

Supporting Information

CO₂ Activation without Metals Enabled by Lewis Acid/Base-Free G13=P Double Bonds

Zheng-Feng Zhang¹ and Ming-Der Su^{1,2*}

¹Department of Applied Chemistry, National Chiayi University, Chiayi 60004,
Taiwan

²Department of Medicinal and Applied Chemistry, Kaohsiung Medical
University, Kaohsiung 80708, Taiwan

*E-mail: midesu@mail.ncyu.edu.tw

(All were calculated at the M06-2X-D3/def2-TZVP level)

Table S1

B=P-Rea

G = -2696.98864688 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
B	0.19724300	0.08589500	-0.01891200
P	0.11509400	0.02582800	1.72780800
C	1.08971200	0.04919300	-1.27964200
C	1.70540900	1.22615900	-1.79661100
C	2.84138700	1.11690400	-2.60657500
H	3.33440300	2.03279700	-2.93516600
C	3.36462500	-0.11924600	-2.96199300
H	4.26526700	-0.18142400	-3.57503300
C	2.73384900	-1.27432100	-2.52002700
H	3.13327600	-2.25352400	-2.78717600
C	1.60718600	-1.21352300	-1.69435200
C	1.30946700	2.64185200	-1.48596000
C	1.85939300	3.26211600	-0.34416900
C	1.64369600	4.63086100	-0.14795100
H	2.06676900	5.12068300	0.73063800
C	0.89943900	5.37271600	-1.05594400
H	0.73317100	6.43800800	-0.88755800
C	0.36734700	4.75561400	-2.18429300
H	-0.20724500	5.35233500	-2.89386700
C	0.57303100	3.39447200	-2.43353900
C	2.75430300	2.50503100	0.62536100
H	2.56211100	1.42960400	0.50348400
C	4.23041000	2.75312100	0.29091000
H	4.88112600	2.19423900	0.97994800
H	4.47004100	3.82373500	0.38414000
H	4.46846800	2.44035500	-0.73549700
C	2.46805000	2.84160800	2.08717300
H	3.02011100	2.14637200	2.73682100
H	1.39718600	2.73748100	2.31469200
H	2.78786200	3.86283200	2.34683800
C	0.08449100	2.79211400	-3.74964400
H	-0.14046900	1.72911500	-3.56335500
C	-1.17555000	3.46389300	-4.30666700
H	-1.57662600	2.86689500	-5.13888300
H	-0.94404600	4.45980700	-4.71355500
H	-1.96729300	3.58519600	-3.55801000
C	1.16220400	2.87791700	-4.84317200
H	0.75719900	2.51355300	-5.79920400
H	2.05209000	2.28459300	-4.61097400
H	1.47188400	3.92523600	-4.98216400
C	1.07626000	-2.54060700	-1.23477400

C	0.16908200	-3.26221600	-2.04749700
C	-0.22505900	-4.53828000	-1.62833600
H	-0.93611900	-5.10845300	-2.22734200
C	0.28552100	-5.10262600	-0.46403200
H	-0.03152900	-6.10106900	-0.15754900
C	1.20886300	-4.40081600	0.30222600
H	1.62241900	-4.86228000	1.20019500
C	1.61915100	-3.11448300	-0.06215700
C	-0.30951600	-2.72804300	-3.39767800
H	-0.44475400	-1.63830500	-3.29273200
C	0.72922600	-2.98244300	-4.50320700
H	0.32633800	-2.66563400	-5.47686300
H	0.95518100	-4.05829200	-4.56216200
H	1.66624000	-2.44199600	-4.33967400
C	-1.62885300	-3.33922300	-3.88448300
H	-2.00197100	-2.76942600	-4.74804800
H	-2.41669400	-3.35350300	-3.12132000
H	-1.47826700	-4.37506100	-4.22441500
C	2.71759500	-2.42172600	0.73869800
H	2.65914900	-1.34248000	0.53325100
C	4.09230900	-2.91863700	0.26962400
H	4.89461100	-2.40371900	0.81878700
H	4.24591900	-2.74521400	-0.80397800
H	4.18940400	-3.99961500	0.45513800
C	2.59162600	-2.59565000	2.25294600
H	3.36422000	-1.99790300	2.75915000
H	2.73633300	-3.64323300	2.56044400
H	1.61689500	-2.25173000	2.62383200
C	-1.57374300	-0.21242700	2.42065200
C	-1.67769600	-0.55438300	3.78800900
C	-2.94377000	-0.69928200	4.37241500
H	-2.99870400	-0.97777100	5.42753200
C	-4.10619400	-0.51423000	3.63589900
H	-5.08319200	-0.62569400	4.10773200
C	-4.00686100	-0.19597500	2.28330600
H	-4.90735500	-0.05579900	1.68209000
C	-2.76077300	-0.05778000	1.67045900
C	-0.47649100	-0.87617300	4.62575700
C	0.33342700	0.15407200	5.16093600
C	1.47053200	-0.20114500	5.88877500
H	2.11497400	0.57542400	6.30048500
C	1.79955300	-1.53875800	6.10313600
H	2.69775800	-1.79511200	6.66746000
C	0.97463500	-2.54056400	5.61327700
H	1.22558400	-3.58718500	5.80085700
C	-0.17824800	-2.23072200	4.87944200
C	-0.06188900	1.61714400	5.00206200
H	-0.40029600	1.75592900	3.96133500
C	-1.23337400	1.96577400	5.93109900
H	-1.51945600	3.02099900	5.80632300

H	-0.93892200	1.81196900	6.98075400
H	-2.11708500	1.34811400	5.72804800
C	1.08610200	2.59340700	5.25448000
H	0.78920800	3.60739200	4.94964100
H	1.98876900	2.31870200	4.69455800
H	1.34365400	2.63445200	6.32418900
C	-1.06803400	-3.37505500	4.40868600
H	-1.93719300	-2.94679100	3.89471500
C	-0.35904500	-4.27322400	3.39522500
H	-1.02315600	-5.09097300	3.07431100
H	0.55381800	-4.72124700	3.82068400
H	-0.07518800	-3.70054700	2.50258300
C	-1.59563600	-4.18214700	5.59915500
H	-2.29241600	-4.96110900	5.25568700
H	-2.12479600	-3.53614700	6.31493400
H	-0.77643000	-4.68024500	6.13992000
C	-2.70933500	0.27031500	0.22193600
C	-2.62295200	1.63233900	-0.14207700
C	-2.58437100	1.96431100	-1.49496600
H	-2.51880100	3.01526200	-1.77541600
C	-2.63328500	0.97385700	-2.47315700
H	-2.61229700	1.24516000	-3.53014000
C	-2.72034200	-0.36246600	-2.10117300
H	-2.77734500	-1.13459900	-2.87099000
C	-2.75850600	-0.74768800	-0.75186500
C	-2.63398900	2.72537200	0.91482800
H	-2.27641500	2.28244600	1.85577800
C	-4.06514200	3.22443400	1.14583600
H	-4.08182700	4.00069700	1.92538000
H	-4.73092700	2.40831500	1.45944100
H	-4.47186400	3.65897200	0.21935400
C	-1.69673600	3.88063200	0.57727400
H	-1.60803000	4.56222600	1.43673300
H	-2.06086700	4.47655200	-0.27404400
H	-0.69490000	3.50641900	0.32800600
C	-2.96868700	-2.23287500	-0.46243800
H	-2.57923600	-2.73920600	-1.35540400
C	-4.46751700	-2.55205200	-0.38479200
H	-4.62212300	-3.63974500	-0.32059100
H	-5.00437100	-2.17529600	-1.26747800
H	-4.91537400	-2.09600600	0.51026200
C	-2.21840300	-2.86363700	0.71348300
H	-2.25071600	-3.95815700	0.60176400
H	-2.67063900	-2.61493200	1.68368100
H	-1.15961900	-2.56290400	0.72707400

Table S2

Al=P-Rea

G = -2914.60659458 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Al	-0.06626200	0.10682500	0.04395800
P	0.20355900	-0.08651700	2.21608700
C	1.08789100	0.08667800	-1.57241400
C	1.71295900	1.25418900	-2.07793700
C	2.78422300	1.15442900	-2.97666500
H	3.28224500	2.06906900	-3.30303300
C	3.24531000	-0.08006500	-3.41404600
H	4.08906700	-0.14375200	-4.10288500
C	2.64027400	-1.23300700	-2.93213700
H	3.02135400	-2.21145400	-3.22784200
C	1.58157700	-1.16826600	-2.01682000
C	1.37695500	2.65885200	-1.65830900
C	1.96095100	3.18329800	-0.48205100
C	1.79204000	4.54316400	-0.19420100
H	2.24446200	4.96129700	0.70573700
C	1.04636300	5.36570700	-1.02901300
H	0.91859100	6.42160600	-0.78488900
C	0.46036700	4.84036100	-2.17692600
H	-0.11991600	5.49656700	-2.82788000
C	0.62785100	3.49539300	-2.52210500
C	2.82730900	2.33254400	0.43918200
H	2.51930300	1.28198100	0.32578500
C	4.30030300	2.41945500	0.02036100
H	4.92321100	1.79578000	0.67875100
H	4.65570800	3.45900700	0.09418400
H	4.44640000	2.07992900	-1.01442000
C	2.66167000	2.69152100	1.91639000
H	3.14610200	1.92669000	2.54121000
H	1.60024700	2.72231800	2.20132500
H	3.12819800	3.65965000	2.15539100
C	0.07770700	2.99367300	-3.85436000
H	-0.06036500	1.90419400	-3.76436400
C	-1.26177400	3.62525900	-4.25194600
H	-1.67901200	3.09604300	-5.12164400
H	-1.13171600	4.67533300	-4.55317400
H	-2.00981300	3.60313000	-3.44873600
C	1.07346600	3.25338700	-4.99539100
H	0.64822400	2.92238800	-5.95474700
H	2.02228100	2.72672400	-4.84789900
H	1.28649400	4.33091200	-5.06933700
C	1.08675000	-2.48495900	-1.48001300
C	0.15994200	-3.25797000	-2.22057200
C	-0.23315800	-4.50177500	-1.71133700
H	-0.95211600	-5.10946200	-2.26302900
C	0.27696100	-4.97803400	-0.50896900
H	-0.05115200	-5.94446600	-0.12178100
C	1.21116400	-4.22842900	0.19770400

H	1.61358000	-4.61874500	1.13280700
C	1.64758500	-2.98711600	-0.27683900
C	-0.35026500	-2.81358000	-3.59076000
H	-0.39955100	-1.71191600	-3.58368500
C	0.61819800	-3.23789700	-4.70663900
H	0.20506200	-2.96744900	-5.68999700
H	0.75869400	-4.32942600	-4.68345900
H	1.59959200	-2.76299500	-4.61328900
C	-1.73299700	-3.36696000	-3.96008400
H	-2.11399000	-2.84605500	-4.85081000
H	-2.47917800	-3.26520900	-3.16102400
H	-1.67294900	-4.43524700	-4.21653600
C	2.79108400	-2.27117500	0.43819500
H	2.64782500	-1.18594100	0.31212500
C	4.13158000	-2.64752000	-0.21186400
H	4.95754300	-2.12940200	0.29780600
H	4.16950500	-2.38433300	-1.27569100
H	4.30000900	-3.73164500	-0.12010100
C	2.87015300	-2.55467000	1.93818500
H	3.61874800	-1.89149200	2.39557000
H	3.18999200	-3.59000100	2.13483300
H	1.91291000	-2.36811600	2.43952700
C	-1.56117300	-0.33956200	2.67497900
C	-1.86324200	-0.68348000	4.02114700
C	-3.18912600	-0.83878600	4.43722200
H	-3.37612100	-1.10429400	5.48092600
C	-4.25653000	-0.66696700	3.55913300
H	-5.28479400	-0.78410300	3.90216200
C	-3.98287000	-0.33980600	2.23458200
H	-4.80103000	-0.19544600	1.52485900
C	-2.66538500	-0.19118400	1.79609000
C	-0.78057600	-0.89482800	5.03671500
C	-0.14492000	0.22262100	5.61741600
C	0.85029500	0.01253600	6.57560500
H	1.34832900	0.86882800	7.03326400
C	1.21558000	-1.27456000	6.95555400
H	1.99709600	-1.42346600	7.70269600
C	0.58103500	-2.37171100	6.38385000
H	0.87404400	-3.37718500	6.68945700
C	-0.42412300	-2.20466500	5.42495500
C	-0.56557400	1.63944800	5.25704700
H	-1.01711100	1.60496200	4.25594700
C	-1.63514400	2.13900100	6.23469400
H	-1.96825700	3.15311100	5.96527400
H	-1.23593600	2.16914000	7.26064900
H	-2.51233500	1.47560100	6.23095800
C	0.61435900	2.60791400	5.17854700
H	0.28929400	3.56658200	4.74642300
H	1.41023700	2.19435200	4.54290100
H	1.03603100	2.82477100	6.17211300

