

Supporting Information

Influence of the Effect of Group 15 Element on the Reactivity of [3 + 2] Cycloaddition Reactions of G15=G15– G15-based 1,3-Dipoles with Clclocyene

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(All were calculated at the M06-2X-D3/Def2-TZVP level of theory.)

NNP-Rea

G = -1183.715135 Hartree

P	3.72146000	8.97549200	6.38099100
N	2.57980600	8.52871600	5.10128200
N	2.44127600	7.32444300	4.87326500
C	1.45208600	6.99417200	3.89996800
C	0.57015700	7.92582500	3.33584200
H	0.63051200	8.96663900	3.65452000
C	-0.35771600	7.50243400	2.39629000
H	-1.04992600	8.22562300	1.95811100
C	-0.43000100	6.15713700	1.99509600
C	-1.44739300	5.72602000	0.97272200
H	-1.30945500	6.27183700	0.02767700
H	-2.46878900	5.93458000	1.32404900
H	-1.37186000	4.65188000	0.76114200
C	0.45659000	5.24286900	2.57021000
H	0.41421300	4.19336300	2.27194200
C	1.38954400	5.65494500	3.52005900
H	2.08827200	4.95525200	3.98066600
C	4.31410000	10.54493600	5.64733600
C	4.17872500	10.85697100	4.28846700
H	3.67475400	10.15519200	3.62204800
C	4.68266200	12.05796000	3.79209700
H	4.57234000	12.29394900	2.73241100
C	5.33020100	12.95426000	4.64324600
H	5.72592600	13.89219100	4.25046300
C	5.46565200	12.65173500	5.99746200
H	5.96484000	13.35201900	6.66888000
C	4.95046300	11.45669900	6.49803600
H	5.04401900	11.22810600	7.56287800
C	5.13529300	7.84353600	6.05976700
C	5.00426700	6.52023900	6.50493800
H	4.09360700	6.21202200	7.02228600
C	6.02474800	5.59746200	6.28646000
H	5.90872800	4.56884700	6.63154200
C	7.19542400	5.99138500	5.63850900

H	7.99909200	5.27155400	5.47524500
C	7.33861700	7.30858900	5.20525500
H	8.25383300	7.62218600	4.70054400
C	6.31285900	8.23128000	5.40947700
H	6.43306600	9.25821200	5.05933200

PPP-Rea

G = -1756.854938 Hartree

P	4.13669500	8.62224100	6.33278900
P	3.30571400	7.93988900	4.36374700
P	1.46294300	7.46940000	5.07453800
C	0.55438200	6.93184400	3.57753200
C	0.89616600	7.23828900	2.24873100
H	1.77586300	7.85170000	2.04035200
C	0.12182700	6.77462500	1.19455100
H	0.40367200	7.02600100	0.16912900
C	-1.02258000	5.99306200	1.41983200
C	-1.84818900	5.50247700	0.26124400
H	-2.23116200	6.34603300	-0.33184900
H	-2.70475000	4.90794600	0.60329100
H	-1.24369500	4.87739900	-0.41245900
C	-1.36877600	5.69775300	2.74015500
H	-2.25765100	5.09607000	2.94162600
C	-0.59767800	6.16560100	3.80345200
H	-0.89350800	5.92730100	4.82844900
C	4.53787200	10.35989600	5.83917900
C	3.52393200	11.17138200	5.31008200
H	2.53689300	10.74621200	5.11140900
C	3.76228800	12.51465100	5.02788200
H	2.96279500	13.12819700	4.60941600
C	5.01562600	13.07226600	5.27898600
H	5.20369100	14.12370300	5.05702400
C	6.02592700	12.27713700	5.81764100
H	7.00882800	12.70513300	6.02188000
C	5.79106400	10.93122000	6.09733800
H	6.59328100	10.32155400	6.51775300

C	5.78757800	7.80760800	6.17925900
C	6.20928400	6.99423600	7.23613900
H	5.56873200	6.87953500	8.11357900
C	7.43794200	6.33279100	7.17708100
H	7.75584200	5.70231900	8.00888700
C	8.25384200	6.48005400	6.05858200
H	9.21411800	5.96412500	6.01025400
C	7.84117500	7.28899300	4.99664800
H	8.47746900	7.40459200	4.11778800
C	6.61636000	7.94670300	5.05530800
H	6.29818600	8.58062200	4.22329400

AsAsP-Rea

G = -5545.645377 Hartree

P	4.20832500	8.71015200	6.32411200
As	3.33921400	8.04288100	4.23667300
As	1.37838800	7.40337500	5.11284300
C	0.40573000	6.82142300	3.52694600
C	0.68263900	7.22529200	2.21083600
H	1.49805700	7.92522800	2.01267700
C	-0.07788800	6.75029100	1.15019200
H	0.15262100	7.07881400	0.13375800
C	-1.14226700	5.85989100	1.35930300
C	-1.95156800	5.35429900	0.19535900
H	-1.32049800	4.77970400	-0.49890900
H	-2.38607900	6.18949300	-0.37321200
H	-2.77027600	4.70437800	0.52945700
C	-1.42373100	5.46724700	2.66976700
H	-2.25097700	4.77969700	2.85921100
C	-0.66647000	5.94519600	3.73918100
H	-0.91489800	5.62488000	4.75451900
C	4.62868600	10.45755300	5.89039400
C	3.63359700	11.29287800	5.36172200
H	2.64897400	10.88134100	5.12466900
C	3.88582300	12.64322900	5.12993800
H	3.10065400	13.27448200	4.71069800

C	5.13473300	13.18533400	5.43177900
H	5.33394400	14.24217000	5.24868300
C	6.12596000	12.36721200	5.97147800
H	7.10502600	12.78260300	6.21616300
C	5.87681700	11.01452700	6.20138000
H	6.66421800	10.38793300	6.62489500
C	5.85128000	7.88062600	6.16286100
C	6.22114200	6.98070500	7.16809900
H	5.54966400	6.81560100	8.01382400
C	7.43698600	6.29720400	7.09831300
H	7.71324100	5.59884600	7.88980500
C	8.29385700	6.50962300	6.02162800
H	9.24453100	5.97703200	5.96544900
C	7.93405200	7.40579800	5.01180500
H	8.60197800	7.57296900	4.16529600
C	6.72121500	8.08428900	5.08023600
H	6.44529800	8.78636300	4.28868200

SbSbP-Rea

G = -1554.750739 Hartree

P	4.57689400	8.63309800	6.25335200
Sb	3.47565300	7.94394000	4.03796100
Sb	1.30539300	7.29120400	5.35435000
C	0.04109300	6.76580800	3.68197900
C	0.15441400	7.32265700	2.39840500
H	0.91051000	8.08541100	2.19370500
C	-0.69524700	6.92560000	1.37143400
H	-0.58806900	7.37458300	0.38071200
C	-1.69141800	5.96248100	1.58476000
C	-2.60275300	5.54506500	0.46137200
H	-2.02619700	5.12410100	-0.37555900
H	-3.16471700	6.40622200	0.07071300
H	-3.32511800	4.78823400	0.79294000
C	-1.81108200	5.41494700	2.86424500
H	-2.58248200	4.66597400	3.05789100
C	-0.96290200	5.81327300	3.89830800

H	-1.09311500	5.36307500	4.88654600
C	4.91870000	10.39435200	5.80879900
C	5.71768800	10.78855100	4.72365200
H	6.20428400	10.02892300	4.10553400
C	5.90215700	12.13695600	4.43363400
H	6.52676900	12.42855000	3.58770800
C	5.28448300	13.11435700	5.21802000
H	5.42754900	14.17111700	4.98724200
C	4.48626200	12.73540300	6.29414200
H	4.00245000	13.49357300	6.91193300
C	4.30720600	11.38243900	6.58888900
H	3.68556100	11.08654400	7.43713800
C	6.23345900	7.84730400	6.03035400
C	6.31686900	6.48304500	5.71396700
H	5.40478700	5.91478200	5.50941600
C	7.54927600	5.83606300	5.65575000
H	7.59044300	4.77603200	5.40004900
C	8.72369400	6.53939300	5.92145000
H	9.68972300	6.03495700	5.87307700
C	8.65254100	7.89165100	6.25249600
H	9.56455700	8.45062100	6.46887200
C	7.41982500	8.54080100	6.31040900
H	7.38285400	9.59947500	6.57487000

BiBiP-Rea

G = -1503.409914 Hartree

P	4.37611200	8.94753100	6.29648000
Bi	3.43966000	8.21805900	3.92454400
Bi	1.13902900	7.44480000	5.22661000
C	0.00352900	6.70305400	3.41744300
C	0.14117000	7.24880400	2.13332500
H	0.82022600	8.08884500	1.96062400
C	-0.58611200	6.74263600	1.05946100
H	-0.46011200	7.18433200	0.06746700
C	-1.48081300	5.67746600	1.22784000
C	-2.27575400	5.15285100	0.06120900

