	-2.15068500	-0.95042300
C	1.33503100	-1.34357800	-2.08272700
C	0.12583900	-1.38098100	-2.76662900
C	-0.94097100	-2.13023400	-2.29906400
H	0.50946900	-3.51002300	0.40868200
H	2.40446500	-2.17432600	-0.42257400
H	-0.00006800	-0.79909500	-3.67129200
H	-1.87734400	-2.11615800	-2.84645400
C	2.47703100	-0.46326700	-2.51319700
H	3.11538900	-0.28662400	-1.64260200
H	3.09860800	-0.99341400	-3.24404900
C	2.06203800	0.88423700	-3.12147900
H	2.97260800	1.46703500	-3.29012200
H	1.61077300	0.73266300	-4.10597800
C	1.10648400	1.66130500	-2.26032200
C	1.48135500	2.12719400	-1.00262000
C	-0.20132700	1.89602500	-2.66843000
C	0.55287100	2.73509600	-0.16584400
H	2.49867500	1.98421400	-0.65247500
C	-1.12396900	2.50633000	-1.83392400
H	-0.51507600	1.57365200	-3.65581200
C	-0.77547900	2.90775800	-0.55070600
H	0.87160900	3.08692300	0.81208900
H	-2.13893100	2.64637200	-2.18703500
C	-1.78180700	3.49192100	0.40329200
H	-1.90493300	4.56363300	0.20850900
H	-1.37658000	3.41722700	1.41659100
C	-3.16847800	2.83368500	0.36440600
H	-3.77216100	3.27131200	1.16595400
H	-3.67489300	3.09094200	-0.56948400
C	-2.05102300	-3.58258000	-0.57211000
H	-2.83801800	-3.59596800	-1.33067200
H	-1.81250200	-4.63014500	-0.36341500
C	-2.58923300	-2.95409700	0.72225300
H	-3.50964100	-3.48034200	1.00097700
H	-1.87845400	-3.14230100	1.53234600
C	-2.84185700	-1.47199900	0.65521100

pCp1M

C	-3.39746100	-0.86514200	-0.46562500
C	-2.49516800	-0.64897900	1.72186600
C	-3.53259800	0.51103500	-0.54088900
H	-3.70874500	-1.47040200	-1.30895000
C	-2.63821700	0.72814400	1.65081600
H	-2.08273600	-1.09571500	2.62130100
C	-3.12890200	1.33787400	0.50172700
H	-3.94122500	0.95551900	-1.44244100
H	-2.33522800	1.33823800	2.49635400
Cl	3.60198100	0.05337900	1.13559100
Tl	1.01561000	-0.08444900	1.43325200

pCp1Ge

SCF Energy = -3925.2787096 au

C	1.22049800	2.76420700	0.88514900
C	1.11099400	2.72272200	-0.50012200
C	1.94047500	1.90834700	-1.25631400
C	2.92240500	1.12108100	-0.66358100
C	3.08143500	1.22452500	0.71389900
C	2.24562000	2.02886400	1.47079100
H	0.33904100	3.29692300	-0.99925000
H	1.80455700	1.86921300	-2.33302100
H	3.85129900	0.64770100	1.21406900
H	2.37965700	2.06572800	2.54746400
C	3.75566700	0.18319400	-1.49340100
H	3.27902600	0.07616900	-2.47176400
H	4.74000000	0.62578500	-1.68528200
C	3.96707300	-1.20707500	-0.87824000
H	4.49796900	-1.82337500	-1.61120200
H	4.62905300	-1.13149500	-0.01162400
C	2.69372100	-1.88504800	-0.45835100
C	1.69552800	-2.19311500	-1.37691000
C	2.45515000	-2.19376500	0.87565500
C	0.48376800	-2.72603700	-0.96437200
H	1.85401400	-1.99333900	-2.43229300
C	1.24767800	-2.73514600	1.28695000
H	3.22450800	-1.98809800	1.61294200
C	0.22165100	-2.97519900	0.38042900
H	-0.28902100	-2.92662600	-1.69830500
H	1.10161400	-2.95296400	2.33884200
C	-1.13965100	-3.45068600	0.81316500
H	-1.12755400	-4.53499800	0.97268000
H	-1.83922500	-3.26913400	-0.00705700
C	-1.68507700	-2.79013400	2.09099700
H	-2.70989700	-3.14255900	2.23990400
H	-1.11371600	-3.13128700	2.95829400
C	0.22129000	3.51781800	1.72004500
H	0.52585100	3.47659700	2.76955400
H	0.22447000	4.57759600	1.44690700

## pCp1M

C	-1.21711700	3.00368000	1.56659100
H	-1.86207900	3.56148200	2.25566600
H	-1.58038400	3.23871600	0.56188400
C	-1.39937300	1.52725800	1.79067900
C	-0.56226000	0.79737100	2.62164500
C	-2.42495500	0.82605300	1.14298100
C	-0.68621500	-0.57703100	2.74295100
H	0.22439700	1.29870200	3.16894000
C	-2.55753200	-0.55690600	1.28119700
H	-3.14497000	1.37189600	0.54124200
C	-1.65678700	-1.28977400	2.04962200
H	0.00757800	-1.11133700	3.38162900
H	-3.35654400	-1.06491600	0.75329700
Cl	-2.57514800	-1.20723400	-2.11352800
Cl	-1.94689900	2.05376200	-2.12387400
Ge	-1.07464900	0.19691900	-1.20395000