C	-1.05710100	-3.42606900	4.77106500
H	-2.06307600	-3.14032000	4.43326900
C	-0.25642000	-3.82498100	3.52681400
H	-0.74241100	-4.65722100	2.99259800
H	0.75971900	-4.14083000	3.81438400
H	-0.16136400	-2.97445500	2.83568400
C	-1.21639200	-4.61443900	5.72008600
H	-1.80816300	-5.40465500	5.23524500
H	-1.72530900	-4.32371700	6.65060000
H	-0.24470300	-5.05661700	5.98679300
C	-2.46024900	0.15516900	0.35894000
C	-2.28739300	1.53379400	0.01462100
C	-2.20961200	1.89400300	-1.33421900
H	-2.07043000	2.94458800	-1.58634000
C	-2.32373700	0.93312200	-2.34013900
H	-2.28735600	1.23255400	-3.38844800
C	-2.47848700	-0.40364500	-2.00483700
H	-2.56974800	-1.15183000	-2.79311600
C	-2.53198400	-0.83105000	-0.66142300
C	-2.33728300	2.60282000	1.09315800
H	-2.00035600	2.13572400	2.02842900
C	-3.78617900	3.07230100	1.27842900
H	-3.83624700	3.82491000	2.07861300
H	-4.45060800	2.24134200	1.55019500
H	-4.16384700	3.53210900	0.35189700
C	-1.41558600	3.78145300	0.80557700
H	-1.37020100	4.44333800	1.68267900
H	-1.76310300	4.38944000	-0.04426800
H	-0.39590200	3.43808000	0.58773100
C	-2.80748500	-2.31376100	-0.42837800
H	-2.34102800	-2.80778800	-1.29048000
C	-4.31499200	-2.58824100	-0.51293200
H	-4.49511400	-3.67326100	-0.50467000
H	-4.75355300	-2.17190600	-1.43202100
H	-4.83924300	-2.15416100	0.35004800
C	-2.19041400	-2.97805400	0.80162900
H	-2.23049500	-4.06833100	0.66112500
H	-2.72183400	-2.73613700	1.73206900
H	-1.13258400	-2.70034400	0.91983200

Table S3

Ga=P-Rea

G = -4597.03858276 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ga	0.07951700	0.07578200	0.07118100
P	0.16663200	-0.03777500	2.26559400
C	1.16522500	0.02859800	-1.60210200

C	1.78539600	1.19004500	-2.11832800
C	2.84388500	1.06896400	-3.02947300
H	3.34835600	1.97457700	-3.37031500
C	3.28445800	-0.17560300	-3.46126600
H	4.12047400	-0.25377300	-4.15792300
C	2.66963700	-1.32030400	-2.97002800
H	3.03342500	-2.30455800	-3.26802400
C	1.62278000	-1.23711500	-2.04333700
C	1.45014400	2.59562900	-1.70317300
C	2.02724000	3.12551000	-0.52603600
C	1.84557300	4.48363500	-0.23878200
H	2.29102800	4.90627900	0.66239900
C	1.09683100	5.29944900	-1.07728600
H	0.95971300	6.35442200	-0.83437400
C	0.51635600	4.76789600	-2.22478000
H	-0.07023200	5.41818100	-2.87573600
C	0.69201200	3.42335900	-2.56754200
C	2.90272700	2.28479700	0.39612300
H	2.60271700	1.23058200	0.29013000
C	4.37247900	2.37469300	-0.03364600
H	5.00347000	1.75814600	0.62376300
H	4.72276900	3.41644800	0.03103600
H	4.51197900	2.03004300	-1.06769500
C	2.74518400	2.65309000	1.87225500
H	3.23235000	1.89319200	2.50099000
H	1.68525300	2.69113100	2.16200600
H	3.21542000	3.62172300	2.10080200
C	0.13428800	2.91320700	-3.89354300
H	-0.01750300	1.82651100	-3.79135400
C	-1.20007300	3.55493300	-4.29148900
H	-1.63084600	3.01559700	-5.14815300
H	-1.05913200	4.59793300	-4.61199000
H	-1.93960800	3.55423400	-3.48074400
C	1.12669000	3.15250400	-5.04200800
H	0.69080600	2.82036900	-5.99615000
H	2.07041400	2.61587600	-4.89865400
H	1.35174800	4.22694200	-5.12500000
C	1.09727000	-2.53058200	-1.48301500
C	0.13094700	-3.28104000	-2.19583400
C	-0.30262200	-4.49680100	-1.65370700
H	-1.05222800	-5.08760500	-2.18211700
C	0.20295700	-4.96569100	-0.44618600
H	-0.15802200	-5.90964100	-0.03369300
C	1.17096000	-4.23641600	0.23518400
H	1.56652000	-4.61967000	1.17614900
C	1.64790300	-3.02328400	-0.27228300
C	-0.38278000	-2.84133100	-3.56597000
H	-0.41687700	-1.73891600	-3.56742900
C	0.56882100	-3.29114000	-4.68631200
H	0.15088700	-3.02252200	-5.66806400

H	0.69136800	-4.38463200	-4.65496100
H	1.55887100	-2.83203800	-4.60711900
C	-1.77684400	-3.37594500	-3.91778100
H	-2.15655300	-2.85782300	-4.81049500
H	-2.51321300	-3.25142000	-3.11332000
H	-1.73624000	-4.44789600	-4.16283600
C	2.82099500	-2.33052200	0.41707400
H	2.72843700	-1.24507400	0.24902900
C	4.14098300	-2.78595600	-0.22372300
H	4.99159500	-2.27989900	0.25658100
H	4.17729000	-2.57000100	-1.29862700
H	4.26677700	-3.87115400	-0.08795500
C	2.88838400	-2.55891900	1.92698700
H	3.67486300	-1.92220800	2.35781400
H	3.15026300	-3.60164000	2.16461500
H	1.94295500	-2.30143800	2.42073800
C	-1.60667300	-0.28412600	2.69230300
C	-1.89622800	-0.62189100	4.04126400
C	-3.21842100	-0.76661200	4.47260800
H	-3.39682800	-1.02931400	5.51838500
C	-4.28979400	-0.58676100	3.60255800
H	-5.31656000	-0.69372700	3.95358200
C	-4.02419200	-0.26401100	2.27502900
H	-4.84773900	-0.11261500	1.57332000
C	-2.71150000	-0.12626900	1.81682300
C	-0.80193700	-0.83652000	5.04393800
C	-0.16399000	0.27951400	5.62521900
C	0.84630300	0.06618800	6.56688100
H	1.34562600	0.92126900	7.02564300
C	1.22508700	-1.22236600	6.92831900
H	2.01872000	-1.37374700	7.66205500
C	0.58863200	-2.31787200	6.35533000
H	0.89246200	-3.32476200	6.64586300
C	-0.43222400	-2.14782500	5.41383700
C	-0.59383800	1.69800400	5.28204900
H	-1.08422400	1.66749800	4.29919400
C	-1.62505100	2.19914200	6.29919000
H	-1.96407700	3.21487100	6.04411100
H	-1.18910900	2.22527100	7.31017400
H	-2.50402400	1.53860300	6.32526200
C	0.58649200	2.66201300	5.16069400
H	0.24895600	3.62343100	4.74472900
H	1.35541700	2.24709500	4.49331200
H	1.04768400	2.87322700	6.13774400
C	-1.06884500	-3.36759300	4.76097000
H	-2.06642800	-3.07377000	4.40593600
C	-0.25502500	-3.78808500	3.53236100
H	-0.74234100	-4.62182300	3.00172600
H	0.75454400	-4.11015700	3.83632200
H	-0.14400400	-2.94699800	2.83214500

C	-1.25513100	-4.54356100	5.72081200
H	-1.84465500	-5.33481700	5.23491500
H	-1.77841300	-4.23716000	6.63819900
H	-0.29215800	-4.99008500	6.01086500
C	-2.52723800	0.21129300	0.37483700
C	-2.35425900	1.58049600	0.01923400
C	-2.26235900	1.92671500	-1.33043300
H	-2.11927700	2.97435400	-1.59406700
C	-2.35830000	0.95456500	-2.32638900
H	-2.30293500	1.23957800	-3.37799500
C	-2.52257300	-0.37798800	-1.97641700
H	-2.60361000	-1.13498500	-2.75779900
C	-2.60172300	-0.78578600	-0.63042700
C	-2.35759800	2.65853500	1.08957300
H	-2.01420800	2.19106600	2.02278300
C	-3.78628700	3.17256300	1.30648400
H	-3.79804900	3.93399700	2.10010300
H	-4.46651500	2.36191400	1.60086900
H	-4.17381400	3.63250100	0.38405300
C	-1.40424400	3.80624600	0.77506300
H	-1.31200200	4.46907400	1.64806900
H	-1.75388700	4.42298700	-0.06761400
H	-0.40258000	3.42808800	0.52882800
C	-2.88006400	-2.26647300	-0.38231400
H	-2.42986800	-2.77055600	-1.24806200
C	-4.38862800	-2.54131700	-0.43759500
H	-4.57209100	-3.62585500	-0.41707600
H	-4.84147600	-2.13057400	-1.35209900
H	-4.89739800	-2.09834800	0.43026000
C	-2.24314000	-2.92452300	0.84156500
H	-2.29400100	-4.01623800	0.71440400
H	-2.75401200	-2.66986300	1.78014800
H	-1.18051900	-2.65500000	0.93711900

Table S4

In=P-Rea

G = -2862.25296933 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
In	0.19281300	0.07096600	0.07251600
P	0.05415700	0.03282000	2.46201600
C	1.33356900	0.01087400	-1.78890500
C	1.93269900	1.17532400	-2.30975400
C	2.96487600	1.05919800	-3.25143700
H	3.46140000	1.96327600	-3.60859600
C	3.39203800	-0.18860600	-3.69359400
H	4.20871600	-0.26517200	-4.41294600
C	2.79501500	-1.33929300	-3.18855600

H	3.15597500	-2.32107000	-3.49976400
C	1.77217300	-1.25390800	-2.23546300
C	1.56942000	2.55607400	-1.84084300
C	2.12085500	3.04707100	-0.63355400
C	1.85360600	4.36899400	-0.25862500
H	2.27572600	4.76147300	0.66709500
C	1.05306600	5.18821300	-1.04483600
H	0.85154000	6.21498300	-0.73513200
C	0.49821500	4.69385100	-2.22085200
H	-0.13488900	5.34447600	-2.82620200
C	0.74736000	3.38372500	-2.64310200
C	3.06999000	2.21153300	0.21918400
H	2.83822500	1.14729400	0.05167500
C	4.51652100	2.41867200	-0.24817900
H	5.20649600	1.80328200	0.34815300
H	4.80392900	3.47452900	-0.12775600
H	4.63847800	2.14889700	-1.30644400
C	2.94005100	2.48118200	1.71987200
H	3.50794500	1.72794100	2.28548600
H	1.89257500	2.42830000	2.05318200
H	3.34804800	3.46694300	1.98925300
C	0.18173500	2.90563900	-3.97641200
H	0.07407700	1.81056500	-3.91268900
C	-1.18673700	3.50773300	-4.31413800
H	-1.62504600	2.97903400	-5.17344600
H	-1.09569400	4.56534600	-4.60344400
H	-1.89701800	3.45146400	-3.47911400
C	1.14025300	3.22573700	-5.13297400
H	0.70268800	2.90574900	-6.09044500
H	2.10899200	2.72691600	-5.02113700
H	1.31716300	4.31113000	-5.18351500
C	1.23774000	-2.51395300	-1.61325100
C	0.20300700	-3.25193800	-2.23678000
C	-0.27528900	-4.40123400	-1.59672300
H	-1.07695900	-4.98160100	-2.05536500
C	0.24609300	-4.81447600	-0.37486900
H	-0.15085000	-5.70602300	0.11404300
C	1.27497500	-4.09628800	0.22264800
H	1.68269500	-4.43534400	1.17530600
C	1.79592500	-2.94842800	-0.38463300
C	-0.34946200	-2.85610200	-3.60340400
H	-0.36099600	-1.75347200	-3.64339000
C	0.55654200	-3.36410500	-4.73530800
H	0.12130500	-3.11013300	-5.71335800
H	0.64952000	-4.45930700	-4.67608000
H	1.56097400	-2.93137300	-4.69151700
C	-1.76656300	-3.37200400	-3.87838100
H	-2.17299100	-2.88116700	-4.77447000
H	-2.46371600	-3.19767100	-3.04790200
H	-1.75896200	-4.45391100	-4.07928100

C	3.01770000	-2.26440300	0.22342700
H	2.99661600	-1.20061800	-0.06480000
C	4.29265600	-2.86722300	-0.38402500
H	5.18472800	-2.36536400	0.01908100
H	4.30751000	-2.77118100	-1.47768400
H	4.35674000	-3.93732500	-0.13377100
C	3.08386100	-2.33028600	1.74981300
H	3.92912700	-1.72324200	2.10611200
H	3.25566200	-3.35815800	2.10370100
H	2.16766700	-1.94412500	2.21988200
C	-1.73504300	-0.24526800	2.79767000
C	-2.03598900	-0.61187700	4.13798000
C	-3.35511500	-0.79009000	4.55878100
H	-3.53490800	-1.08001600	5.59698400
C	-4.42333300	-0.61213600	3.68233900
H	-5.45110300	-0.74466200	4.02151100
C	-4.15079000	-0.26121700	2.36409400
H	-4.97018200	-0.11540700	1.65596500
C	-2.83693700	-0.09187300	1.91597100
C	-0.93660200	-0.83823400	5.13136800
C	-0.37314600	0.26063100	5.81236100
C	0.64007600	0.02796800	6.74616900
H	1.07847700	0.86932400	7.28664300
C	1.10368000	-1.26093400	6.99193200
H	1.90006500	-1.42607200	7.71972700
C	0.55438800	-2.33685000	6.30334200
H	0.93151200	-3.34490400	6.49029400
C	-0.46998900	-2.14690200	5.36986700
C	-0.86306900	1.67936600	5.56360600
H	-1.43927600	1.67168600	4.62709600
C	-1.80640800	2.12468000	6.68590500
H	-2.18685000	3.14020800	6.49782500
H	-1.28198900	2.12879600	7.65437400
H	-2.66618300	1.44412500	6.77011900
C	0.28813400	2.66875400	5.37253700
H	-0.10332000	3.65189000	5.07007300
H	0.97347900	2.31211700	4.58995100
H	0.86099500	2.81506100	6.30117000
C	-1.00972500	-3.34435700	4.60134900
H	-1.88841900	-3.01027100	4.03344200
C	0.02129600	-3.83845700	3.58095000
H	-0.39478700	-4.65911700	2.97430500
H	0.92942800	-4.20807000	4.08533600
H	0.31290200	-3.01973000	2.90607900
C	-1.46438700	-4.47294800	5.52935900
H	-1.91275200	-5.29102300	4.94594500
H	-2.21147700	-4.11553100	6.25285600
H	-0.62043400	-4.89486200	6.09619000
C	-2.64733300	0.24685900	0.47672200
C	-2.45056900	1.60686400	0.11582000