H	-1.62692400	4.97116400	-0.81009700
H	-3.04507400	5.88032000	-0.24752500
H	-2.78379700	4.21151500	0.31583500
C	-1.62233500	5.13733300	2.50849900
H	-2.31315600	4.30555600	2.66665900
C	-0.89552500	5.64414200	3.58748100
H	-1.03929600	5.19045100	4.57257500
C	4.93405000	10.66636300	5.91755900
C	4.03617200	11.57553700	5.33691400
H	3.04483900	11.23476600	5.02451100
C	4.38740300	12.91071700	5.15095400
H	3.67413400	13.59708100	4.69150200
C	5.64383100	13.36762600	5.54765300
H	5.92191800	14.41196100	5.39916100
C	6.53956700	12.47840800	6.13962900
H	7.52284300	12.82577000	6.46161800
C	6.18869800	11.14214500	6.32768100
H	6.90095600	10.46249700	6.79974000
C	5.95661600	7.99362700	6.21011800
C	6.13864800	6.96893100	7.14676800
H	5.37321900	6.79811700	7.90736100
C	7.28319800	6.17017900	7.11891100
H	7.40799600	5.37571900	7.85644900
C	8.26486500	6.39176500	6.15647900
H	9.16173300	5.77081100	6.13453500
C	8.09723200	7.41332100	5.21824600
H	8.86220300	7.59071200	4.46043100
C	6.95201600	8.20382900	5.24175500
H	6.82902800	9.00182100	4.50410500

NNN-Rea

G = -897.158177 Hartree

N	4.27155200	8.91842700	4.91192900
N	3.16079600	8.55658300	4.26090300
N	3.01431000	7.33829200	4.08074900
C	1.81627300	6.98516600	3.41603700

C	0.74792600	7.86446900	3.18026400
H	0.81884600	8.89497900	3.52744300
C	-0.38485900	7.41029000	2.51948300
H	-1.21373700	8.10022300	2.34213900
C	-0.49471500	6.08201600	2.07844900
C	-1.73690100	5.61564900	1.36626700
H	-1.91458700	6.20631800	0.45531000
H	-2.62458100	5.72804000	2.00654000
H	-1.65824300	4.55968900	1.07717400
C	0.57336200	5.21655400	2.32808900
H	0.51037600	4.17728800	1.99830000
C	1.71490700	5.65871900	2.99322700
H	2.55242300	4.98982600	3.19476500
C	4.50582200	10.30578100	5.04753200
C	3.85206100	11.22542700	4.21495900
H	3.16839600	10.86047600	3.45131600
C	4.08544200	12.58795600	4.37275400
H	3.57082300	13.29303000	3.71794100
C	4.97316400	13.05560900	5.34168300
H	5.15594300	14.12461000	5.45404800
C	5.62542500	12.13744400	6.16218800
H	6.32013700	12.48434400	6.92868600
C	5.39531400	10.77085800	6.02548900
H	5.90105600	10.06215000	6.68105800
C	5.21300400	7.95796600	5.40144100
C	4.85521100	7.08386700	6.42889800
H	3.84497200	7.12377400	6.83676200
C	5.78872000	6.16960000	6.90892600
H	5.51024200	5.48382000	7.71014300
C	7.07647800	6.13252600	6.37173300
H	7.80651300	5.41771000	6.75386900
C	7.42882900	7.00897700	5.34646300
H	8.43341000	6.98178700	4.92231300
C	6.49505100	7.91895200	4.85418100
H	6.75283400	8.61137000	4.05106200

NNAs-Rea

G = -3078.094396 Hartree

As	3.68533400	9.00625400	6.55960700
N	2.49938600	8.56863500	5.10900500
N	2.24336600	7.36855200	5.02767400
C	1.33126800	6.99726000	3.98958900
C	0.61843500	7.92073000	3.21435800
H	0.75710700	8.98511200	3.40522200
C	-0.24675300	7.46063500	2.23303200
H	-0.80866500	8.17797400	1.62987400
C	-0.41942500	6.08563000	1.99762100
C	-1.36367200	5.61464500	0.92395200
H	-1.06115900	6.00054700	-0.06077200
H	-2.38562200	5.97373200	1.11548600
H	-1.39137500	4.51906900	0.86764600
C	0.29970300	5.18055600	2.78259000
H	0.17715600	4.10860000	2.61498700
C	1.16657000	5.63078800	3.77688400
H	1.73370500	4.93831300	4.40043100
C	4.34877800	10.65296400	5.76054900
C	4.24915800	10.91586300	4.38868700
H	3.75945000	10.19278500	3.73411700
C	4.77000100	12.09749800	3.86352400
H	4.68898200	12.29613500	2.79349500
C	5.39663200	13.02279200	4.69964600
H	5.80542700	13.94537000	4.28441300
C	5.49562300	12.76858300	6.06652400
H	5.97969700	13.49112900	6.72545900
C	4.96612100	11.59071500	6.59505700
H	5.03634400	11.40253800	7.66981100
C	5.14896600	7.80794300	6.06335000
C	4.98000200	6.44178900	6.32589700
H	4.05531800	6.08612700	6.78443100
C	5.98246600	5.53211400	5.99309700
H	5.83905900	4.46942400	6.19552400
C	7.16851400	5.98026000	5.41212600
H	7.95610300	5.26903600	5.15807400
C	7.34698100	7.33981300	5.16084100

H	8.27380400	7.69563200	4.70781000
C	6.34085800	8.25190800	5.48086600
H	6.48835100	9.31311000	5.27002600

NNSb-Rea

G = -1082.636147 Hartree

Sb	3.62194000	8.98227000	6.80811900
N	2.38756100	8.53070800	5.11782500
N	1.98079800	7.36992300	5.16871300
C	1.16472600	6.94165800	4.06619100
C	0.79282500	7.77887400	3.00778000
H	1.13656100	8.81349600	3.01466500
C	0.00093100	7.27445400	1.98708200
H	-0.29258300	7.92511600	1.15958400
C	-0.43491500	5.93806400	1.99356600
C	-1.29280400	5.41652400	0.87168900
H	-0.77521500	5.51155100	-0.09431300
H	-2.23045700	5.98695800	0.79725300
H	-1.54715000	4.35938800	1.02035200
C	-0.05417000	5.11910800	3.05959200
H	-0.38455000	4.07861400	3.08219500
C	0.73963500	5.61633000	4.09234300
H	1.04290800	4.99089700	4.93334100
C	4.35935000	10.80269200	5.93036100
C	4.39949900	10.95784400	4.53774100
H	4.02975500	10.15783300	3.89185600
C	4.90192200	12.12997300	3.97462100
H	4.92848200	12.24283500	2.88936000
C	5.37290400	13.15665000	4.79492500
H	5.76865700	14.07197000	4.35170300
C	5.33460700	13.01273900	6.18042100
H	5.69852200	13.81451900	6.82519200
C	4.82431700	11.84157600	6.74450500
H	4.79177800	11.74687400	7.83375500
C	5.22866100	7.74712300	6.06012300
C	5.01533100	6.36928400	5.92488800

H	4.03983000	5.93898100	6.16642300
C	6.03481400	5.54042600	5.45660500
H	5.85562800	4.46951400	5.34614600
C	7.28004000	6.07839600	5.13210500
H	8.07872700	5.42917300	4.76958500
C	7.50109700	7.44800900	5.26960800
H	8.47235300	7.87429100	5.01239900
C	6.47913700	8.28068200	5.72812300
H	6.66054400	9.35524500	5.81409100

NNBi-Rea

G = -1056.951019 Hartree

Bi	3.53828500	9.05820800	6.90150500
N	2.30291000	8.59779600	5.07138500
N	1.87250500	7.45189400	5.16314800
C	1.09205900	6.97621200	4.04823000
C	0.79330800	7.75675400	2.92609500
H	1.16613800	8.78071100	2.88881200
C	0.03569900	7.21169900	1.89989800
H	-0.20053100	7.81838600	1.02212700
C	-0.43731400	5.88981000	1.96452400
C	-1.25033800	5.32017200	0.83248600
H	-2.12971300	5.94726600	0.62518700
H	-1.59949800	4.30527300	1.06164300
H	-0.65579900	5.27522100	-0.09227800
C	-0.13008800	5.12802600	3.09479000
H	-0.49115600	4.09976300	3.16375800
C	0.62941400	5.66651200	4.13282300
H	0.87570700	5.08563300	5.02307900
C	4.40987500	10.90656400	5.96684000
C	4.43019100	11.03846700	4.57289200
H	3.99832000	10.25415300	3.94602200
C	4.99194500	12.17081400	3.98284000
H	5.00336500	12.26719400	2.89559800
C	5.54046600	13.17791800	4.77843300
H	5.98219500	14.06143400	4.31455700

C	5.52160700	13.05472200	6.16652400
H	5.94724700	13.84118800	6.79239600
C	4.95385600	11.92339700	6.75780400
H	4.94292200	11.84718600	7.84924800
C	5.18184900	7.73730900	6.10949100
C	4.91798000	6.37583700	5.92362700
H	3.92306000	5.97350200	6.13414800
C	5.91355700	5.52597200	5.43937600
H	5.69753700	4.46661900	5.28920300
C	7.18064500	6.02972800	5.14639900
H	7.95984700	5.36479000	4.77012900
C	7.44831700	7.38580800	5.33006800
H	8.43654800	7.78522700	5.09474700
C	6.45118400	8.23916100	5.80643000
H	6.66789500	9.30423500	5.92652800

Cyclooctyne

G = -311.467791 Hartree

C	0.59381900	-0.26249000	-0.23951600
H	1.60667500	-0.41025100	0.16875100
H	0.40720400	0.82238200	-0.22287900
C	-0.42284800	-0.93901000	0.70617500
H	-1.44261200	-0.58654900	0.48267600
H	-0.21558700	-0.67371700	1.75307500
C	-0.33307900	-2.37762700	0.45589700
C	-0.05954100	-3.39684300	-0.13673000
C	0.50369700	-4.24103700	-1.19048700
H	1.45109100	-4.68427800	-0.84396300
H	-0.15656100	-5.07546300	-1.46821000
C	0.75881800	-3.32009600	-2.40388100
H	1.36549500	-3.87689200	-3.13459500
H	-0.20495600	-3.11027300	-2.89527100
C	1.45526200	-1.98255800	-2.07459500
H	2.20275100	-2.15196500	-1.28079100
H	2.03362200	-1.70048400	-2.96684000
C	0.56354300	-0.76400100	-1.69896300

