Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic Supplementary Information

Mechanistic Study of CuH-Catalyzed Hydroarylation of Alkenes with Polyfluoroarenes Involving C–F Bond Functionalization: Noncovalent Interaction-Controlled Regioselectivity

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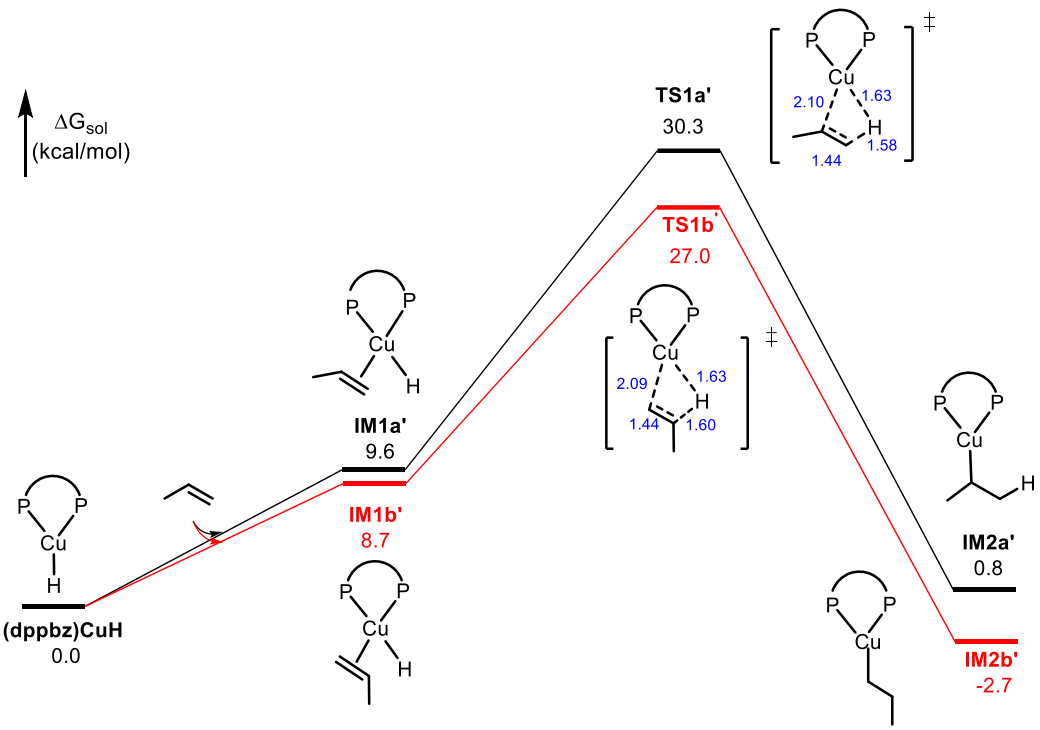

Fig. S1 Energy changes upon replacing groups in TS1a and TS1b.

Cartesian coordinates and energies of the optimized structures

(dppbz)CuH

SCF Energy = -2038.77348873 a.u.

Gibbs Free Energy = -2038.384607 a.u.