C	-2.27707700	1.93746800	-1.23139000
H	-2.10823600	2.97998300	-1.50367000
C	-2.29989800	0.95108100	-2.21769400
H	-2.16622400	1.21755200	-3.26686200
C	-2.47879700	-0.37779700	-1.85792900
H	-2.48994200	-1.14699300	-2.63128700
C	-2.64692900	-0.76521200	-0.51349900
C	-2.46174900	2.69272000	1.17836000
H	-2.14335700	2.22522000	2.12068200
C	-3.88655000	3.22792700	1.36527600
H	-3.90610500	3.99314800	2.15511900
H	-4.58068300	2.42497500	1.64952400
H	-4.25161400	3.68674000	0.43308100
C	-1.48128600	3.82366200	0.88052800
H	-1.40873200	4.49494500	1.74878700
H	-1.79458200	4.43504800	0.01970200
H	-0.47467300	3.43152200	0.67194400
C	-2.89820000	-2.25269500	-0.26609800
H	-2.37335100	-2.75335000	-1.09303700
C	-4.39208600	-2.56432900	-0.42430800
H	-4.55805500	-3.65111600	-0.38180900
H	-4.78382100	-2.19010600	-1.38166800
H	-4.97017500	-2.10268000	0.38925800
C	-2.34450000	-2.88812600	1.01262400
H	-2.33289600	-3.98050700	0.87727000
H	-2.96242400	-2.66330500	1.89262800
H	-1.31152600	-2.56992800	1.22373200

Table S5

Tl=P-Rea

G = -2844.56513726 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Tl	0.29687900	0.05629200	0.09817500
P	0.00155400	0.03431800	2.50441100
C	1.38150200	-0.01915800	-1.83302800
C	1.96807100	1.14656100	-2.35846000
C	2.97403700	1.02705300	-3.32796000
H	3.46890500	1.92859300	-3.69340200
C	3.38156600	-0.22254000	-3.78440500
H	4.18108300	-0.30137900	-4.52246600
C	2.78969400	-1.37262400	-3.27093800
H	3.13900400	-2.35496500	-3.59345700
C	1.79044100	-1.28575900	-2.29291100
C	1.61733800	2.51981100	-1.86018200
C	2.17842800	2.97968900	-0.64535500
C	1.89562700	4.28344300	-0.22213100
H	2.32247600	4.65096200	0.71175100

C	1.07723300	5.11751600	-0.97367500
H	0.86303000	6.12973800	-0.62681400
C	0.52260300	4.65699100	-2.16330300
H	-0.12196800	5.31994300	-2.74261100
C	0.78175600	3.36389400	-2.62993800
C	3.16229400	2.13569300	0.15820700
H	2.96106900	1.07372600	-0.05410000
C	4.59357900	2.40712000	-0.32306700
H	5.31274800	1.78607600	0.23150300
H	4.85253000	3.46457300	-0.16009400
H	4.70198900	2.18951000	-1.39491500
C	3.04979100	2.33613100	1.67132300
H	3.65403800	1.58084800	2.19496300
H	2.01085800	2.23912900	2.02300900
H	3.42883100	3.32289500	1.97654900
C	0.21107700	2.92383500	-3.97387400
H	0.11467500	1.82637300	-3.94553400
C	-1.16554000	3.52221800	-4.28343800
H	-1.60333200	3.01721100	-5.15705000
H	-1.08728200	4.58974700	-4.53807000
H	-1.86981500	3.42940400	-3.44686300
C	1.15938500	3.29262100	-5.12433100
H	0.72263300	2.99464200	-6.08921900
H	2.13670700	2.80676700	-5.03148400
H	1.31943700	4.38165700	-5.14306400
C	1.25953300	-2.53803400	-1.65369400
C	0.20619900	-3.27284200	-2.24825900
C	-0.27450000	-4.40553500	-1.58110700
H	-1.09196500	-4.98232600	-2.01573100
C	0.26379800	-4.80671500	-0.36233000
H	-0.13518200	-5.68563400	0.14724300
C	1.31283900	-4.09299800	0.20453700
H	1.73671200	-4.42458000	1.15294500
C	1.83405100	-2.95986900	-0.42951800
C	-0.36395900	-2.89120800	-3.61137300
H	-0.36579700	-1.78920500	-3.66650500
C	0.52016500	-3.42449600	-4.74889800
H	0.07448100	-3.17798100	-5.72411900
H	0.60105500	-4.51988100	-4.67666300
H	1.53036200	-3.00376900	-4.72471200
C	-1.78980100	-3.39684300	-3.85744100
H	-2.20349600	-2.91711900	-4.75613600
H	-2.47299600	-3.19950700	-3.02075800
H	-1.79616400	-4.48214900	-4.03937200
C	3.07348700	-2.27950300	0.14526800
H	3.08248600	-1.23250000	-0.19740400
C	4.32960400	-2.94550800	-0.43354800
H	5.23718700	-2.44796600	-0.06083500
H	4.33828000	-2.90362300	-1.53126400
H	4.36745900	-4.00365600	-0.13229900

C	3.13451700	-2.26700600	1.67345600
H	4.00208400	-1.67599500	2.00222700
H	3.26220000	-3.27995000	2.08414700
H	2.23127000	-1.82511100	2.12108900
C	-1.79093500	-0.23700600	2.81118300
C	-2.08166300	-0.58943600	4.15636000
C	-3.39679000	-0.77197800	4.58539900
H	-3.57051500	-1.05151300	5.62740500
C	-4.46836300	-0.60661300	3.71017100
H	-5.49431400	-0.74201000	4.05369300
C	-4.20255900	-0.26225700	2.38862300
H	-5.02487300	-0.12203700	1.68289100
C	-2.89224400	-0.09051800	1.93102200
C	-0.96898200	-0.78873000	5.14028000
C	-0.44448100	0.31991600	5.83618800
C	0.58150900	0.10922500	6.76206900
H	0.99049900	0.95708800	7.31551000
C	1.09321400	-1.16559400	6.98433900
H	1.89645000	-1.31317400	7.70837400
C	0.58532700	-2.24968300	6.27592500
H	1.00069700	-3.24640500	6.44336000
C	-0.44574400	-2.08131300	5.34675100
C	-0.98536600	1.72398100	5.60981300
H	-1.58975500	1.70294000	4.69115600
C	-1.90730500	2.13600300	6.76210100
H	-2.32468400	3.13958300	6.58948700
H	-1.35429400	2.15394600	7.71435400
H	-2.74237900	1.42864200	6.86971200
C	0.12954400	2.74878800	5.39000800
H	-0.30119300	3.72518100	5.12112200
H	0.79261500	2.42615700	4.57409800
H	0.73538300	2.89501700	6.29741800
C	-0.95087300	-3.28392500	4.56426000
H	-1.75937400	-2.93854900	3.90616600
C	0.14552100	-3.85512800	3.65999800
H	-0.25387100	-4.67701700	3.04417800
H	0.98796400	-4.24969600	4.25118100
H	0.52876700	-3.07279100	2.98815700
C	-1.53244500	-4.35534400	5.48996800
H	-1.93471800	-5.19529500	4.90383700
H	-2.34476000	-3.94553100	6.10767400
H	-0.76345400	-4.75689200	6.16796300
C	-2.69732600	0.24926900	0.49385400
C	-2.48255300	1.60521000	0.14187900
C	-2.26631800	1.93493900	-1.19908200
H	-2.08055000	2.97592500	-1.46696300
C	-2.26399600	0.94833200	-2.18447100
H	-2.09464000	1.21186600	-3.22936600
C	-2.46456100	-0.37946100	-1.82957900
H	-2.45452200	-1.14900500	-2.60275700

C	-2.67493700	-0.76299700	-0.49200500
C	-2.50581000	2.69177300	1.20457500
H	-2.22487600	2.22114100	2.15708100
C	-3.92568600	3.25145900	1.35125200
H	-3.95733400	4.01715900	2.14044500
H	-4.63998800	2.45851600	1.61392000
H	-4.25682300	3.71477700	0.40863400
C	-1.49529700	3.80493100	0.93949500
H	-1.44333400	4.47861900	1.80755300
H	-1.76563000	4.41761500	0.06517700
H	-0.48867800	3.39382800	0.76951400
C	-2.92033900	-2.25153200	-0.24523000
H	-2.39045600	-2.75053300	-1.07011800
C	-4.41131200	-2.57497600	-0.40458200
H	-4.57148800	-3.66269800	-0.35935800
H	-4.80323400	-2.20522500	-1.36356600
H	-4.99407600	-2.11404700	0.40623300
C	-2.36405300	-2.88261600	1.03542000
H	-2.34137400	-3.97512500	0.90087800
H	-2.98891400	-2.66452300	1.91231500
H	-1.33518300	-2.55363000	1.25282900

Table S6

CO₂

G = -188.596924730 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15618300
O	0.00000000	0.00000000	-1.15618300

Table S7

B=P-TS

G = -2885.54458689 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
O	-0.04761500	-0.33345000	-0.10926500
P	-0.28971000	-0.38382800	2.43184800
C	0.89038000	-0.37232100	0.67922000
O	2.07062100	-0.38735100	0.73110500
B	-1.64302800	-0.89810500	1.35592300
C	0.05696100	-0.96894400	4.12863000
C	-2.67548500	-0.96369100	0.22381900
C	-3.07064200	0.30074000	-0.29675500
C	-3.36607900	0.42668600	-1.65745400

H	-3.64969900	1.40831200	-2.04116300
C	-3.30848700	-0.67165000	-2.50444100
H	-3.49842000	-0.55456800	-3.57241400
C	-3.05996600	-1.93358700	-1.97223000
H	-3.07958800	-2.81363200	-2.61734600
C	-2.77507700	-2.10768100	-0.61599400
C	-3.23866300	1.53950800	0.53056700
C	-2.31426400	2.59819700	0.40861500
C	-2.55726200	3.78693900	1.10753900
H	-1.83719400	4.60541900	1.03720300
C	-3.71216000	3.94764600	1.85897200
H	-3.90052900	4.88659900	2.38229800
C	-4.63995200	2.91196400	1.93712700
H	-5.54431000	3.06634500	2.52398600
C	-4.42119700	1.68612600	1.30167400
C	-1.09719600	2.52428300	-0.50209000
H	-1.02560800	1.50641300	-0.90013800
C	-1.25231300	3.48627800	-1.68576700
H	-0.38841600	3.40249500	-2.36157800
H	-1.31361500	4.53048700	-1.34186400
H	-2.16247000	3.27254200	-2.26485900
C	0.21180700	2.79779300	0.24313500
H	1.07272100	2.58931400	-0.40939700
H	0.31041900	2.16435200	1.13627700
H	0.28372500	3.84887700	0.56733500
C	-5.44318500	0.55415500	1.44740100
H	-4.88113100	-0.33825200	1.77249100
C	-6.50916800	0.83856200	2.50781300
H	-7.09555700	-0.07294300	2.69520800
H	-7.20876100	1.61651300	2.16430800
H	-6.08329300	1.17131200	3.46341700
C	-6.17174400	0.19860500	0.14054800
H	-6.98799000	-0.50799100	0.35671800
H	-5.51981300	-0.27219100	-0.60390400
H	-6.61639500	1.09979400	-0.30989300
C	-2.59504500	-3.52410200	-0.14834600
C	-3.74187900	-4.26709000	0.24006200
C	-3.57331300	-5.61448300	0.57121900
H	-4.43694100	-6.20764500	0.87468200
C	-2.31913100	-6.22181400	0.51916400
H	-2.21320100	-7.27418600	0.78840400
C	-1.21218300	-5.49236600	0.10816800
H	-0.23825700	-5.98090300	0.03458300
C	-1.33261200	-4.14332600	-0.25248200
C	-5.14686900	-3.66097200	0.22008200
H	-5.06224800	-2.61987500	0.57719500
C	-5.73520900	-3.64336600	-1.20138500
H	-6.76404600	-3.25380800	-1.17550900
H	-5.76993500	-4.66852500	-1.60129100
H	-5.16240300	-3.02327600	-1.89666300