H	0.88244000	0.07974000	-2.32868000
H	-0.48173100	-0.96801300	-1.98760600

NNP-TS

G = -1495.139626 Hartree

P	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.82352600
C	1.74306500	0.00000000	-0.51764700
C	-1.22808800	-0.10587500	2.49353900
C	1.18759000	0.03728000	2.56909700
N	-0.61016700	-1.38638900	-0.65960600
C	2.30897500	-1.08452200	-1.20052400
C	2.50733700	1.15660100	-0.30947600
C	-1.26025500	-0.16825400	3.88594200
H	-2.15169700	-0.14784000	1.91787400
C	1.14433900	-0.00955100	3.96032700
H	2.15300600	0.09299600	2.06451800
N	-1.79626400	-1.67494800	-0.29081300
C	3.62716200	-1.01360200	-1.64674200
H	1.70470300	-1.97490400	-1.37616900
C	3.82823600	1.21763200	-0.74849400
H	2.06776600	2.01626100	0.20454500
C	-0.07888100	-0.11219300	4.62286100
H	-2.22013600	-0.25834700	4.39678600
H	2.07496000	0.02551800	4.52883000
C	-2.44530400	-2.60949000	-1.14577600
C	4.39053900	0.13180500	-1.41919700
H	4.06360400	-1.86441400	-2.17246600
H	4.41635500	2.11989700	-0.57439600
H	-0.10949300	-0.15254300	5.71278400
C	-2.05094200	-2.83662500	-2.47216800
C	-3.54845000	-3.29219800	-0.63174500
H	5.42291000	0.18013700	-1.76864500
C	-2.76439300	-3.72753800	-3.26163900
H	-1.19021400	-2.29097000	-2.85965800
C	-4.25761100	-4.18538500	-1.43395400

H	-3.83122600	-3.11264600	0.40691400
C	-3.88093300	-4.41653700	-2.75975400
H	-2.45921500	-3.89220400	-4.29814500
H	-5.11933700	-4.71451000	-1.02129400
C	-4.63499300	-5.38422500	-3.63303200
H	-5.54963600	-5.73801600	-3.13999200
H	-4.91808900	-4.91768900	-4.58770900
H	-4.01640300	-6.26328100	-3.86969600
C	-2.85540000	0.30143600	-0.53297400
C	-4.24969500	-0.01393400	-0.88854600
C	-1.95945900	1.16584900	-0.45375600
C	-4.43833100	0.03859100	-2.42414600
H	-4.89350100	0.74083200	-0.40643600
H	-4.57662200	-0.99277400	-0.50939700
C	-1.69598200	2.60620700	-0.72129800
C	-3.50632900	1.01992100	-3.14666100
H	-4.26625500	-0.96747400	-2.83872800
H	-5.49156900	0.28764400	-2.63022200
C	-2.08258800	2.97029900	-2.16688800
H	-2.30871900	3.20281600	-0.02483000
H	-0.64587100	2.87932400	-0.53307900
C	-3.47291300	2.47033600	-2.60273400
H	-3.79169500	1.03212700	-4.20976800
H	-2.48779900	0.60350900	-3.11540300
H	-2.03334200	4.06637900	-2.26137800
H	-1.32413700	2.56551400	-2.85704300
H	-3.85205700	3.15104800	-3.37925800
H	-4.17022800	2.57752400	-1.75384100

PPP-TS

G = -2068.294794 Hartree

P	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.83680600
C	1.78786000	0.00000000	-0.43087100
C	-0.47930400	1.12399500	2.51533200
C	0.48566700	-1.09064700	2.57223600

P	-0.71060200	-1.90157200	-0.74009700
C	2.14950900	-0.26465500	-1.76061500
C	2.78690600	0.34494000	0.48739100
C	-0.46279700	1.16656100	3.91050200
H	-0.87535600	1.96799100	1.94668600
C	0.50146700	-1.04729600	3.96320700
H	0.84375100	-1.97762400	2.04438600
P	-2.36175800	-1.89779800	0.49727200
C	3.48310000	-0.21334000	-2.15500400
H	1.37737100	-0.52158600	-2.49098400
C	4.12180300	0.40504600	0.08518300
H	2.52528400	0.56364500	1.52434100
C	0.02791400	0.08245000	4.63419300
H	-0.83947900	2.04835100	4.43090600
H	0.88049900	-1.90053700	4.52787400
C	-3.53094700	-2.95426700	-0.44903400
C	4.47529300	0.12302200	-1.23245500
H	3.74908500	-0.43319600	-3.19023000
H	4.89031900	0.67179700	0.81264700
H	0.03777900	0.11312500	5.72494600
C	-3.59057000	-3.01890200	-1.85124300
C	-4.49294500	-3.66249500	0.28584900
H	5.52031700	0.16781600	-1.54239300
C	-4.56199600	-3.78470200	-2.48574100
H	-2.87222100	-2.44883600	-2.44530500
C	-5.46613000	-4.42701700	-0.35519000
H	-4.47771200	-3.61319100	1.37807000
C	-5.51570600	-4.50332300	-1.75042100
H	-4.59241100	-3.81816000	-3.57766400
H	-6.20286900	-4.97249500	0.23880400
C	-6.55490100	-5.33504300	-2.45354700
H	-7.33626800	-5.67003100	-1.75933700
H	-7.03298600	-4.76782300	-3.26473600
H	-6.09752900	-6.22891600	-2.90460100
C	-3.28306700	0.42950300	0.08845700
C	-4.73476800	0.14207600	0.24077800
C	-2.44891300	1.27384200	-0.25675500
C	-5.45769900	0.16301900	-1.12689700

H	-5.13753400	0.93642900	0.88952500
H	-4.93515600	-0.80809700	0.75588000
C	-2.10159500	2.59359000	-0.82276000
C	-4.81036300	1.06653900	-2.18266300
H	-5.49003500	-0.86201400	-1.52886700
H	-6.50353600	0.46240800	-0.95219300
C	-3.06169200	2.96347900	-1.97778100
H	-2.20092800	3.33877400	-0.01406100
H	-1.05994500	2.63982800	-1.16627900
C	-4.52372300	2.53118700	-1.76809100
H	-5.45413800	1.05630300	-3.07568400
H	-3.86525100	0.59421600	-2.49085900
H	-3.00393700	4.05311700	-2.12202000
H	-2.69177800	2.50951300	-2.91085500
H	-5.17060900	3.20489700	-2.34912700
H	-4.79846300	2.69468200	-0.71202900

AsAsP-TS

G = -5857.083139 Hartree

P	-0.10636300	0.00196100	0.05188200
C	-0.11248000	-0.35527200	1.85503300
C	1.64672200	0.39507300	-0.32909700
C	-1.14706100	0.16325100	2.63962000
C	0.85340000	-1.17944800	2.45373100
As	-0.49373700	-1.97095000	-1.03104300
C	2.09809200	0.26750600	-1.65154200
C	2.50773000	0.95262400	0.62613000
C	-1.21376400	-0.12861800	4.00415700
H	-1.91608600	0.78584800	2.17578900
C	0.79035500	-1.46099600	3.81416100
H	1.65329200	-1.60385200	1.84230200
As	-2.51176000	-2.13701800	0.02725800
C	3.38803800	0.65675400	-2.00197800
H	1.43248000	-0.14530600	-2.41499700
C	3.79742100	1.34670100	0.26994000
H	2.17199200	1.07776300	1.65732600

C	-0.24458400	-0.93520900	4.59288700
H	-2.02924900	0.27725400	4.60456200
H	1.54573700	-2.10324700	4.26979500
C	-3.41472900	-3.43560700	-1.12755100
C	4.24427100	1.19661500	-1.04147300
H	3.72541800	0.53959100	-3.03305500
H	4.45687800	1.77394400	1.02725400
H	-0.29556900	-1.16322500	5.65874000
C	-3.07069800	-3.73004700	-2.45646100
C	-4.51945000	-4.09324900	-0.57064300
H	5.25440500	1.50331900	-1.31643000
C	-3.80001200	-4.65886900	-3.18917600
H	-2.22362200	-3.22104700	-2.92415200
C	-5.25144700	-5.02182400	-1.31134900
H	-4.81197600	-3.88101600	0.46138100
C	-4.90409700	-5.32059500	-2.63090100
H	-3.51343400	-4.87450100	-4.22158300
H	-6.10712900	-5.52361200	-0.85395300
C	-5.68631400	-6.31673400	-3.44445600
H	-6.50567700	-6.75484000	-2.86036600
H	-6.11888100	-5.84098300	-4.33709800
H	-5.03778000	-7.13432400	-3.79210500
C	-3.41223000	0.17539300	-0.61539900
C	-4.52060400	-0.17549000	-1.54511100
C	-2.66447900	1.10427500	-0.28518900
C	-3.99485100	-0.16208100	-3.00244200
H	-5.30002300	0.59280000	-1.41719300
H	-4.99268700	-1.14430900	-1.32788600
C	-2.24223000	2.51311100	-0.40969100
C	-2.82674800	0.79494000	-3.28156300
H	-3.66315500	-1.17816100	-3.26610500
H	-4.84624800	0.06563100	-3.66399900
C	-1.93260300	2.80453800	-1.89067600
H	-3.08680900	3.14527900	-0.08466400
H	-1.38258100	2.76615400	0.22552700
C	-3.00522500	2.27649600	-2.86327800
H	-2.61621500	0.74439100	-4.36100400
H	-1.93146400	0.38853200	-2.78523100