## pCp1Sn

SCF Energy = -2062.87771398 au

C	2.91774900	0.89405700	0.94420200
C	2.91282600	0.93006300	-0.44663500
C	2.82690400	-0.23979800	-1.18883800
C	2.76169800	-1.48884900	-0.57614300
C	2.86503600	-1.52425500	0.80953100
C	2.93617600	-0.35713000	1.55191400
H	2.91959300	1.88258100	-0.96414300
H	2.78230500	-0.17414500	-2.27216400
H	2.85957900	-2.47531800	1.32810500
H	2.98535500	-0.42305300	2.63388300
C	2.55822600	-2.73423400	-1.39720900
H	2.13080800	-2.44046100	-2.36047700
H	3.52747100	-3.19191500	-1.62748400
C	1.66441000	-3.80915100	-0.75941000
H	1.53891800	-4.61365900	-1.49072500
H	2.17759900	-4.25601400	0.09619200
C	0.32083000	-3.30470500	-0.31355100
C	-0.64643400	-2.89051400	-1.22522900
C	0.01293800	-3.19421400	1.03730100
C	-1.83338700	-2.31145900	-0.79791800
H	-0.46308000	-2.99723900	-2.29034900
C	-1.17240700	-2.61875500	1.46455400
H	0.72570200	-3.54627300	1.77527800
C	-2.10004000	-2.12086900	0.55707400
H	-2.54963500	-1.95833400	-1.53177500
H	-1.36133900	-2.54064400	2.52812500
C	-3.33211100	-1.37128300	0.99190200
H	-4.15415700	-2.07394400	1.17058300
H	-3.65031800	-0.73686200	0.15982200
C	-3.17014100	-0.50386400	2.25145000

	pCp1M		
H	-4.10697200	0.04101100	2.40058600
H	-3.04494500	-1.14128000	3.13080500
C	2.84273700	2.15595500	1.75945600
H	3.01748100	1.91459000	2.81156700
H	3.64702300	2.83808900	1.46805000
C	1.51599500	2.91581300	1.60540600
H	1.53865400	3.78726100	2.27009200
H	1.44510200	3.31393100	0.58892400
C	0.27415300	2.10881700	1.87400100
C	0.25399600	1.05638400	2.77927800
C	-0.91644200	2.38254600	1.19010400
C	-0.86601200	0.25440400	2.92792300
H	1.13631300	0.83279000	3.36446500
C	-2.04541500	1.57593600	1.34530900
H	-0.96049500	3.23560500	0.51971500
C	-2.02160900	0.46292100	2.18405500
H	-0.82855500	-0.57280000	3.62777000
H	-2.93872300	1.80557000	0.77482600
Cl	-2.65574700	0.92089000	-2.10474300
Cl	0.40474700	2.73022200	-2.15625900
Sn	-0.42929500	0.67629400	-1.14171600

#### pCp1Pb

SCF Energy = -2041.4514647 au

C	2.91420100	1.02926800	0.98273100
C	2.85219900	1.10854500	-0.40511800
C	2.82940000	-0.04132900	-1.18386500
C	2.88892500	-1.31040700	-0.61219800
C	3.04640200	-1.38068900	0.76755800
C	3.05282100	-0.23536800	1.54638100
H	2.76193000	2.07321500	-0.89078200
H	2.74132600	0.05587700	-2.26231400
H	3.13765200	-2.34485100	1.25273200
H	3.14829600	-0.33084500	2.62302900
C	2.76152200	-2.54269000	-1.46735200
H	2.28624600	-2.25627300	-2.41018000
H	3.75713200	-2.91456200	-1.73584900
C	1.97298200	-3.70218100	-0.83907600
H	1.88147900	-4.49021900	-1.59281100
H	2.54683200	-4.13575400	-0.01590200
C	0.61294600	-3.31215900	-0.33350400
C	-0.41478100	-2.94699400	-1.19994500
C	0.34620200	-3.26238800	1.02963700
C	-1.62791000	-2.47510400	-0.71582800
H	-0.26365100	-3.01386500	-2.27347500
C	-0.86332100	-2.79095800	1.51357200
H	1.10910400	-3.57968800	1.73227600
C	-1.85918900	-2.34265500	0.65346900
H	-2.39499800	-2.15804100	-1.41361000

	pCp1M		
H	-1.01924300	-2.75648500	2.58471500
C	-3.13047000	-1.70605200	1.15124100
H	-3.88789800	-2.47752100	1.33105300
H	-3.52436900	-1.07363400	0.35053600
C	-2.99483400	-0.86895700	2.43431900
H	-3.96544400	-0.40334800	2.62839000
H	-2.79327900	-1.52117500	3.28829500
C	2.77702500	2.25612400	1.84219600
H	3.00830600	1.99598300	2.87877900
H	3.51802600	3.00420600	1.54528900
C	1.39375100	2.92026700	1.75878900
H	1.37658600	3.76942200	2.45166500
H	1.25637100	3.34265700	0.75891800
C	0.22535400	2.01451300	2.04204500
C	0.31388200	0.93749300	2.91488300
C	-1.00378200	2.21571900	1.40219000
C	-0.73688600	0.04768000	3.07133600
H	1.22872900	0.76580300	3.46693000
C	-2.06192300	1.31844400	1.56231000
H	-1.13039500	3.07694800	0.75296000
C	-1.92709300	0.18666200	2.36605000
H	-0.61507900	-0.79352900	3.74439100
H	-2.98487600	1.49125800	1.01928500
Cl	-2.79094700	0.63732100	-1.88573500
Cl	0.23632800	2.77494900	-1.97427000
Pb	-0.43847300	0.56055000	-0.92542800