C	-6.16806400	-4.39092400	1.10029000
H	-7.08788000	-3.79109900	1.16225700
H	-5.81962900	-4.58036500	2.12145700
H	-6.44719800	-5.35864300	0.65633200
C	-0.14633900	-3.43692200	-0.89435300
H	-0.38676100	-2.37152900	-0.99089600
C	0.06113700	-3.98872200	-2.31149100
H	0.87184400	-3.44547500	-2.81857900
H	-0.85102300	-3.88952400	-2.91748400
H	0.32946400	-5.05635900	-2.28151100
C	1.15251700	-3.53296100	-0.09219600
H	1.95266000	-2.98930200	-0.61555800
H	1.48201500	-4.57623300	0.03522200
H	1.05343000	-3.08408100	0.90555600
C	1.28197000	-0.52802900	4.67856800
C	1.62652400	-0.93143200	5.97299700
H	2.55998100	-0.56285600	6.40100700
C	0.79019000	-1.75522800	6.72034000
H	1.07517000	-2.05637800	7.72923200
C	-0.43153800	-2.15313500	6.18715000
H	-1.12885600	-2.74781200	6.78026900
C	-0.81196100	-1.75671100	4.90276200
C	2.19429500	0.40410500	3.94053400
C	1.85732000	1.77765900	3.87099600
C	2.71538000	2.63616000	3.18083100
H	2.47121200	3.69593700	3.09993200
C	3.88804800	2.15935800	2.59906000
H	4.54732400	2.84583600	2.06527700
C	4.21548900	0.81340200	2.68940300
H	5.12739600	0.44958600	2.21410000
C	3.37235900	-0.08961500	3.34508400
C	0.63659700	2.33001500	4.60071700
H	-0.13989600	1.55048400	4.60257000
C	0.99032000	2.63022400	6.06297000
H	0.10339100	2.98449800	6.61061500
H	1.76281900	3.41304200	6.11407700
H	1.37621200	1.73776200	6.57495600
C	0.01960200	3.56071500	3.93824700
H	-0.90904600	3.83774800	4.45819500
H	-0.23018600	3.36772400	2.88623700
H	0.69091300	4.43166500	3.98601500
C	3.74081800	-1.56723100	3.40168600
H	2.80964000	-2.13212900	3.57016900
C	4.36582800	-2.08904100	2.10415100
H	4.44952600	-3.18511300	2.15010200
H	5.38377300	-1.69435800	1.96327600
H	3.76147400	-1.81335200	1.23223800
C	4.69065900	-1.84996900	4.57317300
H	4.95167900	-2.91836600	4.60814700
H	4.25231800	-1.57417700	5.54062300

H	5.62165300	-1.27513900	4.44913000
C	-2.19662200	-2.04075300	4.44372400
C	-3.16046000	-1.03156300	4.67431100
C	-4.48335600	-1.27018000	4.29689900
H	-5.24149800	-0.50918200	4.48636000
C	-4.84987900	-2.47528100	3.70438600
H	-5.88790000	-2.64895000	3.41153000
C	-3.89114500	-3.46054400	3.50385300
H	-4.16102600	-4.42064200	3.06442400
C	-2.55311900	-3.27245200	3.86592600
C	-2.81495300	0.26469600	5.39781400
H	-1.73856600	0.26619100	5.61534400
C	-3.54042200	0.33352700	6.74595300
H	-3.24808300	1.24195200	7.29319800
H	-3.29885200	-0.53902800	7.37017000
H	-4.63242700	0.35855700	6.60774400
C	-3.10904100	1.50055400	4.54820900
H	-2.81068000	2.41446400	5.08486700
H	-4.18320000	1.58386500	4.32640300
H	-2.57231600	1.47700100	3.58571400
C	-1.62855200	-4.47000200	3.67678100
H	-2.07100800	-5.02449700	2.83521400
C	-1.68572100	-5.38919200	4.90367300
H	-1.11339600	-6.31027500	4.71674600
H	-2.72053900	-5.66734600	5.14967400
H	-1.24605600	-4.89257900	5.78167600
C	-0.17965800	-4.18196600	3.28243600
H	0.25568800	-5.08250700	2.82270900
H	0.44656600	-3.90738200	4.14305100
H	-0.12694400	-3.37205600	2.54342000

Table S8

Al=P-TS

G = -3103.19127331 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
O	-0.15192200	-0.06456500	-0.04160600
P	0.08005900	-0.17153300	2.71525600
C	0.97725900	0.02306100	0.33880000
O	2.12557300	0.15248600	0.28639100
Al	-1.68345500	-0.80705700	1.53804100
C	0.28948500	-0.85322000	4.39513000
C	-2.92066200	-0.97150700	0.01425200
C	-3.45904200	0.22266200	-0.52073200
C	-3.73625000	0.31152600	-1.89137500
H	-4.12906800	1.24938200	-2.29095900
C	-3.52680500	-0.77524700	-2.73306600
H	-3.71504600	-0.68596200	-3.80396400

C	-3.12332700	-1.99208600	-2.19101900
H	-3.01937100	-2.86989300	-2.83215900
C	-2.84195000	-2.10896300	-0.82510000
C	-3.82713800	1.40118200	0.33921100
C	-3.00522100	2.54543300	0.39036400
C	-3.42712200	3.65073400	1.14290300
H	-2.79244800	4.53789900	1.19179000
C	-4.63962200	3.63592700	1.81516300
H	-4.95434200	4.50350100	2.39756500
C	-5.45901700	2.51017200	1.74530000
H	-6.41539700	2.51735700	2.26945700
C	-5.08099900	1.38482400	1.01048400
C	-1.70589400	2.64827800	-0.39337700
H	-1.49429700	1.66417500	-0.83054500
C	-1.85696400	3.64254800	-1.55048700
H	-0.92839000	3.69272700	-2.13809500
H	-2.07508000	4.65357800	-1.17326400
H	-2.67560500	3.35189100	-2.22450800
C	-0.51890100	3.02374400	0.49844000
H	0.41980400	2.98128400	-0.07559500
H	-0.42761300	2.34384200	1.35934800
H	-0.61553900	4.04846700	0.88956400
C	-6.04889000	0.21395200	0.85961300
H	-5.44410800	-0.70625800	0.86014700
C	-7.08860700	0.10178300	1.97725000
H	-7.63511100	-0.84778000	1.87675900
H	-7.83441100	0.90815700	1.90913000
H	-6.65110200	0.13495300	2.98346500
C	-6.80068000	0.28937800	-0.47838400
H	-7.49069800	-0.56295600	-0.57425800
H	-6.12345500	0.27411500	-1.33939400
H	-7.39386700	1.21578100	-0.52250900
C	-2.52687800	-3.47156600	-0.27314600
C	-3.60111200	-4.28547600	0.17114400
C	-3.31160300	-5.55491200	0.67724300
H	-4.12330500	-6.19541100	1.02605900
C	-1.99903900	-6.01954100	0.74993400
H	-1.79362800	-7.00997900	1.15994000
C	-0.95671200	-5.22768600	0.28751800
H	0.06548000	-5.60948200	0.31843900
C	-1.20304900	-3.95577500	-0.24818700
C	-5.05205900	-3.83645400	0.02008600
H	-5.07192100	-2.74152000	0.14218000
C	-5.56921600	-4.16900200	-1.38809400
H	-6.60919400	-3.82869900	-1.50396200
H	-5.54464800	-5.25817700	-1.54678200
H	-4.96792400	-3.69679300	-2.17280200
C	-6.02307100	-4.44478000	1.03604100
H	-7.00528000	-3.95945100	0.93695500
H	-5.69503800	-4.32736100	2.07658700

H	-6.17802900	-5.51812600	0.84928100
C	-0.06915900	-3.19673500	-0.92078500
H	-0.40633600	-2.16602200	-1.09578700
C	0.20874600	-3.81932700	-2.29578100
H	0.99197800	-3.25582700	-2.82390000
H	-0.69498500	-3.82424400	-2.92146800
H	0.54871400	-4.86079900	-2.18671600
C	1.21388800	-3.13684200	-0.09220100
H	1.97755600	-2.54938400	-0.62388700
H	1.63922500	-4.13799200	0.07710500
H	1.05146600	-2.66884100	0.89216300
C	1.54480500	-0.64103900	5.00852900
C	1.77123400	-1.08895300	6.31364200
H	2.74604900	-0.89946700	6.76916400
C	0.76993500	-1.73033700	7.03805800
H	0.95271100	-2.05869400	8.06182700
C	-0.47594000	-1.92687600	6.44618900
H	-1.28320400	-2.40263100	7.00708000
C	-0.71849200	-1.51028100	5.13612800
C	2.60630700	0.14838300	4.30549000
C	2.66112900	1.54023400	4.51392800
C	3.64960600	2.28018200	3.85481000
H	3.70214100	3.36115400	4.00475400
C	4.55526600	1.66015400	3.00376700
H	5.31873800	2.24991100	2.49361300
C	4.47813100	0.28654900	2.78619300
H	5.17837600	-0.18286700	2.09480100
C	3.50604400	-0.48817500	3.42241600
C	1.65790800	2.26715400	5.39913200
H	0.98289400	1.51776900	5.83640700
C	2.35207200	2.98751400	6.55834100
H	1.61077000	3.46779100	7.21439000
H	3.03218900	3.77123700	6.19070800
H	2.94399900	2.28465100	7.16242100
C	0.79382200	3.23076000	4.57799200
H	0.04501300	3.71869800	5.22107200
H	0.26769600	2.69193500	3.77547600
H	1.40773300	4.02015200	4.11642700
C	3.41361900	-1.98721100	3.17315400
H	2.34149600	-2.24719500	3.19290200
C	3.96597700	-2.40448800	1.81040300
H	3.70247700	-3.45222600	1.60329200
H	5.06448500	-2.33385600	1.78417500
H	3.56147600	-1.77512400	1.00626800
C	4.11307300	-2.78080800	4.28368600
H	4.02088500	-3.86233000	4.10048900
H	3.68343600	-2.56498200	5.27046700
H	5.18425400	-2.52723800	4.31249000
C	-2.05646600	-1.71717700	4.52106300
C	-2.93443400	-0.60748600	4.44370200

C	-4.16429800	-0.76164000	3.79953100
H	-4.82755500	0.09854500	3.71710100
C	-4.54072400	-1.99217600	3.25989600
H	-5.51032300	-2.10233500	2.76874700
C	-3.66762500	-3.06926200	3.33940000
H	-3.93724900	-4.03285500	2.90791000
C	-2.40650600	-2.95556900	3.94689100
C	-2.57094900	0.72455500	5.08241100
H	-1.47602900	0.81327000	5.06654100
C	-3.02236300	0.74041800	6.54798700
H	-2.73542800	1.68809600	7.02765600
H	-2.56502500	-0.08317800	7.11436300
H	-4.11667000	0.63783300	6.61515000
C	-3.12757900	1.92413800	4.32078500
H	-2.69424800	2.85493300	4.71522900
H	-4.22125600	2.00778600	4.41632900
H	-2.88236500	1.86661900	3.24834200
C	-1.54488800	-4.21681400	3.95537700
H	-1.95875200	-4.82687100	3.13750700
C	-1.74404400	-5.01641700	5.24876600
H	-1.24045200	-5.99170100	5.17092800
H	-2.81055600	-5.19303900	5.44999800
H	-1.31251500	-4.48443000	6.10828500
C	-0.05468600	-4.04632100	3.63924500
H	0.35609100	-5.01897200	3.32648500
H	0.52461800	-3.70034300	4.50714800
H	0.10332200	-3.33214500	2.81714200

Table S9

Ga=P-TS

G = -4785.62579148 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
O	0.00681500	0.00832700	0.00001300
P	-0.00172200	0.00939700	2.74647000
C	1.04657800	-0.00403300	0.60831600
O	2.21554900	0.01999500	0.63472100
Ga	-1.74495300	-0.79103800	1.59390300
C	0.26523700	-0.79551600	4.36717300
C	-2.93434600	-0.97436000	0.01921000
C	-3.49449100	0.21082000	-0.50680200
C	-3.79445600	0.28355100	-1.87351400
H	-4.20625500	1.21244600	-2.27396300
C	-3.58188700	-0.80650000	-2.70981000
H	-3.78782500	-0.72784500	-3.77820700
C	-3.14977000	-2.01288100	-2.16673300
H	-3.03944800	-2.89228300	-2.80412500
C	-2.84702700	-2.11895100	-0.80463100

C	-3.85997100	1.38962200	0.35252500
C	-3.02609400	2.52505400	0.40804500
C	-3.44376400	3.63377700	1.15771800
H	-2.80312900	4.51617100	1.20881300
C	-4.65974100	3.62813300	1.82471200
H	-4.97008300	4.49853800	2.40532300
C	-5.48786700	2.50910800	1.75275600
H	-6.44613300	2.52374600	2.27345800
C	-5.11622000	1.38127900	1.01797300
C	-1.72842800	2.61372900	-0.37987700
H	-1.48041100	1.61059500	-0.74980800
C	-1.91202300	3.52640600	-1.59841600
H	-0.98367300	3.57190300	-2.18652700
H	-2.16799900	4.55024700	-1.28414300
H	-2.71695500	3.16512900	-2.25443300
C	-0.55130600	3.08336500	0.47788400
H	0.38569700	3.00990300	-0.09402300
H	-0.44673600	2.46887200	1.38430200
H	-0.66664700	4.13338200	0.78877700
C	-6.09474000	0.22033900	0.85857700
H	-5.49967300	-0.70660400	0.84203100
C	-7.12834300	0.10345700	1.98155400
H	-7.68241100	-0.84103200	1.87504700
H	-7.86872000	0.91569600	1.92643600
H	-6.68427600	0.12413100	2.98497500
C	-6.85620400	0.32338000	-0.47218500
H	-7.55821900	-0.51824500	-0.57431400
H	-6.18635200	0.31168200	-1.33882300
H	-7.43721000	1.25808900	-0.49835000
C	-2.50860600	-3.47378100	-0.25047000
C	-3.57007000	-4.31387000	0.17455200
C	-3.25793200	-5.58346500	0.66731500
H	-4.05860500	-6.24568600	1.00077300
C	-1.93639200	-6.02195000	0.74163100
H	-1.71377600	-7.01456600	1.13716900
C	-0.90632400	-5.20127100	0.30142300
H	0.12321200	-5.56190600	0.33614800
C	-1.17380500	-3.92605700	-0.21592200
C	-5.02942900	-3.89440600	0.01495200
H	-5.07177400	-2.79844700	0.12314100
C	-5.53593300	-4.25658500	-1.38983300
H	-6.58128800	-3.93665800	-1.51444000
H	-5.49142100	-5.34737200	-1.53214000
H	-4.94012600	-3.78624900	-2.17969100
C	-5.99270900	-4.50760100	1.03562900
H	-6.98709400	-4.05293500	0.91550400
H	-5.68035800	-4.35636500	2.07656000
H	-6.11558200	-5.58882400	0.87257000
C	-0.05472600	-3.12542500	-0.86406700
H	-0.39346900	-2.08677400	-0.97814300