H	-1.81817400	3.89355600	-2.00341200
H	-0.95716800	2.35767200	-2.14622700
H	-2.99121000	2.90644600	-3.76468200
H	-4.00127800	2.43251300	-2.41293400

SbSbP-TS

G = -1866.188195 Hartree

P	-0.01017000	-0.01732900	0.11025800
C	0.03908400	-0.34402200	1.92077700
C	1.69432200	0.53226500	-0.29897200
C	-1.04152600	0.08952700	2.69739000
C	1.07701600	-1.05787800	2.54087800
Sb	-0.27495100	-2.25611200	-1.02237000
C	2.12661300	0.45583400	-1.63274700
C	2.52681800	1.15871800	0.63975800
C	-1.08763500	-0.18206200	4.06726900
H	-1.86187700	0.63593200	2.22299000
C	1.03738200	-1.31490900	3.90694500
H	1.91522700	-1.41849500	1.93973000
Sb	-2.65541100	-2.27961100	0.21633200
C	3.36618600	0.96426600	-2.01077100
H	1.48385500	-0.01054100	-2.38561900
C	3.76692200	1.66962100	0.25706100
H	2.20642400	1.24817700	1.67943500
C	-0.04723500	-0.87883300	4.67398300
H	-1.94066200	0.15592000	4.65752500
H	1.85041600	-1.87084400	4.37677100
C	-3.71330000	-3.64543100	-1.09696900
C	4.19408400	1.57164700	-1.06585400
H	3.68678000	0.88578200	-3.05088400
H	4.40333100	2.14869700	1.00310700
H	-0.07968300	-1.08999500	5.74397800
C	-3.32422800	-3.95999700	-2.40828900
C	-4.89034300	-4.22568800	-0.60521900
H	5.16574700	1.96989500	-1.36124200
C	-4.08048200	-4.82859800	-3.18880700

H	-2.41741300	-3.51688700	-2.83075700
C	-5.64901300	-5.09415900	-1.39175300
H	-5.22823600	-4.00446500	0.41142100
C	-5.25735400	-5.40933100	-2.69522300
H	-3.75500900	-5.06076000	-4.20613100
H	-6.56142500	-5.53524900	-0.98361000
C	-6.07162900	-6.33550000	-3.55897600
H	-6.91179900	-6.76777000	-3.00053800
H	-6.48055900	-5.80075900	-4.42938400
H	-5.45351300	-7.15995900	-3.94302300
C	-3.40412800	0.04962500	-0.66789000
C	-4.41803600	-0.24809100	-1.73037500
C	-2.70959700	1.00439300	-0.28799600
C	-3.72829500	-0.24039700	-3.11378100
H	-5.17605000	0.54934800	-1.67761600
H	-4.94735700	-1.20055100	-1.58540700
C	-2.28238300	2.41247500	-0.34134000
C	-2.55856400	0.74187000	-3.27394800
H	-3.34177200	-1.25125500	-3.31882100
H	-4.50567900	-0.04671900	-3.87058900
C	-1.83499400	2.74060900	-1.77931400
H	-3.15943800	3.03097600	-0.08123700
H	-1.48994300	2.65100300	0.38011600
C	-2.79783300	2.21652300	-2.86214800
H	-2.24634600	0.70429600	-4.32885600
H	-1.70581300	0.34641100	-2.70022700
H	-1.73219700	3.83379000	-1.85496200
H	-0.83087000	2.31664000	-1.94626100
H	-2.69630800	2.85736100	-3.74995500
H	-3.83679900	2.36010300	-2.51648400

BiBiP-TS

G = -1814.848846 Hartree

P	0.04097300	-0.03174500	0.09867800
C	0.05124400	-0.33700900	1.91518600
C	1.72954400	0.59532900	-0.25486600

C	-1.02363700	0.13289600	2.67950900
C	1.06247000	-1.07380900	2.55395400
Bi	-0.11841800	-2.37256700	-1.05564000
C	2.17732000	0.58023300	-1.58668500
C	2.53955000	1.20377100	0.71523300
C	-1.09180200	-0.12805500	4.05109000
H	-1.82164200	0.70222400	2.19487100
C	1.00259800	-1.31924100	3.92127400
H	1.89604700	-1.46220000	1.96369300
Bi	-2.60410800	-2.33740200	0.29495500
C	3.40761300	1.13103200	-1.93304100
H	1.55114200	0.12840700	-2.36259800
C	3.77059400	1.75779700	0.36423600
H	2.20813800	1.24499900	1.75442200
C	-0.07815900	-0.84932000	4.67394800
H	-1.94051700	0.23916600	4.63015800
H	1.79605600	-1.89251300	4.40363100
C	-3.76649500	-3.71402900	-1.08631300
C	4.21226700	1.72102800	-0.95704800
H	3.73955100	1.10049400	-2.97215100
H	4.38888900	2.22250100	1.13429100
H	-0.12781000	-1.05207600	5.74491900
C	-3.37243400	-4.03952600	-2.39198900
C	-4.97193100	-4.24646500	-0.61312800
H	5.17676300	2.15322100	-1.22710400
C	-4.15297700	-4.87354900	-3.18810500
H	-2.44302300	-3.63045200	-2.80108400
C	-5.75538800	-5.08055300	-1.41409600
H	-5.31818600	-4.01725400	0.39938600
C	-5.35922300	-5.40702600	-2.71343200
H	-3.82348300	-5.11502600	-4.20218000
H	-6.69110700	-5.48532700	-1.02074200
C	-6.20071000	-6.29417000	-3.59264700
H	-5.60771200	-7.12921300	-3.99295700
H	-7.05235600	-6.71203300	-3.04043400
H	-6.59631600	-5.73254100	-4.45235700
C	-3.31987100	0.03717500	-0.65381300
C	-4.39331500	-0.24542700	-1.66019800

C	-2.57662400	0.97615300	-0.32563300
C	-3.76654400	-0.30157600	-3.07241500
H	-5.11895700	0.58141000	-1.59770700
H	-4.95027300	-1.17366700	-1.46861500
C	-2.15127100	2.38368200	-0.44485600
C	-2.57127300	0.63221400	-3.31112000
H	-3.42750600	-1.33177800	-3.26435800
H	-4.56954500	-0.09888100	-3.79959200
C	-1.73762900	2.65469400	-1.90322800
H	-3.02384600	3.01153600	-0.19151400
H	-1.34340800	2.65046700	0.24863600
C	-2.74684000	2.12647300	-2.94067500
H	-2.30380800	0.55005100	-4.37576300
H	-1.71009900	0.22536000	-2.75819000
H	-1.60758800	3.74182000	-2.01643200
H	-0.75027500	2.19828700	-2.08502300
H	-2.65016800	2.73475600	-3.85167000
H	-3.77013800	2.31676100	-2.57129500

NNN-TS

G = -1208.549039 Hartree

N	1.26926500	0.10686700	0.28006600
N	-0.76074100	0.72624800	0.11532200
C	-0.69020700	-0.13246700	-1.44134400
C	0.50373900	-0.47115200	-1.69412900
C	1.87718800	1.42200800	0.08783100
C	2.15834200	-0.95982400	0.64570700
C	1.59815200	2.22639200	-1.01014200
C	2.69872700	1.89184300	1.11795800
N	0.07353700	0.05955700	0.87557400
C	1.71859300	-2.00103700	1.46852900
C	3.44737400	-0.99385500	0.10384700
C	2.16815500	3.49962300	-1.08893300
H	0.93843500	1.85250700	-1.78969700
C	3.26874300	3.15673800	1.02863400
H	2.88481000	1.25663200	1.98561700

C	2.57406100	-3.06476300	1.74573700
H	0.70960500	-1.96385000	1.87190800
C	4.28709200	-2.07049500	0.37948300
H	3.78952900	-0.17920000	-0.53505600
C	3.00624500	3.96450800	-0.08009600
H	1.94678400	4.13120400	-1.95042600
H	3.91327100	3.51661500	1.83170600
C	-2.07201600	0.82359600	0.66025000
C	3.85674300	-3.11156800	1.20054300
H	2.22630100	-3.87117900	2.39315300
H	5.28794000	-2.09093000	-0.05406200
H	3.45019800	4.95850000	-0.15027800
C	-2.51346600	0.06307000	1.75147800
C	-2.94193400	1.74802000	0.08041200
H	4.51666500	-3.95295200	1.41439100
C	-3.81050900	0.21967500	2.22495200
H	-1.82524700	-0.64091100	2.21731300
C	-4.24472900	1.88693400	0.55571900
H	-2.57551000	2.35881300	-0.74648700
C	-4.70272000	1.12687700	1.63506500
H	-4.14476000	-0.37899000	3.07608500
H	-4.91435700	2.61053800	0.08566500
C	-6.10028200	1.28655200	2.17344900
H	-6.71070600	1.91993000	1.51670100
H	-6.60071000	0.31236900	2.27188400
H	-6.08709400	1.74988800	3.17175100
C	-2.01120800	-0.56039500	-1.98911700
C	-2.43062700	-1.91815300	-1.38629300
H	-1.89429500	-0.65953100	-3.08008400
H	-2.81050100	0.17514800	-1.82550700
C	1.36009800	-1.32592900	-2.53399700
C	-1.28238500	-2.91339400	-1.17399800
H	-2.92040400	-1.74313800	-0.41528700
H	-3.19607600	-2.35951900	-2.04577200
C	1.08046100	-2.81906200	-2.28346000
H	1.15180400	-1.09389200	-3.59456600
H	2.43296900	-1.12364900	-2.37897600
C	-0.39947400	-3.21761700	-2.40905000