# pCp1As

SCF Energy = -4544.21054817 au

C	1.86069100	2.25104300	-1.40675600
C	1.35663700	2.61819800	-0.16337200
C	0.00000000	2.84332600	0.01918000
C	-0.90323700	2.72204100	-1.03485100
C	-0.38633300	2.42292400	-2.28922400
C	0.96726300	2.18844300	-2.46889900
H	2.02703300	2.70718100	0.68428300
H	-0.36783900	3.11572600	1.00333900
H	-1.04984600	2.34529000	-3.14240000
H	1.33362900	1.92822700	-3.45652200
C	-2.37920400	2.89605600	-0.79956100
H	-2.56968100	2.77844400	0.27085500
H	-2.68000100	3.92017300	-1.04953400
C	-3.27490200	1.92440500	-1.58090800
H	-4.30729200	2.07639800	-1.25041900
H	-3.25721900	2.17343500	-2.64521400
C	-2.87980500	0.48588400	-1.40675600
C	-2.94574500	-0.13421800	-0.16337200
C	-2.37887800	-0.25654800	-2.46889900
C	-2.46239300	-1.42166300	0.01918000

## pCp1M

H	-3.35800400	0.40187200	0.68428300
C	-1.90514700	-1.54603600	-2.28922400
H	-2.33670800	0.19084300	-3.45652200
C	-1.90573800	-2.14324700	-1.03485100
H	-2.51437800	-1.87642100	1.00333900
H	-1.50615800	-2.08183800	-3.14240000
C	-1.31845600	-3.50847900	-0.79956100
H	-2.05496900	-4.28103500	-1.04953400
H	-1.12136300	-3.61463200	0.27085500
C	-0.02913200	-3.79835100	-1.58090800
H	0.35543200	-4.76842300	-1.25041900
H	-0.25364100	-3.90755200	-2.64521400
C	3.30403400	1.87394600	-1.58090800
H	3.51085900	1.73411700	-2.64521400
H	3.95186000	2.69202500	-1.25041900
C	3.69766000	0.61242300	-0.79956100
H	4.73497000	0.36086200	-1.04953400
H	3.69104400	0.83618700	0.27085500
C	2.80897500	-0.57879400	-1.03485100
C	2.29148000	-0.87688800	-2.28922400
C	2.46239300	-1.42166300	0.01918000
C	1.41161600	-1.93189500	-2.46889900
H	2.55600300	-0.26345200	-3.14240000
C	1.58910800	-2.48398100	-0.16337200
H	2.88221700	-1.23930500	1.00333900
C	1.01911500	-2.73692700	-1.40675600
H	1.00307900	-2.11907000	-3.45652200
H	1.33097100	-3.10905300	0.68428300
Cl	-0.20187000	-1.87857000	2.86440500
Cl	1.72782400	0.76446000	2.86440500
Cl	-1.52595400	1.11411000	2.86440500
As	0.00000000	0.00000000	1.74882500

## pCp1Sb

SCF Energy = -2548.91119635 au

C	-1.19876300	-2.68730900	-1.42760600
C	-0.59088400	-2.95750300	-0.20507600
C	0.78014000	-2.80575500	-0.03889600
C	1.59720300	-2.38883600	-1.08995000
C	0.99603500	-2.20131100	-2.32824500
C	-0.37231200	-2.34447800	-2.49098400
H	-1.19480800	-3.26337000	0.64190300
H	1.22420400	-3.00749800	0.93068300
H	1.59716800	-1.91524300	-3.18253800
H	-0.80973200	-2.16317100	-3.46702800
C	3.06480500	-2.14180500	-0.86556600
H	3.21972200	-1.96539200	0.20243000
H	3.63574000	-3.04533600	-1.10911000
C	3.65665200	-0.96870500	-1.66108100

## pCp1M

H	4.69488800	-0.83762500	-1.34120800
H	3.69584900	-1.21907000	-2.72452500
C	2.89601300	0.31496900	-1.48592600
C	2.85210400	0.96918900	-0.25826800
C	2.16322700	0.86528300	-2.53069500
C	2.03885700	2.07953800	-0.06814200
H	3.43651800	0.59393900	0.57437400
C	1.35910000	1.97795400	-2.34428000
H	2.20410000	0.40140900	-3.51051200
C	1.24719900	2.58480000	-1.09961600
H	2.01184400	2.55901700	0.90522700
H	0.79245700	2.36057500	-3.18423600
C	0.30423300	3.73060200	-0.84791700
H	0.79597900	4.67852200	-1.09547700
H	0.09656200	3.76913600	0.22499200
C	-1.02391600	3.66184600	-1.61629000
H	-1.64970200	4.49311600	-1.27745500
H	-0.84905700	3.82837600	-2.68252700
C	-2.69332100	-2.70692900	-1.57866000
H	-2.94670800	-2.63211200	-2.63948300
H	-3.09341900	-3.66663500	-1.23760000
C	-3.40125200	-1.59600800	-0.78883100
H	-4.47274200	-1.64249500	-1.01555000
H	-3.30966000	-1.80231200	0.28112800
C	-2.88534800	-0.20494300	-1.04183200
C	-2.44300900	0.20406000	-2.29361700
C	-2.82054000	0.72586000	-0.00486600
C	-1.88518500	1.45798200	-2.48331000
H	-2.50975200	-0.47188200	-3.13725900
C	-2.26953700	1.98651200	-0.19818200
H	-3.20124900	0.45598300	0.97498500
C	-1.75147900	2.36013100	-1.43475400
H	-1.52555700	1.73202100	-3.46943100
H	-2.21854000	2.67445500	0.63829800
Cl	-0.25952300	1.98372100	2.70806900
Cl	-1.53083300	-1.23434500	2.73248200
Cl	1.89221800	-0.72628000	2.68869000
Sb	0.01812000	0.00396300	1.42349700