C	0.20526400	-3.67466300	-2.27348700
H	0.98024200	-3.08130400	-2.78025300
H	-0.70609900	-3.64779100	-2.88732300
H	0.54810600	-4.71982100	-2.22320000
C	1.24213400	-3.10002500	-0.05684100
H	1.98387500	-2.46441100	-0.56186000
H	1.68524500	-4.10295100	0.04256000
H	1.09387800	-2.69310400	0.95582100
C	1.53619200	-0.61237800	4.95384100
C	1.77585700	-1.07328100	6.25261100
H	2.76124800	-0.90271300	6.69219700
C	0.78097800	-1.71392700	6.98611100
H	0.97706500	-2.05319900	8.00382200
C	-0.47248900	-1.90287700	6.40899200
H	-1.27165100	-2.38907800	6.97246700
C	-0.73402900	-1.46300600	5.11018600
C	2.61629300	0.14475900	4.24160000
C	2.69152400	1.54112100	4.41713600
C	3.73524400	2.24035700	3.80243700
H	3.80916400	3.32235200	3.93305900
C	4.67646200	1.57573800	3.02569800
H	5.48632200	2.13337100	2.55234700
C	4.57293000	0.20182300	2.82980300
H	5.29513400	-0.29980900	2.18546800
C	3.54194000	-0.53340800	3.41901500
C	1.67376800	2.30255500	5.25484700
H	0.87514100	1.60157500	5.53808200
C	2.31023100	2.81945700	6.54870000
H	1.56583300	3.34187400	7.16827700
H	3.12594000	3.52556100	6.32851400
H	2.73125100	1.99217100	7.13838400
C	1.01665800	3.43613800	4.46211900
H	0.23598800	3.92187000	5.06723900
H	0.55162300	3.04827500	3.54396300
H	1.74747100	4.20936800	4.17964100
C	3.40938300	-2.02981800	3.16709300
H	2.32745100	-2.24672000	3.12964100
C	4.01846600	-2.47258400	1.83606100
H	3.72579000	-3.51073200	1.61942300
H	5.11866400	-2.44703300	1.87321600
H	3.68258200	-1.83144600	1.01104200
C	4.02087000	-2.85523200	4.30653400
H	3.90582500	-3.93114900	4.10405500
H	3.54855500	-2.63951900	5.27290300
H	5.09661700	-2.63664400	4.39344500
C	-2.07997000	-1.67448300	4.51256900
C	-2.98150200	-0.58283700	4.47513100
C	-4.21855900	-0.74726900	3.84651100
H	-4.89964100	0.10156900	3.79709500
C	-4.57887500	-1.97141100	3.28222000

H	-5.55227700	-2.09001000	2.80050500
C	-3.68385000	-3.03260600	3.32535100
H	-3.93967100	-3.99199000	2.87689200
C	-2.41659400	-2.90820100	3.91782200
C	-2.63651500	0.74060600	5.13976300
H	-1.54201900	0.83295000	5.14818000
C	-3.11596600	0.72971300	6.59636800
H	-2.84560000	1.67128200	7.09683800
H	-2.66331000	-0.10021300	7.15756700
H	-4.21045900	0.61763000	6.64108700
C	-3.18379100	1.94830600	4.38330100
H	-2.76354500	2.87562900	4.79964400
H	-4.27959000	2.02497500	4.45800800
H	-2.91630600	1.90681000	3.31564000
C	-1.53650600	-4.15602800	3.89277600
H	-1.94186800	-4.74998100	3.05934200
C	-1.72504600	-4.99082200	5.16535400
H	-1.20453500	-5.95493500	5.06413900
H	-2.78872400	-5.19082100	5.35927700
H	-1.30463800	-4.47310000	6.03912300
C	-0.04913900	-3.95714700	3.58234200
H	0.37169500	-4.91058100	3.22692900
H	0.52924200	-3.63981600	4.46160800
H	0.09924800	-3.20927700	2.78914300

Table S10

In=P-TS

G = -3050.84803305 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
O	0.18152900	0.09975600	0.05884700
P	0.05552200	0.10159700	2.86736300
C	1.19084800	0.08705400	0.70901800
O	2.35530000	0.11592400	0.80487700
In	-1.80497000	-0.77307500	1.57689300
C	0.30028900	-0.75062700	4.47145900
C	-3.05208500	-0.97609900	-0.18909000
C	-3.66437600	0.18865300	-0.69028400
C	-4.05319000	0.23559400	-2.03577500
H	-4.50941200	1.14727600	-2.42752500
C	-3.86554900	-0.86522400	-2.86687200
H	-4.14638800	-0.80964400	-3.91958300
C	-3.35371800	-2.04992000	-2.34274800
H	-3.25186800	-2.93105500	-2.97936900
C	-2.96379500	-2.12414900	-1.00040300
C	-3.98056500	1.35039600	0.21017400
C	-3.08635600	2.43489800	0.33214700
C	-3.43970000	3.51052000	1.15851500

H	-2.75654900	4.35497500	1.26025000
C	-4.64431000	3.51714400	1.84739000
H	-4.90179300	4.36070200	2.49018800
C	-5.52121200	2.44135100	1.72717800
H	-6.46405500	2.45926200	2.27569100
C	-5.21439200	1.34868500	0.91221000
C	-1.79567000	2.50065600	-0.47002300
H	-1.53046800	1.48053700	-0.78138500
C	-2.01514400	3.32699400	-1.74358700
H	-1.09212800	3.36533100	-2.34046600
H	-2.30361600	4.35848700	-1.48797400
H	-2.81103700	2.89778100	-2.36835700
C	-0.61724600	3.05180800	0.33555500
H	0.31348700	2.93308900	-0.23762400
H	-0.49759100	2.52146700	1.29316000
H	-0.73640500	4.12490000	0.54968200
C	-6.23242900	0.22795800	0.72738100
H	-5.66665300	-0.70611300	0.57890600
C	-7.17129000	0.03120000	1.92031400
H	-7.74692000	-0.89719800	1.79000600
H	-7.90001400	0.85215700	1.99540300
H	-6.63794900	-0.03126700	2.87792400
C	-7.08619300	0.47084300	-0.52600400
H	-7.81331600	-0.34465400	-0.65790800
H	-6.47694800	0.53327800	-1.43482700
H	-7.64387100	1.41414100	-0.42090100
C	-2.55207900	-3.44236700	-0.41107700
C	-3.56543400	-4.32136000	0.04358800
C	-3.18602800	-5.53836100	0.61815300
H	-3.95175900	-6.23119400	0.97148600
C	-1.84244500	-5.88018500	0.75466100
H	-1.56579100	-6.82965400	1.21664500
C	-0.85467200	-5.01527900	0.29839700
H	0.19455900	-5.29811100	0.39451300
C	-1.18974100	-3.79534600	-0.30372300
C	-5.04409900	-3.99987300	-0.15076000
H	-5.14367800	-2.90361600	-0.18640000
C	-5.53445800	-4.56405800	-1.49187100
H	-6.59251600	-4.30978500	-1.65405100
H	-5.43969600	-5.66097700	-1.49489300
H	-4.95506500	-4.17283300	-2.33665200
C	-5.95813900	-4.51478500	0.96441200
H	-6.98002800	-4.14139200	0.80267900
H	-5.63733800	-4.19051600	1.96316300
H	-6.01643400	-5.61347700	0.96717600
C	-0.10952500	-2.94232100	-0.95115900
H	-0.47448700	-1.90728800	-1.01450700
C	0.11872900	-3.42490600	-2.39017500
H	0.87394800	-2.80058700	-2.88946500
H	-0.80931900	-3.37886800	-2.97709700

H	0.47266900	-4.46746100	-2.39343500
C	1.20953200	-2.91882400	-0.18118600
H	1.90268700	-2.20329000	-0.64730500
H	1.70691600	-3.90067200	-0.18733000
H	1.07427500	-2.61438300	0.86964700
C	1.57827000	-0.59974800	5.05763100
C	1.81455000	-1.06688200	6.35444000
H	2.80644700	-0.91834200	6.78763700
C	0.81240800	-1.69094000	7.09271700
H	1.00606400	-2.03486100	8.10924800
C	-0.44356900	-1.86148700	6.51611500
H	-1.24720500	-2.34124800	7.07894100
C	-0.70297300	-1.41435500	5.21935200
C	2.68671300	0.11155900	4.33996600
C	2.81438000	1.50693200	4.48935800
C	3.90116500	2.15073600	3.88882100
H	4.01652900	3.23105300	4.00115800
C	4.83482900	1.43313600	3.15058000
H	5.67987500	1.94791600	2.69031200
C	4.67692200	0.06202400	2.97403000
H	5.39154000	-0.48207100	2.35571000
C	3.60008100	-0.61710500	3.54789500
C	1.80730300	2.32140400	5.28865200
H	0.95317000	1.66794900	5.51949400
C	2.41134100	2.77929900	6.61982900
H	1.67435300	3.34492400	7.20979200
H	3.28334600	3.42968000	6.44873200
H	2.74520300	1.91880100	7.21770600
C	1.26236300	3.50470600	4.48442700
H	0.47130800	4.01862400	5.05149000
H	0.83667400	3.15998700	3.53072600
H	2.04809600	4.24439600	4.26746000
C	3.40261100	-2.10735100	3.30542600
H	2.31334600	-2.27992800	3.29687200
C	3.95367900	-2.57462100	1.95700300
H	3.61074500	-3.59957300	1.74936200
H	5.05453600	-2.59588000	1.95890300
H	3.62075200	-1.91803000	1.14247500
C	4.00927800	-2.95368700	4.43138500
H	3.84455700	-4.02503200	4.23824700
H	3.57075100	-2.71288700	5.40813200
H	5.09510300	-2.77976800	4.49049300
C	-2.04735400	-1.62553200	4.61469900
C	-2.95139500	-0.53806100	4.57535500
C	-4.15506200	-0.67786100	3.87442900
H	-4.83740700	0.17085800	3.81592300
C	-4.47327200	-1.87452200	3.23138100
H	-5.40839900	-1.96915400	2.67511400
C	-3.58250500	-2.94190500	3.28947700
H	-3.81290700	-3.87894500	2.78111000

C	-2.35656200	-2.84353300	3.96939600
C	-2.63229700	0.76645500	5.28724300
H	-1.53834100	0.85314900	5.33951300
C	-3.16906000	0.71544000	6.72293600
H	-2.91705800	1.64141500	7.26039600
H	-2.73972000	-0.13143800	7.27698800
H	-4.26465000	0.60467800	6.72207000
C	-3.14595000	1.99704900	4.54357100
H	-2.75513200	2.91000400	5.01634800
H	-4.24487200	2.06681600	4.55809000
H	-2.81490100	1.99421500	3.49338400
C	-1.48114500	-4.09532500	3.96302400
H	-1.88751300	-4.70131300	3.13876000
C	-1.67289300	-4.91168600	5.24692500
H	-1.16087700	-5.88123400	5.15506300
H	-2.73762700	-5.10070900	5.44576300
H	-1.24468200	-4.38791300	6.11273300
C	0.00696400	-3.90306500	3.65083800
H	0.43015500	-4.86509200	3.32206600
H	0.58127800	-3.56324000	4.52425900
H	0.15904200	-3.17402600	2.83996900

Table S11

Tl=P-TS

G = -3033.15818522 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
O	0.32289400	0.17609700	0.11898900
P	0.05267200	0.21464600	2.89059400
C	1.24895300	0.10722300	0.89359000
O	2.41821100	0.07331600	1.02783600
Tl	-1.79402000	-0.70293900	1.54700300
C	0.30313000	-0.73103100	4.44779600
C	-3.09036400	-0.96948600	-0.20504200
C	-3.73206100	0.18170400	-0.69303200
C	-4.16762200	0.19985100	-2.02484800
H	-4.64695000	1.09978300	-2.41556500
C	-3.99078800	-0.91114900	-2.84486200
H	-4.30866000	-0.87636000	-3.88778900
C	-3.43742500	-2.07764800	-2.32329400
H	-3.33820800	-2.96502500	-2.95131600
C	-2.99959800	-2.12872800	-0.99391900
C	-4.02290500	1.35346400	0.20214400
C	-3.09915400	2.41395700	0.32293800
C	-3.42435600	3.49771300	1.14959300
H	-2.71949000	4.32341100	1.25342700
C	-4.62876400	3.53516500	1.83893500
H	-4.86382100	4.38527600	2.48169500