H	-1.72485900	-3.85068100	-0.80324600
H	-0.64344500	-2.54058800	-0.35778800
H	1.67897000	-3.39766500	-3.00460600
H	1.45027600	-3.09197500	-1.28043900
H	-0.43764100	-4.29790200	-2.61335300
H	-0.82245700	-2.73736500	-3.30907600

NNAs-TS

G = -3389.511988 Hartree

As	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.96496000
C	1.98953000	0.00000000	-0.13137600
C	-0.81328300	-0.85836600	2.70994200
C	0.84012500	0.89879000	2.63671300
N	0.06685900	-1.90227300	-0.47346800
C	2.81482200	-0.99395800	0.41195900
C	2.58191200	1.08151100	-0.78710300
C	-0.79229400	-0.81291300	4.10617300
H	-1.46532300	-1.56689700	2.19723700
C	0.84598800	0.95406200	4.02820400
H	1.50185800	1.55627900	2.06751400
N	-0.91701600	-2.60469200	-0.36459600
C	4.19975600	-0.90257300	0.30195900
H	2.36694700	-1.84684100	0.92770300
C	3.97264300	1.18088000	-0.89548800
H	1.94896900	1.86031600	-1.22319800
C	0.02923700	0.09636700	4.76745800
H	-1.42496600	-1.49468000	4.67730700
H	1.49655100	1.66649700	4.53825100
C	-0.81784900	-3.95824200	-0.83083900
C	4.78177000	0.18758300	-0.35131400
H	4.83238800	-1.68263300	0.72985200
H	4.42103000	2.03309900	-1.40950700
H	0.03915900	0.13527200	5.85793900
C	-0.07294300	-4.27614500	-1.96843200
C	-1.48212800	-4.95188700	-0.11636000

H	5.86766600	0.25866400	-0.43472100
C	-0.01040200	-5.59793900	-2.39089600
H	0.44868700	-3.47723000	-2.49682000
C	-1.39517700	-6.27550700	-0.54202200
H	-2.04925300	-4.67947500	0.77566800
C	-0.66766800	-6.61813000	-1.68681500
H	0.56485600	-5.84981000	-3.28469300
H	-1.90395100	-7.05750000	0.02494700
C	-0.59250900	-8.04291300	-2.16704400
H	-1.05013500	-8.73258800	-1.44656300
H	-1.11574500	-8.15888000	-3.12797400
H	0.45136100	-8.35040200	-2.32311600
C	-2.65793800	-1.64649000	-0.27521000
C	-3.64005600	-2.50604500	-0.97486800
C	-2.39037500	-0.47565300	0.08316700
C	-3.69375000	-2.16444700	-2.48002600
H	-4.61557900	-2.28719400	-0.51057700
H	-3.47203600	-3.58189600	-0.83924800
C	-3.04252800	0.85332500	0.18505700
C	-3.46174400	-0.68290800	-2.80544200
H	-2.93167400	-2.75726900	-3.01225300
H	-4.66958200	-2.49585100	-2.87035100
C	-3.50019900	1.35822600	-1.19523900
H	-3.91809600	0.76651800	0.84992700
H	-2.36574400	1.59919100	0.63956100
C	-4.31289500	0.34162700	-2.01534200
H	-3.63071800	-0.54897500	-3.88482600
H	-2.39669100	-0.45759700	-2.64136300
H	-4.09414200	2.27257400	-1.04009800
H	-2.61271700	1.65950400	-1.77613000
H	-4.94481000	0.89958500	-2.72204100
H	-5.01705600	-0.17743600	-1.34234800

NNSb-TS

G = -1394.066619 Hartree

Sb	0.17346200	-0.00113600	-0.14710200
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C	0.05764600	-0.05412100	2.01581400
C	2.35882400	-0.10460100	-0.09790000
C	-0.85854700	-0.86004600	2.70058900
C	0.92930200	0.75819300	2.75408300
N	0.32149600	-2.20720100	-0.37588800
C	3.07073800	-1.13951000	0.52447800
C	3.07789100	0.94351100	-0.68240800
C	-0.90965900	-0.84429800	4.09647800
H	-1.53460400	-1.51104400	2.14128400
C	0.87115400	0.78093000	4.14667600
H	1.67424200	1.37298000	2.24079500
N	-0.66668800	-2.88617200	-0.48564600
C	4.46371900	-1.12121700	0.56330800
H	2.52783800	-1.97153200	0.97960200
C	4.47525400	0.96829700	-0.64474500
H	2.54586000	1.76066300	-1.18096600
C	-0.05042800	-0.02085400	4.82103500
H	-1.62421100	-1.48334600	4.61866500
H	1.55356600	1.42202300	4.70755300
C	-0.50310800	-4.30816600	-0.63014400
C	5.16858400	-0.06583200	-0.02083400
H	5.00547900	-1.93235400	1.05390800
H	5.02048100	1.79413200	-1.10579300
H	-0.09279200	-0.00797700	5.91145400
C	0.55607100	-4.84001600	-1.36736000
C	-1.42634800	-5.14482100	-0.00750000
H	6.25955400	-0.05248300	0.01125800
C	0.67387800	-6.21923200	-1.48829000
H	1.27321300	-4.15757200	-1.82518500
C	-1.28274100	-6.52576300	-0.12036600
H	-2.23685600	-4.70519800	0.57706100
C	-0.24063200	-7.08395600	-0.86907700
H	1.49777700	-6.63932900	-2.06968400
H	-1.99476100	-7.18354700	0.38211400
C	-0.10877500	-8.57531100	-1.02788400
H	-0.69268000	-9.11108000	-0.26847600
H	-0.47083100	-8.89478500	-2.01719800
H	0.94034300	-8.89091500	-0.94449300

C	-2.54802100	-1.88615000	-0.60963900
C	-3.39150400	-2.78423600	-1.42606900
C	-2.36145700	-0.75114300	-0.13166400
C	-3.61410000	-2.21184600	-2.84791500
H	-4.35957100	-2.86522300	-0.90353300
H	-2.99702400	-3.80542300	-1.49928600
C	-3.04955900	0.53663100	0.14525100
C	-3.57765700	-0.68312900	-2.94974400
H	-2.84100700	-2.61362000	-3.52115900
H	-4.57620500	-2.59848500	-3.21999500
C	-3.71384300	1.12811500	-1.11201700
H	-3.82223800	0.33439600	0.90551600
H	-2.36978200	1.28575500	0.58958700
C	-4.47661300	0.10278900	-1.96581900
H	-3.83658900	-0.41147900	-3.98463500
H	-2.53543800	-0.35817300	-2.81066900
H	-4.39132100	1.93304000	-0.78727300
H	-2.94160900	1.60744100	-1.73595900
H	-5.25720800	0.63167000	-2.53230600
H	-5.01579300	-0.58875300	-1.29561000

NNBi-TS

G = -1368.383713 Hartree

Bi	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.25864700
C	2.28615400	0.00000000	-0.04355700
C	-0.89878200	-0.77713400	2.99651500
C	0.91658500	0.81175200	2.93763300
N	0.34836100	-2.33660800	-0.02559700
C	3.06712100	-0.96113200	0.61063300
C	2.93095600	1.04119100	-0.71910000
C	-0.88953900	-0.73163600	4.39268200
H	-1.60558700	-1.43215700	2.48007800
C	0.92040600	0.86170100	4.33198200
H	1.65007700	1.40198200	2.38061500
N	-0.58784800	-3.07926600	-0.11419300

C	4.45923100	-0.87815600	0.59020400
H	2.58100700	-1.78728600	1.13549000
C	4.32625000	1.12969600	-0.74241000
H	2.34690900	1.80606100	-1.24326300
C	0.01549000	0.09056200	5.06168400
H	-1.59114500	-1.34693200	4.95930200
H	1.63890700	1.49970200	4.84993300
C	-0.35694600	-4.50207700	-0.06797000
C	5.09103100	0.16795500	-0.08611600
H	5.05702200	-1.63231000	1.10630800
H	4.81421000	1.94889200	-1.27438000
H	0.02193200	0.12506600	6.15247500
C	0.73827200	-5.06886400	-0.71909800
C	-1.24571200	-5.29574200	0.65293900
H	6.18060400	0.23179200	-0.10030800
C	0.92809700	-6.44479900	-0.65627500
H	1.42857800	-4.41597900	-1.25479900
C	-1.03025400	-6.66976700	0.72379400
H	-2.08654000	-4.82626700	1.16737700
C	0.04975100	-7.26702800	0.06319200
H	1.78196300	-6.89323800	-1.16914000
H	-1.71498700	-7.29182200	1.30390500
C	0.25444100	-8.75826900	0.10271900
H	-0.24432400	-9.20646600	0.97190500
H	-0.15924500	-9.23203400	-0.80097000
H	1.32244500	-9.01117600	0.14759200
C	-2.52369100	-2.28362100	-0.31121600
C	-3.28827800	-3.31081800	-1.05618800
C	-2.48362700	-1.11099900	0.11222800
C	-3.64699600	-2.83330100	-2.48517300
H	-4.21383200	-3.49433200	-0.48460100
H	-2.77121300	-4.27661300	-1.11757700
C	-3.30482700	0.10325400	0.34783500
C	-3.81319500	-1.31963100	-2.64975600
H	-2.86032000	-3.16332400	-3.18119900
H	-4.56708400	-3.35485400	-2.79338500
C	-4.10593900	0.54455900	-0.89223100
H	-4.00627200	-0.13832200	1.16410900