## pCp1Bi

SCF Energy = -2523.30369491 au

C	2.90283700	0.38980800	-1.58875500
C	2.82473400	1.03682100	-0.35850400
C	1.98257100	2.12801700	-0.17603700
C	1.19391300	2.61912800	-1.21774100
C	1.33891000	2.01981500	-2.46321500
C	2.17289200	0.92775200	-2.64209800
H	3.40635400	0.67331400	0.48128600
H	1.93137100	2.60349000	0.79838400

pCp1M

H	0.77658300	2.39343300	-3.31017600
H	2.24109100	0.47097300	-3.62364000
C	0.22121200	3.74143300	-0.97461300
H	0.00000000	3.77256600	0.09586100
H	0.69307400	4.70101400	-1.21530400
C	-1.09541500	3.64057700	-1.75889000
H	-1.74733200	4.45291000	-1.42387300
H	-0.91397600	3.81523000	-2.82269900
C	-1.78900300	2.31902600	-1.58875500
C	-2.31028100	1.92788100	-0.35850400
C	-1.88990300	1.41790300	-2.64209800
C	-2.83420200	0.65294900	-0.17603700
H	-2.28628400	2.61333200	0.48128600
C	-2.41866600	0.14962300	-2.46321500
H	-1.52842000	1.70535500	-3.62364000
C	-2.86518700	-0.27560500	-1.21774100
H	-3.22037400	0.37087200	0.79838400
H	-2.46106500	-0.52417600	-3.31017600
C	-3.35078200	-1.67914200	-0.97461300
H	-4.41773400	-1.75028700	-1.21530400
H	-3.26713800	-1.88628300	0.09586100
C	-2.60512400	-2.76894600	-1.75889000
H	-2.98266700	-3.73968900	-1.42387300
H	-2.84709800	-2.69914200	-2.82269900
C	3.70053900	-0.87163100	-1.75889000
H	3.76107400	-1.11608800	-2.82269900
H	4.73000000	-0.71322100	-1.42387300
C	3.12957000	-2.06229100	-0.97461300
H	3.72466000	-2.95072600	-1.21530400
H	3.26713800	-1.88628300	0.09586100
C	1.67127500	-2.34352300	-1.21774100
C	1.07975600	-2.16943800	-2.46321500
C	0.85163100	-2.78096500	-0.17603700
C	-0.28298900	-2.34565500	-2.64209800
H	1.68448300	-1.86925700	-3.31017600
C	-0.51445400	-2.96470200	-0.35850400
H	1.28900300	-2.97436100	0.79838400
C	-1.11383400	-2.70883500	-1.58875500
H	-0.71267100	-2.17632800	-3.62364000
H	-1.12007000	-3.28664600	0.48128600
Bi	0.00000000	0.00000000	1.23990800
Cl	-0.33611500	2.05299800	2.57618600
Cl	-1.60989100	-1.31758300	2.57618600
Cl	1.94600600	-0.73541500	2.57618600



## pCp-Mn+

pCp-Ga+

SCF Energy = -2852.74255678 au

C	-2.85105400	-0.68383100	0.09669000
C	-2.54082600	-0.17411300	-1.16396500
C	-2.17496200	1.15609900	-1.33174500
C	-2.11586600	2.04101900	-0.25415100
C	-2.51550200	1.55447600	0.99143700
C	-2.86974100	0.22024900	1.16170900
H	-2.54868100	-0.82777400	-2.02839700
H	-1.90911100	1.50890800	-2.32235000
H	-2.52098600	2.21586500	1.85149800
H	-3.13610100	-0.13422500	2.15194900
C	-1.60507300	3.44379300	-0.43754500
H	-1.46321200	3.62893700	-1.50464300
H	-2.36536300	4.15767400	-0.10799600
C	-0.30733900	3.76604500	0.32540900
H	0.00000000	4.77927000	0.04616800
H	-0.51461400	3.80229100	1.39795100
C	0.83331200	2.81100000	0.09669000
C	1.11962600	2.28747600	-1.16396500
C	1.62561200	2.37514500	1.16170900
C	2.08869200	1.30552300	-1.33174500
H	0.55746700	2.62111000	-2.02839700
C	2.60396600	1.40125100	0.99143700
H	1.45180800	2.78305600	2.15194900
C	2.82550700	0.81188400	-0.25415100
H	2.26130800	0.89888400	-2.32235000
H	3.17948800	1.07530500	1.85149800
C	3.78494900	-0.33186300	-0.43754500
H	4.78333300	-0.03037300	-0.10799600
H	3.87435800	-0.54729000	-1.50464300
C	3.41516000	-1.61685900	0.32540900
H	4.13896900	-2.38963500	0.04616800
H	3.55018800	-1.45547700	1.39795100
C	-3.10782100	-2.14918500	0.32540900
H	-3.03557400	-2.34681400	1.39795100
H	-4.13896900	-2.38963500	0.04616800
C	-2.17987600	-3.11193000	-0.43754500
H	-2.41797000	-4.12730100	-0.10799600
H	-2.41114600	-3.08164700	-1.50464300
C	-0.70964100	-2.85290300	-0.25415100
C	-0.08846500	-2.95572600	0.99143700
C	0.08627000	-2.46162200	-1.33174500
C	1.24413000	-2.59539300	1.16170900
H	-0.65850200	-3.29117000	1.85149800
C	1.42119900	-2.11336300	-1.16396500
H	-0.35219800	-2.40779300	-2.32235000
C	2.01774200	-2.12716900	0.09669000
H	1.68429300	-2.64883100	2.15194900