C	-5.53192500	2.48182300	1.72141500
H	-6.47240200	2.52238900	2.27281100
C	-5.25312500	1.38025800	0.90757500
C	-1.80847500	2.44239100	-0.48251000
H	-1.52578900	1.40783000	-0.72652400
C	-2.03835700	3.17725700	-1.80960300
H	-1.11394300	3.18993700	-2.40521600
H	-2.34377700	4.21847000	-1.62255700
H	-2.82467900	2.69424100	-2.40620400
C	-0.63567800	3.06367400	0.27783200
H	0.29559600	2.89555900	-0.28023700
H	-0.51638200	2.61431600	1.27598300
H	-0.76066900	4.15040900	0.40033800
C	-6.29514600	0.27967200	0.73616600
H	-5.75090700	-0.66404200	0.56835600
C	-7.20853300	0.09119400	1.95025800
H	-7.80221100	-0.82690500	1.82907000
H	-7.92165600	0.92340100	2.04775100
H	-6.65200500	0.01492700	2.89332300
C	-7.17482600	0.54958200	-0.49340500
H	-7.92303800	-0.24859200	-0.61173500
H	-6.58856000	0.60544300	-1.41751500
H	-7.70854300	1.50421500	-0.36816400
C	-2.54602100	-3.43248500	-0.40504100
C	-3.53241300	-4.34906900	0.03328500
C	-3.11528800	-5.55882300	0.59769400
H	-3.85956700	-6.28189400	0.93630500
C	-1.76215700	-5.85803800	0.73530000
H	-1.45610400	-6.80350400	1.18690200
C	-0.80119400	-4.95592200	0.29291200
H	0.25611700	-5.20575400	0.38972100
C	-1.17267000	-3.74008300	-0.29480400
C	-5.02061800	-4.08775600	-0.18155000
H	-5.16063400	-2.99983000	-0.27302100
C	-5.47842000	-4.73758900	-1.49523000
H	-6.53993800	-4.52023700	-1.68558500
H	-5.35608600	-5.83027400	-1.43726800
H	-4.89581700	-4.38036000	-2.35321400
C	-5.92435200	-4.57529100	0.95392800
H	-6.96418000	-4.28417400	0.74481900
H	-5.64884300	-4.14950900	1.92730700
H	-5.91132900	-5.67154500	1.04521100
C	-0.11796400	-2.84332800	-0.92610200
H	-0.49364200	-1.80984600	-0.93773600
C	0.08654500	-3.25804900	-2.38981400
H	0.82428000	-2.60186500	-2.87390900
H	-0.85306800	-3.19733100	-2.95669700
H	0.45293800	-4.29477100	-2.44586500
C	1.21774000	-2.83473000	-0.18540500
H	1.88202300	-2.07533300	-0.62194200

H	1.73425800	-3.80397200	-0.25914800
H	1.10099500	-2.59387500	0.88372700
C	1.58195400	-0.60610900	5.03628300
C	1.80926400	-1.09842600	6.32607600
H	2.80185700	-0.96699700	6.76276800
C	0.79992900	-1.72485300	7.05082800
H	0.98750000	-2.08845200	8.06167100
C	-0.45509700	-1.87352400	6.46741500
H	-1.26507100	-2.35737900	7.01730800
C	-0.70924300	-1.39792600	5.17939200
C	2.71221400	0.09376900	4.34169300
C	2.84864700	1.48943700	4.48296500
C	3.96584500	2.11474900	3.91980800
H	4.08817100	3.19500300	4.02326400
C	4.92587100	1.37702300	3.23713800
H	5.79641200	1.87739200	2.80964700
C	4.76364400	0.00510700	3.07354400
H	5.50002600	-0.55491600	2.49617600
C	3.65224500	-0.65442600	3.60115000
C	1.83043100	2.31990700	5.25181500
H	0.94805700	1.68893300	5.43468800
C	2.39082800	2.73336300	6.61651400
H	1.64678200	3.31011800	7.18651100
H	3.28854900	3.35913900	6.49407300
H	2.67290800	1.85166300	7.21014500
C	1.35514500	3.53537600	4.45203300
H	0.54926800	4.05472700	4.99243700
H	0.96908200	3.22733300	3.46937300
H	2.16759600	4.26067600	4.29336700
C	3.44230200	-2.14154000	3.34916700
H	2.35168200	-2.30290900	3.32606200
C	4.00290700	-2.60549300	2.00283000
H	3.64856500	-3.62436200	1.78387400
H	5.10326300	-2.64204700	2.01722400
H	3.68622100	-1.93717400	1.19158000
C	4.02661600	-3.00254000	4.47571400
H	3.85753400	-4.07074900	4.26963700
H	3.57665000	-2.76877000	5.44898600
H	5.11271200	-2.83707500	4.55182600
C	-2.06055100	-1.59737500	4.58478100
C	-2.96951500	-0.51441600	4.57842700
C	-4.19343000	-0.65862600	3.91532500
H	-4.88302800	0.18604000	3.88565600
C	-4.52697800	-1.85525900	3.28100100
H	-5.48039200	-1.95357900	2.75722600
C	-3.63032900	-2.91796900	3.30774700
H	-3.87125300	-3.85613500	2.80593600
C	-2.38367700	-2.81475700	3.94608600
C	-2.64166200	0.78625700	5.29432200
H	-1.54761500	0.86050000	5.36296100

C	-3.19673600	0.74290600	6.72314700
H	-2.94039500	1.66562600	7.26422000
H	-2.78508600	-0.10968900	7.28207600
H	-4.29346900	0.64506500	6.70876100
C	-3.13097100	2.02251500	4.54279500
H	-2.73922700	2.93206400	5.02163700
H	-4.22921600	2.10190900	4.53921000
H	-2.78395500	2.01686600	3.49784400
C	-1.50223300	-4.06149300	3.90334000
H	-1.91038900	-4.64690300	3.06552100
C	-1.68255900	-4.91375400	5.16549400
H	-1.16607900	-5.87784400	5.04493000
H	-2.74525300	-5.11369700	5.36438500
H	-1.25301600	-4.41169800	6.04362100
C	-0.01671000	-3.85617900	3.58857400
H	0.40639700	-4.80536200	3.22430900
H	0.56333000	-3.54489800	4.46878100
H	0.13028300	-3.10114000	2.80064500

Table S12

B=P-Prod

G = -2885.62192872 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
B	2.82304100	-0.21843300	1.62129600
P	1.77921000	0.92319700	2.90369100
C	3.88894800	-0.21623600	0.46738700
C	4.66944100	0.93838100	0.23444400
C	5.85509800	0.84451500	-0.51002300
H	6.44373000	1.75122300	-0.66649100
C	6.27571800	-0.36618600	-1.04158000
H	7.20364800	-0.42443800	-1.61251900
C	5.48931400	-1.50065800	-0.85984000
H	5.77975600	-2.45093300	-1.31258500
C	4.30579200	-1.44267400	-0.12191300
C	4.32554100	2.31376700	0.72604600
C	4.66267900	2.71175000	2.03608700
C	4.47674500	4.05097600	2.39419800
H	4.75514000	4.38253900	3.39466900
C	3.96946800	4.97322700	1.48658900
H	3.83904600	6.01544800	1.78396300
C	3.63453600	4.56949100	0.19773100
H	3.23928400	5.30414200	-0.50384100
C	3.80176400	3.24145700	-0.20445800
C	5.29752000	1.74410300	3.02690200
H	4.94016900	0.72909500	2.78967600
C	6.82253700	1.73585100	2.85651400
H	7.28516200	1.02327700	3.55533600

H	7.23023100	2.73701300	3.06485700
H	7.11300600	1.45416600	1.83506100
C	4.92465800	2.02938600	4.48340400
H	5.27644700	1.21043300	5.12781700
H	3.83651400	2.12081800	4.61532700
H	5.39887400	2.95338400	4.84941200
C	3.39865400	2.79147100	-1.60418500
H	4.17587000	2.10248200	-1.96752100
C	2.07486100	2.02008100	-1.55834700
H	1.79564600	1.65769900	-2.55978800
H	1.26900400	2.67322300	-1.19856100
H	2.12254600	1.15202000	-0.88428200
C	3.29823800	3.93471900	-2.61247600
H	3.13525700	3.52807200	-3.62057100
H	4.21165000	4.54655900	-2.63134700
H	2.44666500	4.59528900	-2.38744500
C	3.44971000	-2.67514500	-0.11372900
C	2.58296700	-2.87147200	-1.20999500
C	1.76209300	-4.00494700	-1.22525500
H	1.08491100	-4.16915700	-2.06657000
C	1.80792200	-4.93121700	-0.18973200
H	1.15669400	-5.80684900	-0.20934700
C	2.70367500	-4.75345300	0.86117800
H	2.75687000	-5.50229100	1.65283000
C	3.54900800	-3.64073900	0.90990500
C	2.56681800	-1.93118800	-2.40918300
H	3.18310400	-1.05272200	-2.17211200
C	3.19290000	-2.61666100	-3.62812500
H	3.22329000	-1.92882600	-4.48625300
H	2.60950300	-3.50299300	-3.92166800
H	4.21940300	-2.94735700	-3.41363000
C	1.16604700	-1.41063100	-2.71600000
H	1.18671200	-0.72001800	-3.57314800
H	0.76813000	-0.86035400	-1.85372200
H	0.46737800	-2.22635800	-2.96147600
C	4.62510600	-3.55257100	1.98084700
H	4.93116600	-2.50081000	2.06064200
C	5.85030300	-4.36370200	1.53903700
H	6.65208600	-4.29248700	2.28926200
H	6.24543800	-4.00199800	0.57884300
H	5.58711100	-5.42587600	1.41732200
C	4.14749100	-4.00365800	3.36155400
H	4.92173400	-3.78882900	4.11291300
H	3.96409900	-5.08868700	3.39094400
H	3.22604300	-3.48442300	3.65784900
C	-0.06337300	0.95405300	3.18625100
C	-0.38712200	1.06154600	4.56934700
C	-1.72861100	0.98880900	4.96118600
H	-1.96079000	1.09769900	6.02021900
C	-2.75208900	0.83561900	4.03656200

H	-3.79143300	0.78363500	4.36308900
C	-2.43423800	0.81208500	2.68703100
H	-3.22537300	0.77057500	1.93621200
C	-1.10586100	0.88411000	2.24132900
C	0.60103700	1.35061100	5.67278600
C	1.19384400	2.64041500	5.74271600
C	2.06741100	2.92439300	6.79486400
H	2.53926500	3.90418100	6.85658300
C	2.34741300	1.97865900	7.77619300
H	3.03891600	2.21776800	8.58578000
C	1.72538700	0.74123200	7.73068500
H	1.92389100	0.01237200	8.51791000
C	0.83565000	0.40644100	6.70073700
C	0.84681900	3.74353400	4.74662900
H	0.81846100	3.29741800	3.74299100
C	-0.54024500	4.33531700	5.02970100
H	-0.77734500	5.11455700	4.28794600
H	-0.56079800	4.79735800	6.02881000
H	-1.33070300	3.57416200	4.98730400
C	1.88312400	4.86507200	4.70151500
H	1.68441100	5.52768400	3.84666100
H	2.89932900	4.46472400	4.59013800
H	1.84824700	5.48401800	5.61105700
C	0.11975900	-0.93593800	6.80627500
H	-0.31792900	-1.16894400	5.82748600
C	1.06167100	-2.08708100	7.18296900
H	0.55078000	-3.04880000	7.02862900
H	1.34656100	-2.03896800	8.24522700
H	1.97132300	-2.08449300	6.57274600
C	-1.00298000	-0.86601200	7.85270600
H	-1.52254500	-1.83383400	7.91838000
H	-1.75039600	-0.09427700	7.62815400
H	-0.58401900	-0.63954800	8.84551000
C	-1.00436400	1.10122700	0.75872800
C	-1.06581300	2.44982400	0.33005000
C	-1.28616400	2.72582300	-1.02214100
H	-1.33140100	3.76305200	-1.35945600
C	-1.46236000	1.69868200	-1.94090900
H	-1.65240200	1.92519100	-2.99125300
C	-1.39608300	0.37919500	-1.51189000
H	-1.53497000	-0.42960300	-2.23270000
C	-1.16058100	0.04913200	-0.17030900
C	-0.89837200	3.61521400	1.29729400
H	-1.03363400	3.24020100	2.32116300
C	-1.94155000	4.71566100	1.09125900
H	-1.85112700	5.47212400	1.88469600
H	-2.96174900	4.30681600	1.12110800
H	-1.80858800	5.23412800	0.13005900
C	0.52199100	4.17655300	1.19588800
H	0.67791900	4.99226700	1.91889000

H	0.71279400	4.57823600	0.18728500
H	1.28576800	3.40433500	1.38657600
C	-1.13363800	-1.43689300	0.18059800
H	-1.00777300	-1.95124600	-0.78624100
C	-2.45436800	-1.94732100	0.77181400
H	-2.45271600	-3.04729900	0.78726600
H	-3.31486400	-1.61301000	0.17394800
H	-2.59132300	-1.60094400	1.80509700
C	0.05195700	-1.85548900	1.04775100
H	0.12334200	-2.95209000	1.10010500
H	-0.03943500	-1.47712400	2.07503400
H	0.99543500	-1.50013600	0.60392600
C	2.05666800	-0.81161800	3.52138500
O	2.98229700	-1.21193900	2.57270300
O	1.61636700	-1.53573800	4.34656400

Table S13

Al=P-Prod

G = -3103.24348082 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Al	2.69346300	-0.01876500	1.37877500
P	1.58669900	1.28970000	2.98183100
C	4.07292800	-0.32052600	0.02161900
C	4.96916200	0.76315000	-0.08938100
C	6.15737700	0.63682600	-0.81540400
H	6.82770800	1.49475900	-0.90257100
C	6.47626500	-0.57632800	-1.42010600
H	7.40254400	-0.67820100	-1.98777500
C	5.61657300	-1.66433600	-1.29007700
H	5.86725200	-2.62070100	-1.75517800
C	4.42017700	-1.55274900	-0.57027300
C	4.63199500	2.05673200	0.58988300
C	4.98737300	2.26092400	1.94450300
C	4.63757200	3.47371900	2.54765800
H	4.89640300	3.64787800	3.59300000
C	3.95011100	4.45508500	1.84167700
H	3.68110300	5.39170900	2.33278600
C	3.58607000	4.23472500	0.51761500
H	3.02530100	5.00139300	-0.02190800
C	3.91767300	3.03959500	-0.12687500
C	5.76088500	1.21387800	2.73539100
H	5.50617900	0.22384400	2.32698500
C	7.27032300	1.41345800	2.54962800
H	7.83060500	0.65380700	3.11459200
H	7.57059000	2.40706500	2.91645800
H	7.55899300	1.33761100	1.49216700
C	5.39823000	1.20007900	4.22244000