H	-2.70330300	0.95564900	0.71650100
C	-4.76515200	-0.61235000	-1.65750400
H	-4.14605500	-1.12921900	-3.68170000
H	-2.81666700	-0.85911800	-2.57109000
H	-4.86696600	1.26842000	-0.56188200
H	-3.44049600	1.09168200	-1.58052900
H	-5.63561600	-0.22097300	-2.20435000
H	-5.17209700	-1.33476700	-0.92938600

NNP-Prod

G = -1495.24077 Hartree

P	3.97378000	8.65218200	5.45199700
N	3.08630200	8.17372100	4.17909000
N	1.89335100	7.65366900	4.68736400
C	1.69264100	7.80252300	6.02207300
C	0.34189100	7.66470800	6.66425400
H	0.49370100	7.53243300	7.74466200
C	2.81622200	8.79406500	8.13087700
H	2.28965100	8.07147000	8.77821600
C	0.97580700	7.15445300	3.74056200
C	2.77496200	8.33711900	6.69928000
C	0.81495900	7.82970300	2.52314200
H	1.42627000	8.711172500	2.33675300
C	-0.09080300	7.35951600	1.58178300
H	-0.20625900	7.89816100	0.63802500
C	-0.85961400	6.21004200	1.81370900
C	-1.85684200	5.73105800	0.79157500
H	-1.41618400	5.71323600	-0.21548900
H	-2.73370600	6.39579800	0.75384900
H	-2.21355300	4.71962500	1.02678400
C	-0.66270100	5.52856100	3.01675100
H	-1.21826500	4.60792700	3.20918600
C	0.25553400	5.97818600	3.96481700
H	0.44120400	5.39382300	4.86600400
C	4.50349200	10.39443600	5.26653200
C	3.83858400	11.18247000	4.32335600

H	3.10453700	10.70377600	3.67080800
C	4.12187800	12.54453800	4.23062800
H	3.61164400	13.15736600	3.48590600
C	5.05178000	13.12431000	5.09388700
H	5.26602300	14.19219700	5.02697700
C	5.70943200	12.34124600	6.04409300
H	6.43607700	12.79569000	6.71928700
C	5.44252500	10.97582400	6.12687000
H	5.96835400	10.36004200	6.86145200
C	5.55655000	7.79042800	5.80517300
C	5.55032300	6.71522400	6.69937700
H	4.61974100	6.45223500	7.20974400
C	6.71687900	5.98735800	6.92998600
H	6.70932700	5.15533200	7.63579500
C	7.89030500	6.32005400	6.25382400
H	8.80228200	5.74727600	6.42979800
C	7.89882300	7.38284000	5.34905000
H	8.81524600	7.63932400	4.81533300
C	6.73690600	8.11896000	5.12752300
H	6.74730500	8.95604500	4.42508900
C	-0.50346400	8.92231600	6.40614500
H	2.49324500	10.50023200	9.40266800
C	0.19569600	10.24293100	6.74070300
H	1.02229100	10.41369800	6.03101000
C	0.72805900	10.35811700	8.18432700
H	0.20117300	9.63689900	8.83515000
C	2.24246500	10.19943700	8.37221300
H	2.76033700	10.91167400	7.70623100
H	-0.20479700	6.78374500	6.31140000
H	3.86433300	8.78443300	8.47591800
H	0.46086700	11.35085800	8.57686100
H	-1.42965900	8.83806500	6.99837900
H	-0.80851100	8.93282400	5.34694000
H	-0.52893700	11.05030100	6.55669600

PPP-Prod

G = -2068.389334 Hartree

P	3.75632400	9.37048400	4.86111000
P	3.14144900	9.88184500	2.90380300
P	1.05104300	9.37290700	3.36869800
C	1.11688400	9.14179900	5.21085000
C	-0.20968700	9.04935900	5.91145600
H	-0.09527300	8.51519200	6.86718900
C	2.43605900	9.08035800	7.39052700
H	1.74988900	8.31390400	7.78773200
C	0.80370600	7.56702800	2.98580200
C	2.27827400	9.16864100	5.88862500
C	-0.50440200	7.10615500	2.80643100
H	-1.33652400	7.81488100	2.84152000
C	-0.76046300	5.75333300	2.57417800
H	-1.79061500	5.41408200	2.44180300
C	0.28274500	4.82788600	2.49564400
C	0.02050000	3.37093200	2.21722300
H	0.33206500	3.10508600	1.19548800
H	-1.04615700	3.13066400	2.31628500
H	0.58417800	2.72777300	2.90818200
C	1.59390600	5.29883800	2.65321200
H	2.42856200	4.59588600	2.58472300
C	1.85328800	6.64488700	2.88951700
H	2.88401500	6.99616600	2.98486000
C	4.76437000	10.67534300	5.66426600
C	4.54710100	12.00539300	5.28838100
H	3.86706500	12.21593000	4.45904300
C	5.19394300	13.03601800	5.96848400
H	5.02305300	14.07135700	5.67023400
C	6.05545200	12.74496800	7.02607700
H	6.55904400	13.55317400	7.55879000
C	6.27766700	11.41967700	7.40013400
H	6.95467000	11.18872700	8.22382300
C	5.63651900	10.38463700	6.72116200
H	5.81830300	9.34893800	7.01609400
C	4.74102800	7.84266500	5.10574700
C	4.12934200	6.67264500	5.56793000
H	3.07600000	6.68693100	5.85912700

C	4.85608000	5.48366100	5.63612100
H	4.37272400	4.57525900	5.99864800
C	6.19135400	5.45625800	5.23790100
H	6.75796000	4.52538100	5.29014200
C	6.80254700	6.61965400	4.76585400
H	7.84546300	6.59931400	4.44636700
C	6.08036900	7.80782600	4.69588000
H	6.55955500	8.71540600	4.31917200
C	-0.79245100	10.44941700	6.16533400
H	2.56053100	10.26625000	9.17026600
C	0.16240900	11.42230200	6.86248000
H	0.97799600	11.69556000	6.17221700
C	0.76407400	10.92249000	8.19036900
H	0.11121000	10.14683600	8.62930100
C	2.20699800	10.40458300	8.13599400
H	2.85332500	11.18139000	7.69278000
H	-0.91680300	8.46516600	5.30221100
H	3.45188300	8.72193300	7.62325700
H	0.75592600	11.75248900	8.91285500
H	-1.70662600	10.33410600	6.77049700
H	-1.10207000	10.88432100	5.20193300
H	-0.39631500	12.35211400	7.04666100

AsAsP-Prod

G = -5857.174946 Hartree

P	3.75525900	9.42556000	4.82172300
As	3.26750800	10.03451100	2.72176900
As	0.95937100	9.47859800	3.16247500
C	1.07045400	9.27265900	5.13120400
C	-0.25326200	9.20946200	5.84031800
H	-0.14973100	8.67136800	6.79530000
C	2.37907100	9.15544600	7.30744700
H	1.66840500	8.40305200	7.68748800
C	0.80188000	7.52343600	2.88731900
C	2.23384400	9.26901500	5.80248500
C	-0.48219900	6.97140900	2.83503000

H	-1.35956600	7.62287000	2.88685400
C	-0.66194300	5.59297600	2.70965700
H	-1.67370800	5.18130400	2.67682800
C	0.43435300	4.73080700	2.61659400
C	0.24699800	3.24590100	2.44495300
H	0.33193400	2.96119000	1.38468000
H	-0.74209800	2.92425900	2.79730700
H	1.01145300	2.68227300	2.99767300
C	1.71740800	5.29205300	2.65025700
H	2.59153500	4.63974000	2.57275700
C	1.90164500	6.66683600	2.77873400
H	2.91262300	7.08400800	2.78559300
C	4.79292200	10.65239400	5.70834000
C	4.63795800	12.00592400	5.38800900
H	3.98580600	12.28359200	4.55585200
C	5.31065200	12.97831500	6.12610400
H	5.18690400	14.03183100	5.87148100
C	6.13874200	12.60612500	7.18494200
H	6.66360600	13.36885000	7.76228600
C	6.30094400	11.25768800	7.50220700
H	6.95246000	10.96274000	8.32600700
C	5.63215200	10.28054900	6.76635300
H	5.76652400	9.22650200	7.01822100
C	4.64336000	7.84010200	5.05697400
C	3.96287700	6.69838000	5.49174200
H	2.90650500	6.76276800	5.76342100
C	4.62513600	5.47153800	5.55255600
H	4.08666700	4.58460400	5.88971500
C	5.96397000	5.37948900	5.17797400
H	6.47973200	4.41925500	5.22503700
C	6.64429900	6.51619500	4.73525600
H	7.69035000	6.44579400	4.43371000
C	5.98638200	7.74084700	4.66933300
H	6.51785000	8.62650300	4.31092000
C	-0.80251400	10.62155600	6.10221300
H	2.53119500	10.30572500	9.10728600
C	0.17301300	11.56387700	6.81235900
H	0.99698900	11.82600500	6.12788300