			pCp-Mn+
H	1.99121400	-1.79333600	-2.02839700
Ga	0.00000000	0.00000000	0.40536600

pCp-In+

SCF Energy = -1118.29403846 au

C	0.00000000	2.95744100	-0.10974400
C	0.36198100	2.39711300	-1.33315200
C	1.57294900	1.74030400	-1.49633600
C	2.48900300	1.61590500	-0.45227400
C	2.18452900	2.28458400	0.73597100
C	0.96551600	2.93904600	0.90245100
H	-0.32058100	2.44638100	-2.17159500
H	1.80234600	1.29980100	-2.45981000
H	2.89411900	2.27293300	1.55719000
H	0.74618400	3.41390700	1.85365700
C	3.73003500	0.77871300	-0.61729300
H	3.89188700	0.59953300	-1.68282600
H	4.60097500	1.34321200	-0.27358700
C	3.73462300	-0.56512200	0.13910300
H	4.66402800	-1.08379900	-0.11967400
H	3.79475000	-0.37291700	1.21438400
C	2.56121900	-1.47872000	-0.10974400
C	1.89497000	-1.51204100	-1.33315200
C	2.06253000	-2.30568400	0.90245100
C	0.72067300	-2.23236600	-1.49633600
H	2.27891900	-0.94555900	-2.17159500
C	0.88624300	-3.03415000	0.73597100
H	2.58343800	-2.35316800	1.85365700
C	0.15491300	-2.96349200	-0.45227400
H	0.22448800	-2.21077800	-2.45981000
H	0.52135800	-3.64284700	1.55719000
C	-1.19063200	-3.61966100	-0.61729300
H	-1.13723200	-4.65616700	-0.27358700
H	-1.42673300	-3.67023900	-1.68282600
C	-2.35672100	-2.95171700	0.13910300
H	-3.27061200	-3.49726700	-0.11967400
H	-2.22033000	-3.09989200	1.21438400
C	-1.37790100	3.51683900	0.13910300
H	-1.57442000	3.47280800	1.21438400
H	-1.39341600	4.58106600	-0.11967400
C	-2.53940300	2.84094800	-0.61729300
H	-3.46374300	3.31295500	-0.27358700
H	-2.46515400	3.07070700	-1.68282600
C	-2.64391600	1.34758700	-0.45227400
C	-3.07077200	0.74956600	0.73597100
C	-2.29362200	0.49206200	-1.49633600
C	-3.02804600	-0.63336200	0.90245100
H	-3.41547700	1.36991500	1.55719000
C	-2.25695100	-0.88507100	-1.33315200

	pCp-Mn+		
H	-2.02683400	0.91097700	-2.45981000
C	-2.56121900	-1.47872000	-0.10974400
H	-3.32962200	-1.06073900	1.85365700
H	-1.95833800	-1.50082200	-2.17159500
In	0.00000000	0.00000000	0.94713700

pCp-Tl+

SCF Energy = -1100.67990157 au

C	-2.91819600	-0.44322700	-0.28324000
C	-2.41202800	-0.00314000	-1.50404300
C	-1.94705300	1.29285400	-1.66807300
C	-1.96844800	2.21929400	-0.62673400
C	-2.58820800	1.81982800	0.55958300
C	-3.05179900	0.51567100	0.72648300
H	-2.35572000	-0.68607500	-2.34154100
H	-1.54440600	1.58499300	-2.63101400
H	-2.69295000	2.52662100	1.37685200
H	-3.49944800	0.23046900	1.67371500
C	-1.32883900	3.57240800	-0.79178900
H	-1.17634400	3.75977200	-1.85730700
H	-2.01710200	4.34880800	-0.44711200
C	0.00000000	3.77669900	-0.03670500
H	0.37687600	4.77121900	-0.29884000
H	-0.19873200	3.81249800	1.03862800
C	1.07525300	2.74884500	-0.28324000
C	1.20329400	2.09044700	-1.50404300
C	1.97248300	2.38510000	0.72648300
C	2.09317100	1.03977000	-1.66807300
H	0.58370100	2.38315100	-2.34154100
C	2.87012200	1.33154000	0.55958300
H	1.94931600	2.91537600	1.67371500
C	2.90618900	0.59507900	-0.62673400
H	2.14484700	0.54499800	-2.63101400
H	3.53459400	1.06885300	1.37685200
C	3.75821600	-0.63539600	-0.79178900
H	4.77472900	-0.42754200	-0.44711200
H	3.84423000	-0.86114200	-1.85730700
C	3.27071700	-1.88834900	-0.03670500
H	3.94355800	-2.71199400	-0.29884000
H	3.40108600	-1.73414200	1.03862800
C	-3.27071700	-1.88834900	-0.03670500
H	-3.20235400	-2.07835600	1.03862800
H	-4.32043500	-2.05922500	-0.29884000
C	-2.42937700	-2.93701300	-0.79178900
H	-2.75762700	-3.92126500	-0.44711200
H	-2.66788600	-2.89863000	-1.85730700
C	-0.93774100	-2.81437300	-0.62673400
C	-0.28191300	-3.15136800	0.55958300
C	-0.14611800	-2.33262400	-1.66807300