H	5.78166600	0.28406800	4.69322300
H	4.31018500	1.23561800	4.38022100
H	5.84331300	2.05535700	4.75368300
C	3.45444300	2.80541100	-1.55553600
H	3.90608600	1.86993400	-1.91361200
C	1.93555600	2.62995400	-1.58570300
H	1.58000700	2.38840700	-2.59880700
H	1.42823800	3.54992800	-1.25669500
H	1.59725600	1.82333400	-0.91154400
C	3.90180800	3.92286400	-2.50066800
H	3.59897300	3.69385800	-3.53290900
H	4.99407800	4.04614600	-2.48076400
H	3.44692300	4.88704200	-2.22780100
C	3.52685100	-2.75067500	-0.44459400
C	2.65791200	-3.07367600	-1.50879500
C	1.77833000	-4.15169900	-1.35825400
H	1.09059200	-4.40600200	-2.16673600
C	1.77819300	-4.91414200	-0.19433700
H	1.08818300	-5.75347500	-0.09133400
C	2.66987800	-4.61640800	0.83179300
H	2.67723900	-5.23305900	1.73099400
C	3.55951500	-3.54047200	0.72852400
C	2.63347700	-2.24765100	-2.78748800
H	3.59466000	-1.72270500	-2.86725300
C	2.47203100	-3.09889700	-4.04818400
H	2.59675400	-2.47247400	-4.94326700
H	1.47251800	-3.55498000	-4.10817000
H	3.21706200	-3.90635800	-4.08543900
C	1.53374300	-1.18923600	-2.70326800
H	1.51737900	-0.55093700	-3.60030300
H	1.66489600	-0.53403900	-1.82732200
H	0.55399600	-1.68275400	-2.61605000
C	4.60738000	-3.31411400	1.80974800
H	4.83359000	-2.23939200	1.84326900
C	5.89757800	-4.05353400	1.42903000
H	6.67495600	-3.88409600	2.18883700
H	6.28656400	-3.71404100	0.45879800
H	5.71246200	-5.13686000	1.36205000
C	4.14895500	-3.72340300	3.20913800
H	4.88973800	-3.38744400	3.94894800
H	4.06561700	-4.81705600	3.30536700
H	3.18958100	-3.25894800	3.47303500
C	-0.21573800	1.06888600	3.34201500
C	-0.59744800	1.17224700	4.70934600
C	-1.94844600	1.04491400	5.04797200
H	-2.23246900	1.16066800	6.09399100
C	-2.92492200	0.81156400	4.08535500
H	-3.97211800	0.71212200	4.37397300
C	-2.55510400	0.76236800	2.74964400
H	-3.31201300	0.64664300	1.97111400

C	-1.21480700	0.91009900	2.36183600
C	0.35264400	1.50919900	5.82886700
C	0.91399700	2.80885600	5.88777300
C	1.78041600	3.12596700	6.93745800
H	2.22655200	4.11912100	6.98826800
C	2.07253000	2.19949800	7.93205900
H	2.75329900	2.46248100	8.74347700
C	1.47946200	0.94538900	7.89642600
H	1.69421300	0.22891900	8.69073900
C	0.61214300	0.57701000	6.86154300
C	0.52073100	3.90269900	4.90183400
H	0.30253500	3.43392100	3.93462600
C	-0.76523400	4.59694400	5.36584800
H	-1.07578600	5.36382300	4.63830800
H	-0.61010500	5.08832400	6.33880200
H	-1.58732000	3.87451200	5.47589000
C	1.63603100	4.91637600	4.65227200
H	1.36436700	5.57938000	3.81782800
H	2.57245400	4.40165100	4.39214600
H	1.81600500	5.55619600	5.52919100
C	-0.04861000	-0.79424600	6.94121000
H	-0.44713100	-1.03240400	5.94609300
C	0.92714000	-1.91242900	7.32667700
H	0.43255900	-2.88840500	7.20965800
H	1.23367900	-1.83269900	8.38100700
H	1.81796100	-1.89863700	6.68984200
C	-1.20174800	-0.77693400	7.95570300
H	-1.69472600	-1.76021400	7.99267000
H	-1.96418600	-0.02229600	7.72260100
H	-0.81664700	-0.55427200	8.96313500
C	-1.02731100	1.13218200	0.88739500
C	-1.15361700	2.47152200	0.44793200
C	-1.24762400	2.73800300	-0.92191600
H	-1.34780200	3.77166600	-1.26089900
C	-1.24200400	1.70837700	-1.85198400
H	-1.34370100	1.92370600	-2.91691500
C	-1.10363200	0.39597400	-1.41476900
H	-1.10876500	-0.41382500	-2.14495800
C	-0.97956300	0.07953400	-0.05613400
C	-1.23802500	3.64648000	1.41498600
H	-1.27359500	3.25473800	2.43984700
C	-2.52031300	4.45819900	1.21121100
H	-2.59249000	5.25049000	1.97091300
H	-3.40935900	3.81706100	1.29874500
H	-2.54436200	4.94078500	0.22237600
C	0.00816600	4.52940200	1.30878500
H	-0.05189600	5.36284300	2.02553600
H	0.10406400	4.96138200	0.29883800
H	0.92435700	3.95586500	1.52355000
C	-0.82666800	-1.39812200	0.29585400

H	-0.73788100	-1.91761700	-0.67145600
C	-2.03100000	-2.01832500	1.01515300
H	-1.93902300	-3.11450400	1.01039700
H	-2.96988300	-1.75047100	0.50987500
H	-2.09262200	-1.69003900	2.06084400
C	0.45767100	-1.71004400	1.06448600
H	0.62204100	-2.79318400	1.15728300
H	0.43951300	-1.27963000	2.07550300
H	1.32539100	-1.35417900	0.45925700
C	2.18603700	-0.37218600	3.69778000
O	3.16293100	-0.82297900	2.90161700
O	1.72691800	-0.98643200	4.61479700

Table S14

Ga=P-Prod

G = -4785.65246106 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
Ga	2.69612800	0.09202400	1.33840700
P	1.55324800	1.24331700	3.04154600
C	4.11551700	-0.25693800	0.00582400
C	5.00254400	0.82740600	-0.13347300
C	6.18707100	0.67734000	-0.86111400
H	6.85862300	1.53126700	-0.97374800
C	6.50019600	-0.55252000	-1.43454900
H	7.42287300	-0.67063600	-2.00475600
C	5.63954300	-1.63547600	-1.27295400
H	5.88336000	-2.60229100	-1.71927000
C	4.44673600	-1.50630400	-0.54958600
C	4.66413500	2.13452000	0.51768900
C	4.98250600	2.34689100	1.88039900
C	4.62209300	3.56642300	2.46391100
H	4.85429300	3.74791200	3.51403500
C	3.96167100	4.54638200	1.73087200
H	3.68196500	5.48705000	2.20845100
C	3.63980800	4.32045400	0.39656400
H	3.10070500	5.08689300	-0.16433800
C	3.98101200	3.11811600	-0.22924900
C	5.73556700	1.30575300	2.69910100
H	5.47567300	0.30989400	2.30868200
C	7.24862400	1.48695700	2.52264600
H	7.79597600	0.73128500	3.10519000
H	7.55605700	2.48356900	2.87501400
H	7.54532900	1.38992100	1.46904600
C	5.35994200	1.32196000	4.18264600
H	5.73124300	0.41083100	4.67190600
H	4.27067500	1.36652100	4.33021400
H	5.80719400	2.18303100	4.70270000

C	3.54606200	2.86673700	-1.66429300
H	4.05309900	1.95977900	-2.02143000
C	2.03856300	2.60602400	-1.70477800
H	1.70073800	2.35532400	-2.72195100
H	1.48224300	3.49403600	-1.36796600
H	1.74279600	1.77523600	-1.04122800
C	3.93293100	4.00997500	-2.60484400
H	3.66613700	3.75618600	-3.64109200
H	5.01323400	4.20978400	-2.56573300
H	3.40597400	4.94109500	-2.34785800
C	3.53776700	-2.68815800	-0.40361600
C	2.65427300	-3.00058800	-1.45700100
C	1.75556900	-4.06113400	-1.29143300
H	1.05374800	-4.30429600	-2.09199900
C	1.75082600	-4.81327400	-0.12249900
H	1.04328900	-5.63606900	-0.00504700
C	2.65720100	-4.52543100	0.89433000
H	2.65774300	-5.13367400	1.79914800
C	3.56850800	-3.47110900	0.77501000
C	2.62771400	-2.19254000	-2.74616800
H	3.52960100	-1.56724500	-2.77643600
C	2.64473700	-3.07819200	-3.99385400
H	2.71910300	-2.45718300	-4.89851900
H	1.72527700	-3.67615500	-4.08101600
H	3.49842900	-3.77076400	-3.97956700
C	1.42082600	-1.25637800	-2.74636000
H	1.40272100	-0.61877700	-3.64398700
H	1.42608200	-0.59899200	-1.86316700
H	0.48848200	-1.84218800	-2.72339800
C	4.63349300	-3.25808800	1.84145400
H	4.86273500	-2.18402200	1.88020100
C	5.91446500	-4.00156300	1.43756600
H	6.70229800	-3.84285800	2.18890600
H	6.29444200	-3.65792600	0.46537000
H	5.72185600	-5.08318800	1.36492600
C	4.19500300	-3.67809200	3.24384800
H	4.94631000	-3.34758500	3.97547000
H	4.11462600	-4.77281100	3.33146300
H	3.23907700	-3.21681700	3.52457900
C	-0.25163400	1.03234300	3.37328900
C	-0.63155200	1.15505600	4.73882500
C	-1.98648900	1.07549800	5.07506700
H	-2.26942700	1.21010100	6.11915900
C	-2.96649100	0.86918000	4.10992400
H	-4.01778200	0.81072300	4.39479200
C	-2.59405000	0.79119100	2.77588500
H	-3.35187300	0.69068600	1.99640700
C	-1.24918200	0.88919200	2.39001500
C	0.33315000	1.46499500	5.85342000
C	0.91605200	2.75445600	5.91890200

C	1.80083500	3.04543700	6.96099000
H	2.26287300	4.03115100	7.01787800
C	2.09020300	2.10187800	7.94007200
H	2.78528300	2.34393500	8.74584400
C	1.47802600	0.85669600	7.89683700
H	1.69388600	0.12685100	8.67839100
C	0.59220600	0.51442800	6.86907500
C	0.52704300	3.86535900	4.95047400
H	0.24904400	3.40797700	3.99290300
C	-0.71045700	4.60676900	5.46989000
H	-1.02453000	5.38487500	4.75623900
H	-0.49462800	5.09061700	6.43498700
H	-1.55244500	3.91448600	5.61686500
C	1.67024300	4.83466200	4.65456900
H	1.38172000	5.52343000	3.84708400
H	2.56734500	4.28532600	4.33317600
H	1.92639800	5.45104200	5.52920000
C	-0.08843300	-0.84765800	6.93231300
H	-0.47505600	-1.07396900	5.92939300
C	0.86461900	-1.98206300	7.32641200
H	0.35943200	-2.94985900	7.18931800
H	1.14949200	-1.91710700	8.38786000
H	1.76827600	-1.97385200	6.70785300
C	-1.25660900	-0.81950400	7.92917100
H	-1.75763700	-1.79889000	7.95946900
H	-2.00964900	-0.05992800	7.68321700
H	-0.88419100	-0.59888500	8.94182300
C	-1.03967800	1.06812400	0.91409500
C	-1.08962300	2.40033600	0.43963000
C	-1.14477200	2.63546600	-0.93797800
H	-1.18606300	3.66369900	-1.30496300
C	-1.17873100	1.58192700	-1.84054200
H	-1.25072100	1.77334700	-2.91255000
C	-1.12433000	0.27613400	-1.36636900
H	-1.16641800	-0.55196800	-2.07446200
C	-1.03585100	-0.01278500	0.00118100
C	-1.14366400	3.60216100	1.37546700
H	-1.20266200	3.23780800	2.40926200
C	-2.39940800	4.44558000	1.13667500
H	-2.45497500	5.26154300	1.87240700
H	-3.30783700	3.83362900	1.23331300
H	-2.39962700	4.89866100	0.13365900
C	0.12826000	4.44588500	1.26137400
H	0.08603600	5.29846100	1.95658600
H	0.24678900	4.85036800	0.24255200
H	1.02639600	3.85351200	1.49927900
C	-0.98924500	-1.48812500	0.39409600
H	-0.88720400	-2.03254900	-0.55910300
C	-2.27686300	-2.00187800	1.05237600
H	-2.27549900	-3.10189800	1.05507500

H	-3.16691800	-1.66167200	0.50344500
H	-2.35987000	-1.66586200	2.09429400
C	0.22800500	-1.87368600	1.23530100
H	0.22842500	-2.95335700	1.44117000
H	0.24662300	-1.35283200	2.20301100
H	1.16320600	-1.69073800	0.66741700
C	2.20477600	-0.41997700	3.72886600
O	3.20119000	-0.79923000	2.94595100
O	1.75579000	-1.04570100	4.64407600