C	0.75871800	11.03318800	8.13497700
H	0.08228500	10.27365200	8.56626000
C	2.18525800	10.47268400	8.07464200
H	2.85581300	11.23778500	7.64794200
H	-0.97946200	8.64375600	5.23573600
H	3.38120200	8.76266100	7.54247600
H	0.77603400	11.85583500	8.86566700
H	-1.72151100	10.52310700	6.70295900
H	-1.10027300	11.07347000	5.14249400
H	-0.36432600	12.50418300	7.00660900

SbSbP-Prod

G = -1866.275558 Hartree

P	3.41811400	9.53619900	4.77919000
Sb	3.08210400	10.66349700	2.55700400
Sb	0.52970900	9.59294900	2.92593100
C	0.70136800	9.56827700	5.13054000
C	-0.59600800	9.65880100	5.88934300
H	-0.51478500	9.16553700	6.87110900
C	2.04268700	9.40832000	7.28200200
H	1.27137500	8.73131400	7.68477700
C	0.99781100	7.45765900	2.86929800
C	1.87920200	9.51160500	5.77466300
C	0.20581700	6.56518500	3.59941400
H	-0.65009900	6.92851500	4.17718000
C	0.49288900	5.19863300	3.61759100
H	-0.13475800	4.52228300	4.20376300
C	1.57198400	4.68208800	2.89530400
C	1.91626700	3.21681100	2.93208300
H	1.98980700	2.79962400	1.91726100
H	1.16337600	2.64026500	3.48572300
H	2.89224300	3.06091400	3.41918300
C	2.35167700	5.57488100	2.15016800
H	3.20503500	5.19505700	1.58146800
C	2.07293300	6.93954400	2.13792100
H	2.72331700	7.61575800	1.57524700

C	4.67198600	10.40640600	5.79923700
C	4.75615600	11.80183300	5.71222600
H	4.11454600	12.33666100	5.00664200
C	5.65087100	12.50032100	6.52067700
H	5.71054800	13.58704600	6.44691000
C	6.46802600	11.81225800	7.41745800
H	7.16894300	12.36018200	8.04909600
C	6.39381000	10.42240600	7.50123900
H	7.03614100	9.88004400	8.19647200
C	5.50123100	9.71847600	6.69384800
H	5.45312100	8.62928600	6.75903400
C	3.99404500	7.79663600	4.76859700
C	3.26924200	6.77729100	5.39159500
H	2.32825700	7.00194100	5.89735900
C	3.73023600	5.46118200	5.33660200
H	3.15165000	4.66861000	5.81429900
C	4.91023800	5.15947500	4.66100900
H	5.26917200	4.12951100	4.61996100
C	5.62866700	6.17488400	4.02524900
H	6.54621400	5.94081900	3.48343600
C	5.17013200	7.48778100	4.07298300
H	5.72047100	8.27906900	3.55697700
C	-0.99307400	11.13079300	6.09506300
H	2.32074700	10.55452400	9.06949600
C	0.07947100	11.99459200	6.76413100
H	0.91616400	12.15277800	6.06370300
C	0.62512400	11.44769600	8.09684900
H	-0.11830300	10.77260000	8.55731400
C	1.98689600	10.74514400	8.03698600
H	2.72877400	11.43361000	7.59935500
H	-1.40657800	9.14978200	5.34501500
H	3.00776400	8.92835200	7.50766600
H	0.73413200	12.28475200	8.80290500
H	-1.91345300	11.15234600	6.70151600
H	-1.25255800	11.57501900	5.11966300
H	-0.36141700	12.98837400	6.93366200

BiBiP-Prod

G = -1814.927408 Hartree

P	-1.36660200	0.69986400	-0.00180200
Bi	-0.30018800	-0.01454900	-2.29448500
Bi	1.42921300	-1.60506200	-0.53827800
C	0.21699600	-1.11896900	1.35188900
C	0.67463000	-1.92544500	2.53830900
H	0.45718100	-1.39687700	3.48013900
C	-1.56127900	0.03678800	2.74488500
H	-0.84371500	0.11492800	3.57803500
C	2.95555800	-0.07057000	0.17383100
C	-0.80245700	-0.24978500	1.45437100
C	4.09423200	-0.52531000	0.84541000
H	4.27170000	-1.59824900	0.97401300
C	5.02894200	0.37510500	1.36372600
H	5.91315100	-0.00221900	1.88449200
C	4.85047800	1.75396100	1.22413200
C	5.86986900	2.72994700	1.75272300
H	6.49920900	3.11910700	0.93735600
H	6.53347400	2.25525500	2.48793400
H	5.38507200	3.59248300	2.23173700
C	3.70723600	2.20573600	0.55038200
H	3.54599200	3.28082900	0.42790300
C	2.77606100	1.30898100	0.02798000
H	1.90100800	1.69191200	-0.50911600
C	-3.19714900	0.52034500	0.04114000
C	-3.75362700	-0.58622000	-0.61213700
H	-3.10664600	-1.23762400	-1.20648900
C	-5.11783600	-0.85068000	-0.50511100
H	-5.54203000	-1.71706500	-1.01473800
C	-5.93699500	-0.00839700	0.24659400
H	-7.00525700	-0.21503000	0.32870100
C	-5.38996300	1.10295200	0.88751900
H	-6.02828200	1.76770900	1.47149200
C	-4.02469500	1.36880200	0.78743400
H	-3.60534300	2.23919400	1.29634400
C	-1.07025700	2.44940100	0.45123400

C	-0.10428700	2.78126400	1.40720600
H	0.43429700	1.99099400	1.93594900
C	0.18709700	4.12030200	1.67056100
H	0.94402600	4.36937200	2.41586900
C	-0.48180000	5.13187000	0.98428600
H	-0.25409200	6.17823500	1.19315200
C	-1.44088200	4.80446500	0.02359900
H	-1.96213000	5.59278300	-0.52155000
C	-1.72940200	3.47004400	-0.24762400
H	-2.47361800	3.21903000	-1.00820900
C	-0.00036400	-3.30535500	2.56936600
H	-3.26310700	-0.53391000	3.90939400
C	-1.52937200	-3.26243700	2.51963200
H	-1.85837500	-2.93972100	1.51780400
C	-2.19230600	-2.36541100	3.58118000
H	-1.52105100	-2.25539300	4.45157600
C	-2.65362800	-0.98172100	3.10781400
H	-3.33041600	-1.10645100	2.24593000
H	1.76855000	-2.05933300	2.50712900
H	-2.03128500	1.02984000	2.67338900
H	-3.08645200	-2.87904600	3.96564400
H	0.32248500	-3.82282800	3.48764000
H	0.36924500	-3.91157700	1.72533900
H	-1.89242900	-4.29451200	2.63759000

NNN-Prod

G = -1208.599861 Hartree

N	3.86779200	8.89107400	5.55482200
N	3.12284000	8.65277800	4.33493200
N	2.15375400	7.71490700	4.79502900
C	1.89526100	7.91604300	6.12220300
C	0.60822700	7.62684400	6.82768300
H	0.80602000	7.63791100	7.90958400
C	2.94563400	9.35651600	7.99176600
H	2.58172500	8.64354200	8.75200500
C	1.30751500	7.17031500	3.83245200

C	2.86405900	8.69555600	6.65460300
C	1.20765500	7.77979600	2.57093600
H	1.80961900	8.66416200	2.37178600
C	0.36034600	7.24585500	1.60591100
H	0.29641100	7.73522200	0.63066200
C	-0.41089000	6.10353200	1.84816800
C	-1.35553400	5.56134800	0.80735900
H	-0.97993100	5.74884500	-0.20803900
H	-2.34725400	6.03493600	0.88417600
H	-1.49838100	4.47817700	0.92420100
C	-0.27271500	5.48629300	3.09632600
H	-0.82548600	4.56664900	3.30354400
C	0.58358200	5.99114100	4.06951400
H	0.73095000	5.44248300	4.99905000
C	4.38965600	10.28589400	5.54137800
C	3.72129500	11.24651200	4.78931100
H	2.87862800	10.92130500	4.18240300
C	4.15909000	12.56903800	4.83789300
H	3.64239100	13.32500700	4.24495000
C	5.24502100	12.92800400	5.63528800
H	5.57893700	13.96569000	5.67385400
C	5.90956700	11.95209100	6.37620800
H	6.76713700	12.21987900	6.99459000
C	5.49097800	10.62329800	6.32554500
H	6.02442200	9.85811000	6.89000100
C	5.01235700	7.91732300	5.65137500
C	5.18686000	7.09744000	6.75530900
H	4.49135800	7.14609400	7.59269800
C	6.26113500	6.20015500	6.76821000
H	6.40459400	5.54803900	7.63091900
C	7.13354100	6.13242200	5.68802600
H	7.96706900	5.42897700	5.70152600
C	6.93147300	6.95878300	4.57691900
H	7.60489600	6.89873100	3.72087700
C	5.86535200	7.84815200	4.55151800
H	5.65483700	8.47702200	3.68607500
C	-0.43973200	8.69694500	6.47750900
H	2.37729000	11.11207600	9.09734200

C	0.05426800	10.14090100	6.61847700
H	0.81287700	10.34033300	5.84431200
C	0.61936000	10.51854400	8.00608500
H	0.26756400	9.79357500	8.76246900
C	2.14398300	10.66310200	8.11814200
H	2.49940300	11.37706600	7.35639500
H	0.21390300	6.63291200	6.58994800
H	3.99732400	9.55206500	8.25169900
H	0.18616000	11.48349300	8.30930800
H	-1.31664200	8.54056500	7.12727600
H	-0.78137900	8.53449000	5.44252200
H	-0.79671100	10.79824600	6.38535900