pCp-Mn+

C	1.07931600	-2.90077100	0.72648300
H	-0.84164300	-3.59547400	1.37685200
C	1.20873300	-2.08730700	-1.50404300
H	-0.60044100	-2.12999100	-2.63101400
C	1.84294400	-2.30561900	-0.28324000
H	1.55013200	-3.14584600	1.67371500
H	1.77201800	-1.69707500	-2.34154100
Tl	0.00000000	0.00000000	0.93458200

pCp-Ge2+

SCF Energy = -3004.50389051 au

C	-2.85740300	0.01833500	0.17785000
C	-2.56607300	0.50805700	-1.09919200
C	-1.86718400	1.70227000	-1.27190300
C	-1.44458000	2.46541600	-0.17785000
C	-1.72302600	1.96825600	1.09919200
C	-2.40780100	0.76589400	1.27190300
H	-2.89194900	-0.04086800	-1.97597700
H	-1.66314100	2.05536500	-2.27717500
H	-1.41058200	2.52493500	1.97597700
H	-2.61156900	0.41264000	2.27717500
C	-0.67332800	3.73354400	-0.37162700
H	-0.52003100	3.90141100	-1.43913000
H	-1.26474300	4.58115400	-0.01352900
C	0.67332800	3.73354400	0.37162700
H	1.26474300	4.58115400	0.01352900
H	0.52003100	3.90141100	1.43913000
C	1.44458000	2.46541600	0.17785000
C	1.72302600	1.96825600	-1.09919200
C	1.86718400	1.70227000	1.27190300
C	2.40780100	0.76589400	-1.27190300
H	1.41058200	2.52493500	-1.97597700
C	2.56607300	0.50805700	1.09919200
H	1.66314100	2.05536500	2.27717500
C	2.85740300	0.01833500	-0.17785000
H	2.61156900	0.41264000	-2.27717500
H	2.89194900	-0.04086800	1.97597700
C	3.57000800	-1.28365300	-0.37162700
H	4.59976700	-1.19527800	-0.01352900
H	3.63873700	-1.50034500	-1.43913000
C	2.89668000	-2.44989200	0.37162700
H	3.33502500	-3.38587600	0.01352900
H	3.11870500	-2.40106600	1.43913000
C	-3.57000800	-1.28365300	0.37162700
H	-3.63873700	-1.50034500	1.43913000
H	-4.59976700	-1.19527800	0.01352900
C	-2.89668000	-2.44989200	-0.37162700
H	-3.33502500	-3.38587600	-0.01352900
H	-3.11870500	-2.40106600	-1.43913000

pCp-Mn+

C	-1.41282300	-2.48375100	-0.17785000
C	-0.84304600	-2.47631300	1.09919200
C	-0.54061700	-2.46816400	-1.27190300
C	0.54061700	-2.46816400	1.27190300
H	-1.48136700	-2.48406700	1.97597700
C	0.84304600	-2.47631300	-1.09919200
H	-0.94842800	-2.46800500	-2.27717500
C	1.41282300	-2.48375100	0.17785000
H	0.94842800	-2.46800500	2.27717500
H	1.48136700	-2.48406700	-1.97597700
Ge	0.00000000	0.00000000	0.00000000

pCp-Sn2+

SCF Energy = -1142.11431938 au

C	-2.93868300	0.05664300	0.17446600
C	-2.68687000	0.57809700	-1.10122000
C	-1.98729300	1.77546300	-1.26935400
C	-1.51839600	2.51665300	-0.17446600
C	-1.84408100	2.03784900	1.10122000
C	-2.53124200	0.83331500	1.26935400
H	-3.02159400	0.03918200	-1.98127300
H	-1.79460900	2.13586800	-2.27456500
H	-1.54472900	2.59718600	1.98127300
H	-2.74702100	0.48624300	2.27456500
C	-0.67270800	3.74297200	-0.37741100
H	-0.50173400	3.87800200	-1.44731600
H	-1.23154600	4.62530000	-0.05111200
C	0.67270800	3.74297200	0.37741100
H	1.23154600	4.62530000	0.05111200
H	0.50173400	3.87800200	1.44731600
C	1.51839600	2.51665300	0.17446600
C	1.84408100	2.03784900	-1.10122000
C	1.98729300	1.77546300	1.26935400
C	2.53124200	0.83331500	-1.26935400
H	1.54472900	2.59718600	-1.98127300
C	2.68687000	0.57809700	1.10122000
H	1.79460900	2.13586800	2.27456500
C	2.93868300	0.05664300	-0.17446600
H	2.74702100	0.48624300	-2.27456500
H	3.02159400	0.03918200	1.98127300
C	3.57786300	-1.28890400	-0.37741100
H	4.62140100	-1.24610000	-0.05111200
H	3.60931500	-1.50448700	-1.44731600
C	2.90515500	-2.45406800	0.37741100
H	3.38985500	-3.37920000	0.05111200
H	3.10758100	-2.37351600	1.44731600
C	-3.57786300	-1.28890400	0.37741100
H	-3.60931500	-1.50448700	1.44731600
H	-4.62140100	-1.24610000	0.05111200

## pCp-Mn+

C	-2.90515500	-2.45406800	-0.37741100
H	-3.38985500	-3.37920000	-0.05111200
H	-3.10758100	-2.37351600	-1.44731600
C	-1.42028700	-2.57329600	-0.17446600
C	-0.84278800	-2.61594600	1.10122000
C	-0.54394900	-2.60877800	-1.26935400
C	0.54394900	-2.60877800	1.26935400
H	-1.47686400	-2.63636800	1.98127300
C	0.84278800	-2.61594600	-1.10122000
H	-0.95241200	-2.62211100	-2.27456500
C	1.42028700	-2.57329600	0.17446600
H	0.95241200	-2.62211100	2.27456500
H	1.47686400	-2.63636800	-1.98127300
Sn	0.00000000	0.00000000	0.00000000