Table S15

In=P-Prod

G = -3050.86723299 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
In	2.41957000	0.33147200	1.20219700
P	1.46089000	1.33327500	3.32078700
C	3.98565000	-0.18922400	-0.21959500
C	4.94479300	0.83948800	-0.30145100
C	6.15273200	0.61277900	-0.96819800
H	6.89986700	1.40693700	-1.02279800
C	6.40372800	-0.62668800	-1.55303500
H	7.34905100	-0.80574800	-2.06717600
C	5.45097800	-1.63894900	-1.47887000
H	5.65050800	-2.61007600	-1.93830900
C	4.23326500	-1.43931400	-0.81197000
C	4.60554900	2.16415800	0.32239900
C	4.85041300	2.38599100	1.69953700
C	4.38009500	3.57363500	2.27668700
H	4.54142100	3.75414400	3.33965100
C	3.69098500	4.51479000	1.52223400
H	3.31610100	5.42334900	1.99710300
C	3.46922200	4.29616900	0.16483700
H	2.93006100	5.04592600	-0.41563400
C	3.92068500	3.12908900	-0.45782800
C	5.63943500	1.38885400	2.53973600
H	5.37340800	0.37477500	2.20278500
C	7.14445400	1.58191800	2.30892500
H	7.71667900	0.86416900	2.91480100
H	7.44663500	2.59865300	2.60353000
H	7.41792200	1.43466800	1.25588800
C	5.32572900	1.47056000	4.03462600
H	5.71883400	0.58089100	4.54492800
H	4.24524300	1.51780400	4.22994700
H	5.79498200	2.35466600	4.49378700
C	3.73062800	2.93007900	-1.95552100
H	3.62335200	1.84872400	-2.13522800
C	2.48836700	3.62137000	-2.51621700

H	2.31145900	3.29285900	-3.55086900
H	2.60814200	4.71511200	-2.53933100
H	1.59666900	3.38765100	-1.92057600
C	4.97447300	3.41123000	-2.71466700
H	4.85210300	3.25178600	-3.79630000
H	5.87875300	2.88137800	-2.39040200
H	5.12931200	4.48703200	-2.53986100
C	3.21842600	-2.54303700	-0.75203100
C	2.44478200	-2.84438000	-1.89957000
C	1.43536400	-3.80659500	-1.79046400
H	0.81948200	-4.04727400	-2.65741400
C	1.21409800	-4.48049500	-0.59172400
H	0.41547600	-5.22145500	-0.52310400
C	2.03575000	-4.23971900	0.50329300
H	1.89004400	-4.80967300	1.42131200
C	3.06207100	-3.28812700	0.44119700
C	2.71963200	-2.16514500	-3.23957600
H	3.80749600	-2.02710500	-3.30752200
C	2.29948600	-3.00694400	-4.44447000
H	2.66877000	-2.54195100	-5.36971900
H	1.20458000	-3.07518900	-4.53090700
H	2.70244500	-4.02804200	-4.38705500
C	2.08996600	-0.77289600	-3.32387500
H	2.41462100	-0.25554800	-4.23963700
H	2.37298400	-0.15578400	-2.45897600
H	0.99144900	-0.85194200	-3.35207400
C	4.08475400	-3.19440900	1.56830200
H	4.39801900	-2.14671000	1.67046600
C	5.31939600	-4.02281400	1.18042400
H	6.08231700	-3.95933000	1.97025300
H	5.76897100	-3.67238700	0.24149600
H	5.04332700	-5.08109000	1.05299800
C	3.57295500	-3.64739100	2.93469500
H	4.33198000	-3.42008700	3.69588300
H	3.39382500	-4.73396700	2.95840900
H	2.66099300	-3.11989700	3.24182000
C	-0.31925900	1.01942000	3.71856400
C	-0.69992600	1.18376500	5.07256500
C	-2.05287200	1.07304700	5.41609400
H	-2.34143400	1.24485800	6.45376700
C	-3.02545500	0.79070300	4.46208500
H	-4.07455300	0.71946700	4.75208900
C	-2.65291200	0.63808800	3.13057500
H	-3.40694900	0.46195200	2.36093400
C	-1.31283900	0.75478600	2.75320800
C	0.28067700	1.55452000	6.14993700
C	0.78549600	2.87540200	6.19214200
C	1.68193000	3.22333600	7.20629400
H	2.07685800	4.23913800	7.25296900
C	2.06964200	2.29641700	8.16723300

H	2.77312100	2.58250400	8.95102600
C	1.55367800	1.00718700	8.13045100
H	1.85835600	0.28685100	8.89075800
C	0.65496700	0.61108600	7.13405100
C	0.31421000	3.95371800	5.22363600
H	-0.08821300	3.46183100	4.32739900
C	-0.83235500	4.75456500	5.85174000
H	-1.21172900	5.51170100	5.14792700
H	-0.49097100	5.27080100	6.76230700
H	-1.66583400	4.09312300	6.13029600
C	1.44420600	4.87153900	4.75527700
H	1.07369200	5.56573600	3.98628300
H	2.26431900	4.27953400	4.32112000
H	1.84656900	5.48270600	5.57677800
C	0.08270100	-0.79983200	7.18207900
H	-0.27517100	-1.04452100	6.17219800
C	1.12078800	-1.85815600	7.56851000
H	0.69407600	-2.86133700	7.41967300
H	1.39799100	-1.78163300	8.63139200
H	2.01923800	-1.77122100	6.94797800
C	-1.09512800	-0.87213600	8.16421500
H	-1.50944200	-1.89137600	8.19107400
H	-1.90729400	-0.18236100	7.90146100
H	-0.75706800	-0.61662200	9.18078400
C	-0.94341400	0.77584600	1.30665000
C	-0.85631200	2.04358400	0.69754300
C	-0.37119300	2.13759100	-0.61221300
H	-0.32222600	3.11651600	-1.09288200
C	0.05602600	1.01088700	-1.29924500
H	0.45797500	1.10543100	-2.30869100
C	-0.05584300	-0.24611900	-0.69822400
H	0.25455100	-1.14270600	-1.24144300
C	-0.58216100	-0.39497300	0.59462300
C	-1.25571400	3.32954200	1.40811000
H	-1.54795200	3.08251600	2.43757700
C	-2.47475300	3.96175100	0.72847500
H	-2.78688900	4.86769600	1.26817000
H	-3.32285400	3.26234300	0.70879900
H	-2.24808300	4.24920100	-0.30998000
C	-0.08634100	4.31591200	1.48820800
H	-0.38873300	5.21530100	2.04623700
H	0.24062200	4.63715100	0.48607200
H	0.78210500	3.86978800	1.99864800
C	-0.75272900	-1.82150100	1.11088900
H	-0.33352100	-2.45715900	0.31475400
C	-2.23005300	-2.20754400	1.25150900
H	-2.31576100	-3.29625500	1.38364200
H	-2.80577300	-1.92374400	0.35868200
H	-2.68527000	-1.73048000	2.12964000
C	0.02666000	-2.16375700	2.38144000

H	-0.10474500	-3.23180600	2.61261500
H	-0.29825500	-1.58796800	3.25834400
H	1.10977100	-2.01466700	2.24888300
C	2.27775700	-0.32576700	3.86975300
O	3.20275500	-0.64198600	3.01847500
O	1.91947300	-0.94757400	4.83550100

Table S16

TI=P-Prod

G = -3033.16467902 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
TI	2.38964800	0.39527800	1.18514400
P	1.43479100	1.26232900	3.35291200
C	4.06575100	-0.13329000	-0.14061900
C	5.00923800	0.90811100	-0.19160100
C	6.23900200	0.68196600	-0.81685500
H	6.97626400	1.48598800	-0.86176800
C	6.52028200	-0.56308500	-1.37639900
H	7.48308000	-0.73923800	-1.85792200
C	5.57448600	-1.58230600	-1.32413900
H	5.79404100	-2.55534200	-1.77000300
C	4.32915600	-1.38794800	-0.70573700
C	4.63967300	2.24490800	0.38496400
C	4.84955100	2.51412100	1.75829900
C	4.36489800	3.72075600	2.27936200
H	4.50286300	3.94075800	3.33815700
C	3.69352400	4.63367700	1.47423500
H	3.30883800	5.55936900	1.90633300
C	3.50101000	4.36369700	0.12227400
H	2.97318100	5.08894300	-0.49865400
C	3.96691300	3.17353500	-0.44484600
C	5.60557600	1.54106600	2.65402600
H	5.34464500	0.51833200	2.34003700
C	7.11867300	1.72235900	2.47213700
H	7.66546700	1.02010800	3.11824400
H	7.41507700	2.74602700	2.74832500
H	7.42993900	1.54440900	1.43432100
C	5.23839000	1.66564700	4.13348200
H	5.61949700	0.79425400	4.68266800
H	4.15062700	1.70309600	4.28624300
H	5.68242100	2.56787200	4.58270800
C	3.80097500	2.91612200	-1.93630600
H	3.77186000	1.82611900	-2.08630600
C	2.50972600	3.49314200	-2.51546700
H	2.36632700	3.13344800	-3.54507400
H	2.53541400	4.59257500	-2.55645100
H	1.63816000	3.19139200	-1.91895300

C	5.01504900	3.45808100	-2.70142000
H	4.91626000	3.25587300	-3.77830800
H	5.94915200	3.00007500	-2.35004300
H	5.09711400	4.54682900	-2.56052000
C	3.31783400	-2.49525400	-0.69154600
C	2.58829100	-2.77953800	-1.87115800
C	1.59446100	-3.76226400	-1.81988900
H	1.01277500	-3.99239300	-2.71323000
C	1.34758700	-4.46986000	-0.64589600
H	0.56325300	-5.22868300	-0.62253200
C	2.12357300	-4.23734400	0.48384900
H	1.95501900	-4.82868500	1.38428700
C	3.13102600	-3.26430900	0.48087800
C	2.88966900	-2.05648400	-3.18126400
H	3.96803500	-1.84792500	-3.19137500
C	2.58520800	-2.89755300	-4.42129300
H	2.97201600	-2.39254100	-5.31803900
H	1.50275100	-3.03131600	-4.56693400
H	3.04728700	-3.89303500	-4.35930900
C	2.17342400	-0.70717600	-3.26864900
H	2.51344800	-0.14244300	-4.15040000
H	2.35695700	-0.09583900	-2.37258800
H	1.08701900	-0.86162100	-3.36399500
C	4.09676900	-3.15781600	1.65518000
H	4.37899100	-2.10372500	1.78125600
C	5.36769400	-3.95557700	1.32509900
H	6.08829400	-3.87924700	2.15251200
H	5.85628600	-3.59026400	0.41169300
H	5.12258800	-5.01911000	1.17916700
C	3.53006500	-3.62984500	2.99323600
H	4.24336500	-3.38317700	3.79127000
H	3.37800800	-4.72092300	3.00440800
H	2.58977100	-3.12963800	3.25836300
C	-0.35668800	0.94406800	3.66335500
C	-0.76245700	1.11848900	5.00966100
C	-2.11963800	1.00485800	5.33085900
H	-2.42705300	1.18146700	6.36223100
C	-3.07260800	0.71041300	4.36095400
H	-4.12649200	0.63430000	4.63154300
C	-2.67422800	0.55320800	3.03777800
H	-3.41313600	0.36917400	2.25542000
C	-1.32862100	0.67433900	2.67902800
C	0.20563300	1.50364300	6.09412600
C	0.72072900	2.82221000	6.11653700
C	1.62593500	3.17594300	7.12119200
H	2.03159100	4.18789000	7.15111700
C	2.00810200	2.25957900	8.09418000
H	2.71937300	2.54971200	8.86937300
C	1.47451500	0.97694800	8.08288300
H	1.77152000	0.26683000	8.85566400

C	0.56823900	0.57408500	7.09641400
C	0.24636500	3.89345300	5.14097000
H	-0.13901600	3.39668800	4.24003800
C	-0.91954100	4.67619500	5.75644200
H	-1.30204000	5.42767800	5.04835900
H	-0.59605100	5.19685100	6.67096900
H	-1.74605900	4.00201000	6.02487200
C	1.36628900	4.82908400	4.68460100
H	0.99426500	5.51159500	3.90624100
H	2.20413400	4.25169600	4.26481500
H	1.74460100	5.45259900	5.50824400
C	-0.02968000	-0.82416300	7.17830100
H	-0.39904700	-1.08384400	6.17666000
C	0.98852400	-1.89467200	7.58328700
H	0.53810500	-2.89137000	7.46386600
H	1.27684700	-1.79755100	8.64154900
H	1.88207500	-1.84346500	6.95176600
C	-1.20190400	-0.84732700	8.16981700
H	-1.64376700	-1.85412800	8.21686800
H	-1.99665200	-0.13922000	7.90210500
H	-0.84944500	-0.58420300	9.17953100
C	-0.96362200	0.69223600	1.23055800
C	-0.88906200	1.95883900	0.61352300
C	-0.48139500	2.04075500	-0.72266500
H	-0.44319600	3.01660800	-1.21128300
C	-0.12498500	0.90234400	-1.43220900
H	0.20788400	0.98730400	-2.46730800
C	-0.20880100	-0.34728000	-0.81781500
H	0.06711700	-1.24909600	-1.37076700
C	-0.64719100	-0.48388200	0.50779100
C	-1.23826400	3.25256000	1.33718100
H	-1.49766300	3.01203700	2.37696000
C	-2.47041500	3.90834000	0.70508600
H	-2.74910700	4.81531800	1.26123800
H	-3.32936900	3.22201900	0.71195200
H	-2.27710900	4.19916900	-0.33903500
C	-0.04823900	4.21671500	1.37164800
H	-0.32038500	5.13489800	1.91452500
H	0.26457300	4.50820600	0.35595700
H	0.82200300	3.76669700	1.87624200
C	-0.76708500	-1.90526000	1.05149900
H	-0.35447200	-2.54301700	0.25361600
C	-2.22747200	-2.33140400	1.24593700
H	-2.27737600	-3.41939200	1.40086900
H	-2.83857900	-2.08156400	0.36650400
H	-2.66965900	-1.85089900	2.12891700
C	0.06002100	-2.20324000	2.30248300
H	-0.01312000	-3.27504500	2.54212700
H	-0.26822600	-1.64168400	3.18690200
H	1.13121300	-2.00291800	2.14108700

C	2.28844400	-0.40416300	3.94551400
O	3.30459200	-0.61771300	3.22150000
O	1.79605600	-1.04638100	4.84068100