NNAs-Prod

G = -3389.584853 Hartree

As	0.01222800	-0.92211400	0.74227000
C	0.10796300	-0.42122300	2.62561700
C	1.40160300	0.18338300	-0.03635600
C	-1.07450400	-0.44479700	3.36992100
C	1.32044300	-0.11429600	3.25151100
N	0.24017700	-2.57229300	0.18040700
C	2.16388000	-0.36426300	-1.07066800
C	1.58380500	1.51651800	0.34533700
C	-1.04865200	-0.14618200	4.73178700
H	-2.01442100	-0.70457500	2.87366300
C	1.34558700	0.17357200	4.61538100
H	2.24781800	-0.09747100	2.67319300
N	-1.00962800	-2.98700900	-0.29067900
C	3.12282000	0.41914700	-1.71215700
H	1.99037300	-1.40599900	-1.35316400
C	2.53164900	2.30076400	-0.31058700
H	0.99000100	1.94313500	1.15862300
C	0.16135500	0.16157100	5.35379100
H	-1.97373900	-0.15787500	5.31030500
H	2.29232000	0.40892200	5.10415300
C	-1.08442400	-4.34486300	-0.67626400

C	3.30295900	1.75039300	-1.33561900
H	3.72868700	-0.00877600	-2.51244400
H	2.67199600	3.34279900	-0.01907300
H	0.18305100	0.39024400	6.42053900
C	-0.03581500	-4.90160500	-1.41917300
C	-2.15189400	-5.15846300	-0.29020500
H	4.04768100	2.36446700	-1.84462400
C	-0.08900100	-6.23439300	-1.80529000
H	0.81557500	-4.26867400	-1.66681900
C	-2.19967800	-6.49076900	-0.69883900
H	-2.93093900	-4.75398000	0.35686300
C	-1.17644600	-7.05217500	-1.46601300
H	0.73526900	-6.65513200	-2.38634900
H	-3.04223800	-7.11338000	-0.38957800
C	-1.22859000	-8.48853600	-1.91642900
H	-2.02381100	-9.04039200	-1.39642100
H	-1.42477100	-8.55576300	-2.99864400
H	-0.27349000	-8.99970000	-1.72407500
C	-2.00849100	-2.07387600	-0.39988500
C	-3.22233900	-2.32261800	-1.25306100
C	-1.74510300	-0.81913200	0.12565900
C	-2.88536200	-2.11260600	-2.73759700
H	-4.00687000	-1.61776200	-0.94490900
H	-3.63088400	-3.32979500	-1.11676700
C	-2.58760400	0.41789800	-0.01223200
C	-2.18805700	-0.78723200	-3.05682400
H	-2.24875600	-2.94615400	-3.07677300
H	-3.82325400	-2.17996200	-3.31356200
C	-2.41092300	1.17568100	-1.33706500
H	-3.65463800	0.16877200	0.12205300
H	-2.34408200	1.10745900	0.81398900
C	-2.94018000	0.47891100	-2.59742700
H	-2.04829200	-0.74798000	-4.14762900
H	-1.17382000	-0.78961000	-2.62402200
H	-2.91850800	2.15009000	-1.24642300
H	-1.33786100	1.39629200	-1.47574900
H	-2.90492500	1.22051000	-3.40977000
H	-4.01210800	0.24653700	-2.46210400

NNSb-ProdG = -1394.118837 Hartree

Sb	4.49177300	8.27688200	4.67613800
N	2.33145100	8.78097800	3.37482100
N	1.50411800	8.12061100	3.98827500
C	1.57185000	7.93267800	5.45175800
C	0.25052800	7.99066200	6.16612200
H	0.37875800	7.58929300	7.17993600
C	2.92165700	7.99082500	7.53324800
H	2.20179900	7.29133300	7.99138800
C	0.43067200	7.42838200	3.27377500
C	2.78083700	7.99133600	6.02961200
C	-0.22229400	8.09830600	2.24361800
H	0.06353600	9.12694000	2.02092900
C	-1.20186600	7.43311600	1.51634800
H	-1.72375300	7.95800000	0.71312200
C	-1.52808400	6.09683400	1.79019700
C	-2.58529000	5.39129700	0.98282100
H	-2.29680500	5.33749000	-0.07726500
H	-3.54335500	5.92861500	1.03503900
H	-2.74718600	4.36773300	1.34371500
C	-0.84237300	5.44381900	2.81894900
H	-1.07194200	4.39945600	3.03935700
C	0.13342900	6.10234000	3.56621400
H	0.66748400	5.58786300	4.36773900
C	4.69605600	10.42745900	4.87571100
C	4.28354500	11.22920300	3.80257600
H	3.86356500	10.76355400	2.90851400
C	4.38568700	12.61896400	3.87171700
H	4.05905800	13.22844300	3.02711400
C	4.90133100	13.22874700	5.01505900
H	4.97942800	14.31589900	5.06962400
C	5.31803400	12.44183900	6.08730900
H	5.72306400	12.90990300	6.98642700
C	5.21810800	11.05082700	6.01553500

H	5.55350800	10.45027300	6.86456400
C	6.02698000	7.72632600	6.15300000
C	5.91314600	6.49301000	6.81163800
H	5.00044600	5.89653800	6.69971900
C	6.94163900	5.99784600	7.61352100
H	6.82360200	5.03904000	8.12207900
C	8.12267100	6.72589300	7.75808200
H	8.93084400	6.34291400	8.38342200
C	8.26781900	7.93975400	7.08856900
H	9.19432400	8.50921000	7.18445900
C	7.23148400	8.43005200	6.29088200
H	7.37466500	9.37960600	5.76749500
C	-0.24893000	9.44226700	6.24506000
H	3.10653600	9.30294900	9.21467300
C	0.77519300	10.42118200	6.82398600
H	1.59977200	10.56956100	6.10564000
C	1.35562800	10.00571200	8.18929800
H	0.65092100	9.32983400	8.70666200
C	2.75648100	9.38168900	8.17318300
H	3.44096000	10.08231300	7.67073100
H	-0.51137000	7.37054600	5.67616300
H	3.91958600	7.62533700	7.80694800
H	1.42141300	10.89958500	8.82780100
H	-1.16331500	9.45595200	6.86064000
H	-0.54893700	9.77935600	5.23845100
H	0.28157300	11.39983400	6.91828200

NNBi-Prod

G = -1368.435783 Hartree

Bi	4.38349600	8.72854500	4.31129500
N	1.72287600	9.33680300	3.22979400
N	1.22579600	8.43521000	3.88050200
C	1.44871400	8.28229400	5.34257300
C	0.17807600	8.26930900	6.14649600
H	0.40368600	7.90127400	7.15689700
C	2.96323000	8.50836300	7.30614900

H	2.36187500	7.76406300	7.85876600
C	0.36925200	7.41661300	3.25467700
C	2.68935300	8.40823800	5.82310000
C	-0.37189700	7.77633100	2.13256200
H	-0.30541500	8.80424200	1.77489700
C	-1.14632400	6.81606600	1.49459000
H	-1.73574000	7.09631700	0.61858100
C	-1.18088600	5.48934000	1.95020700
C	-2.02859600	4.46440700	1.24450500
H	-1.77982800	4.41817200	0.17446900
H	-3.09610300	4.71900400	1.32205600
H	-1.88602800	3.46416500	1.67282900
C	-0.41367700	5.15307200	3.06885100
H	-0.41615000	4.12355200	3.43241300
C	0.35866100	6.10959400	3.72839100
H	0.95544500	5.83906600	4.60157700
C	4.77832900	10.78381600	5.16572700
C	3.95159000	11.81932700	4.71188800
H	3.19540900	11.61933000	3.94696100
C	4.06218900	13.10010700	5.25571600
H	3.40693700	13.89853500	4.90221800
C	5.00417500	13.35826300	6.25210200
H	5.08919100	14.35889200	6.67926100
C	5.83521300	12.33292000	6.70147200
H	6.57121800	12.52864400	7.48364000
C	5.72164300	11.04891700	6.16217300
H	6.36169300	10.25036200	6.54536000
C	5.92414400	7.63508600	5.58821200
C	5.57055800	6.49096600	6.31481500
H	4.52208000	6.17876100	6.36911300
C	6.53486200	5.73498800	6.98387900
H	6.23753500	4.84925700	7.54870100
C	7.87672700	6.11109000	6.93047500
H	8.63237800	5.52348400	7.45444500
C	8.24846600	7.23900300	6.20002400
H	9.29780200	7.53577500	6.14822000
C	7.27866700	7.98890400	5.53088200
H	7.59614400	8.86728000	4.95950800

C	-0.42829100	9.67799300	6.22950100
H	3.15543000	9.89083700	8.92480200
C	0.56010500	10.74231000	6.70831600
H	1.31461700	10.92234000	5.92399600
C	1.27274100	10.40245800	8.03128400
H	0.66945100	9.67943100	8.60971100
C	2.71818800	9.90466500	7.91348700
H	3.29631100	10.64759500	7.34299100
H	-0.55969400	7.57840500	5.71374700
H	4.01482400	8.25095700	7.49943200
H	1.30938100	11.31067500	8.65162600
H	-1.29412700	9.63911000	6.91079700
H	-0.82354300	9.96452500	5.24076300
H	0.00729900	11.68715900	6.81896600