## pCp-Pb2+

SCF Energy = -1120.6971224 au

C	-2.94239800	0.05883700	0.17405700
C	-2.69230300	0.58182800	-1.10131200
C	-1.99338900	1.77939700	-1.26901800
C	-1.52215400	2.51877300	-0.17405700
C	-1.85003000	2.04068900	1.10131200
C	-2.53769700	0.83662800	1.26901800
H	-3.02924200	0.04427000	-1.98149700
H	-1.80344300	2.14192100	-2.27411900
H	-1.55296000	2.60126600	1.98149700
H	-2.75668000	0.49086700	2.27411900
C	-0.67310500	3.74360900	-0.37708900
H	-0.50209000	3.87770800	-1.44715400
H	-1.23021800	4.62725500	-0.05147900
C	0.67310500	3.74360900	0.37708900
H	1.23021800	4.62725500	0.05147900
H	0.50209000	3.87770800	1.44715400
C	1.52215400	2.51877300	0.17405700
C	1.85003000	2.04068900	-1.10131200
C	1.99338900	1.77939700	1.26901800
C	2.53769700	0.83662800	-1.26901800
H	1.55296000	2.60126600	-1.98149700
C	2.69230300	0.58182800	1.10131200
H	1.80344300	2.14192100	2.27411900
C	2.94239800	0.05883700	-0.17405700
H	2.75668000	0.49086700	-2.27411900
H	3.02924200	0.04427000	1.98149700
C	3.57861300	-1.28887900	-0.37708900
H	4.62243000	-1.24822700	-0.05147900
H	3.60923900	-1.50403100	-1.44715400
C	2.90550800	-2.45473100	0.37708900
H	3.39221100	-3.37902800	0.05147900
H	3.10714800	-2.37367700	1.44715400

pCp-Mn+			
C	-3.57861300	-1.28887900	0.37708900
H	-3.60923900	-1.50403100	1.44715400
H	-4.62243000	-1.24822700	0.05147900
C	-2.90550800	-2.45473100	-0.37708900
H	-3.39221100	-3.37902800	-0.05147900
H	-3.10714800	-2.37367700	-1.44715400
C	-1.42024400	-2.57761000	-0.17405700
C	-0.84227400	-2.62251700	1.10131200
C	-0.54430800	-2.61602400	-1.26901800
C	0.54430800	-2.61602400	1.26901800
H	-1.47628200	-2.64553500	1.98149700
C	0.84227400	-2.62251700	-1.10131200
H	-0.95323700	-2.63278800	-2.27411900
C	1.42024400	-2.57761000	0.17405700
H	0.95323700	-2.63278800	2.27411900
H	1.47628200	-2.64553500	-1.98149700
Pb	0.00000000	0.00000000	0.00000000

pCp-As3+

SCF Energy = -3162.78300725 au

C	-2.76727700	-0.75501000	0.13100000
C	-2.89024000	-0.12192700	-1.10397100
C	-2.52251400	1.21350100	-1.28121200
C	-2.05105800	2.00221100	-0.22616900
C	-1.94165500	1.38792700	1.02906700
C	-2.24907500	0.01412100	1.19965000
H	-3.29383400	-0.66896700	-1.95030300
H	-2.62943400	1.65890000	-2.26569400
H	-1.65337100	1.96295100	1.90193500
H	-2.22186000	-0.40315500	2.20196000
C	-1.64245700	3.42344500	-0.42749100
H	-1.54129400	3.62397300	-1.49572900
H	-2.43749400	4.08744200	-0.06889700
C	-0.34373000	3.79135400	0.32188400
H	0.00000000	4.75687900	-0.06136500
H	-0.53586400	3.94015700	1.38592100
C	0.72978100	2.77403700	0.13100000
C	1.33952900	2.56398500	-1.10397100
C	1.13676700	1.94069600	1.19965000
C	2.31217900	1.57781100	-1.28121200
H	1.06757400	3.18702700	-1.95030300
C	2.17280700	0.98755900	1.02906700
H	0.76178800	2.12576500	2.20196000
C	2.75949500	0.77516300	-0.22616900
H	2.75136700	1.44770600	-2.26569400
H	2.52665100	0.45038600	1.90193500
C	3.78601900	-0.28931300	-0.42749100
H	4.75857600	0.06721100	-0.06889700
H	3.90909900	-0.47718600	-1.49572900

	pCp-Mn+		
C	3.45527400	-1.59799800	0.32188400
H	4.11957800	-2.37843900	-0.06136500
H	3.68020900	-1.50600700	1.38592100
C	-3.11154400	-2.19335600	0.32188400
H	-3.14434400	-2.43415100	1.38592100
H	-4.11957800	-2.37843900	-0.06136500
C	-2.14356200	-3.13413200	-0.42749100
H	-2.32108200	-4.15465300	-0.06889700
H	-2.36780500	-3.14678600	-1.49572900
C	-0.70843700	-2.77737400	-0.22616900
C	-0.23115300	-2.37548600	1.02906700
C	0.21033500	-2.79131100	-1.28121200
C	1.11230900	-1.95481700	1.19965000
H	-0.87328000	-2.41333700	1.90193500
C	1.55071200	-2.44205800	-1.10397100
H	-0.12193300	-3.10660700	-2.26569400
C	2.03749700	-2.01902700	0.13100000
H	1.46007300	-1.72261000	2.20196000
H	2.22625900	-2.51806000	-1.95030300
As	0.00000000	0.00000000	0.22687400

pCp-Sb3+

SCF Energy = -1167.5106511 au

C	-2.87895200	0.01854000	0.17627800
C	-2.58802400	0.51802500	-1.10451800
C	-1.88491800	1.71809000	-1.27560600
C	-1.45553200	2.48397600	-0.17627800
C	-1.74263500	1.98228200	1.10451800
C	-2.43036800	0.77334200	1.27560600
H	-2.92131300	-0.02204800	-1.98529100
H	-1.69103500	2.07550300	-2.28248800
H	-1.44156300	2.54095600	1.98529100
H	-2.64295500	0.42672800	2.28248800
C	-0.67852200	3.74552100	-0.36896700
H	-0.53954700	3.92953200	-1.43554300
H	-1.26342700	4.59068300	0.00916100
C	0.67852200	3.74552100	0.36896700
H	1.26342700	4.59068300	-0.00916100
H	0.53954700	3.92953200	1.43554300
C	1.45553200	2.48397600	0.17627800
C	1.74263500	1.98228200	-1.10451800
C	1.88491800	1.71809000	1.27560600
C	2.43036800	0.77334200	-1.27560600
H	1.44156300	2.54095600	-1.98529100
C	2.58802400	0.51802500	1.10451800
H	1.69103500	2.07550300	2.28248800
C	2.87895200	0.01854000	-0.17627800
H	2.64295500	0.42672800	-2.28248800
H	2.92131300	-0.02204800	1.98529100



pCp-Mn+			
C	3.58297700	-1.28514300	-0.36896700
H	4.60736200	-1.20118200	0.00916100
H	3.67284800	-1.49750400	-1.43554300
C	2.90445500	-2.46037800	0.36896700
H	3.34393500	-3.38950100	-0.00916100
H	3.13330100	-2.43202700	1.43554300
C	-3.58297700	-1.28514300	0.36896700
H	-3.67284800	-1.49750400	1.43554300
H	-4.60736200	-1.20118200	-0.00916100
C	-2.90445500	-2.46037800	-0.36896700
H	-3.34393500	-3.38950100	0.00916100
H	-3.13330100	-2.43202700	-1.43554300
C	-1.42342000	-2.50251600	-0.17627800
C	-0.84539000	-2.50030700	1.10451800
C	-0.54545000	-2.49143200	-1.27560600
C	0.54545000	-2.49143200	1.27560600
H	-1.47975100	-2.51890800	1.98529100
C	0.84539000	-2.50030700	-1.10451800
H	-0.95192100	-2.50223000	-2.28248800
C	1.42342000	-2.50251600	0.17627800
H	0.95192100	-2.50223000	2.28248800
H	1.47975100	-2.51890800	-1.98529100
Sb	0.00000000	0.00000000	0.00000000

pCp-Bi3+

SCF Energy = -1141.91848668 au

C	-2.90340500	0.02973200	0.17507300
C	-2.62614800	0.54037300	-1.10538900
C	-1.92346500	1.74178600	-1.27489100
C	-1.47745100	2.49955600	-0.17507300
C	-1.78105000	2.00412400	1.10538900
C	-2.47016300	0.79487700	1.27489100
H	-2.96636400	0.00571300	-1.98701200
H	-1.73778200	2.10464400	-2.28151600
H	-1.48813000	2.56609000	1.98701200
H	-2.69156600	0.45264100	2.28151600
C	-0.67816400	3.74995800	-0.37045800
H	-0.53340200	3.92352000	-1.43818100
H	-1.25446300	4.60567200	-0.00310100
C	0.67816400	3.74995800	0.37045800
H	1.25446300	4.60567200	0.00310100
H	0.53340200	3.92352000	1.43818100
C	1.47745100	2.49955600	0.17507300
C	1.78105000	2.00412400	-1.10538900
C	1.92346500	1.74178600	1.27489100
C	2.47016300	0.79487700	-1.27489100
H	1.48813000	2.56609000	-1.98701200
C	2.62614800	0.54037300	1.10538900
H	1.73778200	2.10464400	2.28151600

			pCp-Mn+
C	2.90340500	0.02973200	-0.17507300
H	2.69156600	0.45264100	-2.28151600
H	2.96636400	0.00571300	1.98701200
C	3.58664100	-1.28767100	-0.37045800
H	4.61586000	-1.21643900	-0.00310100
H	3.66456900	-1.49982000	-1.43818100
C	2.90847600	-2.46228600	0.37045800
H	3.36139700	-3.38923300	0.00310100
H	3.13116700	-2.42370000	1.43818100
C	-3.58664100	-1.28767100	0.37045800
H	-3.66456900	-1.49982000	1.43818100
H	-4.61586000	-1.21643900	0.00310100
C	-2.90847600	-2.46228600	-0.37045800
H	-3.36139700	-3.38923300	-0.00310100
H	-3.13116700	-2.42370000	-1.43818100
C	-1.42595300	-2.52928800	-0.17507300
C	-0.84509700	-2.54449700	1.10538900
C	-0.54669800	-2.53666200	-1.27489100
C	0.54669800	-2.53666200	1.27489100
H	-1.47823400	-2.57180400	1.98701200
C	0.84509700	-2.54449700	-1.10538900
H	-0.95378400	-2.55728500	-2.28151600
C	1.42595300	-2.52928800	0.17507300
H	0.95378400	-2.55728500	2.28151600
H	1.47823400	-2.57180400	-1.98701200
Bi	0.00000000	0.00000000	0.00000000