Cu	-0.00740900	-0.69020400	-2.11283100
C	-0.79541700	-0.96096200	1.08594700
C	-1.52324800	-1.42373600	2.19033200
C	-0.86341500	-1.89329800	3.32713100
C	0.53253100	-1.90466700	3.37051700
C	1.26945400	-1.45055400	2.27560100
C	0.62059300	-0.97809100	1.12635800
H	-2.60864000	-1.42155000	2.16073100
H	-1.43933300	-2.25175700	4.17557900
H	1.04853300	-2.27153200	4.25313500
H	2.35421900	-1.47235800	2.31366100
P	-1.59393800	-0.30648600	-0.44880300
P	1.52883900	-0.40788800	-0.37938500
C	-1.73921100	1.48961800	-0.08527400
C	-2.05107200	1.99215100	1.18830700
C	-2.06886600	3.36873300	1.41468700
C	-1.76242000	4.25422800	0.37709300
C	-1.44591700	3.76169900	-0.89087400
C	-1.43546700	2.38519300	-1.12202500
H	-2.26156100	1.30984100	2.00647000
H	-2.30915600	3.74963300	2.40337100
H	-1.76146500	5.32500900	0.56017000
H	-1.19312900	4.44552900	-1.69574500
H	-1.16891600	1.99826000	-2.10254100
C	-3.29279100	-0.99801000	-0.39737500
C	-3.46209300	-2.29044700	-0.92275500
C	-4.71759600	-2.89747000	-0.91280600
C	-5.82099100	-2.21361300	-0.39363600
C	-5.66332300	-0.92239000	0.11492500
C	-4.40518200	-0.31509100	0.11646000
H	-2.60884900	-2.81588100	-1.34546600
H	-4.83658900	-3.89796800	-1.31892000
H	-6.80082100	-2.68269700	-0.39338300
H	-6.51968400	-0.38487400	0.51265700
H	-4.29565100	0.68854200	0.51415200
C	1.84815900	1.37793100	-0.09506000
C	1.53280000	2.04030000	1.09931900
C	1.73310500	3.41806500	1.21169900
C	2.26097700	4.14217900	0.14090400
C	2.58300000	3.48685700	-1.05134700
C	2.36859700	2.11446400	-1.17347700
H	1.11669500	1.48839300	1.93566300
H	1.47250300	3.92457000	2.13658400
H	2.41420500	5.21384000	0.23126100
H	2.98909000	4.04581700	-1.88967100
H	2.59848500	1.61136700	-2.10933500
C	3.17426700	-1.20781500	-0.24697100
C	4.26028400	-0.62581200	0.42529400
C	5.48106700	-1.29956800	0.49873600
C	5.62640100	-2.55692000	-0.09381800
C	4.54975700	-3.13973100	-0.76812600
C	3.33094200	-2.46539200	-0.85147300
H	4.15409400	0.35056000	0.88863000
H	6.31789700	-0.84235400	1.01938600
H	6.57774700	-3.07822900	-0.03564800
H	4.66173700	-4.11279700	-1.23794200
H	2.49864000	-2.91008200	-1.39194400
H	0.04172900	-1.00488000	-3.64568200

S1

SCF Energy = -540.8768568 a.u.

Gibbs Free Energy = -540.6999078 a.u.

C	0.69698900	-1.04843700	-0.30977000
C	-0.08986800	0.07230700	0.02140000
C	0.57880300	1.25933500	0.36498600
C	1.96952200	1.32127800	0.37622800
C	2.75640800	0.20287400	0.04805500
C	2.08496000	-0.98631600	-0.29650700
H	0.21178900	-1.97394200	-0.60563800
H	0.00504300	2.13655100	0.64884200
H	2.45961300	2.25149400	0.65371700
C	4.22239000	0.32616900	0.07957800
C	5.12400300	-0.63270400	-0.17291200

H	4.58691900	1.31943200	0.34159900
H	2.65277200	-1.87102200	-0.56864600
H	4.84669400	-1.64976100	-0.43761800
H	6.18800500	-0.42095600	-0.12002000
C	-1.57213600	0.00098500	0.00381800
C	-2.34443000	1.10458400	-0.40300500
C	-2.24450300	-1.17210200	0.39312600
C	-3.73754300	1.03728800	-0.41899500
H	-1.84888700	2.01308900	-0.73268300
C	-3.63759200	-1.23942200	0.37529200
H	-1.67188400	-2.02928800	0.73494900
C	-4.39126300	-0.13495800	-0.03037900
H	-4.31309800	1.89977200	-0.74398300
H	-4.13511900	-2.15358700	0.68752100
H	-5.47629700	-0.18706800	-0.04352900

IM1a

SCF Energy = -2579.666711 a.u.

Gibbs Free Energy = -2579.074346 a.u.

C	-1.66001800	1.60203800	1.30881800
C	-1.73482900	2.56770000	2.32206800
C	-2.79864200	2.57243700	3.22413300
C	-3.80126000	1.60466300	3.12553900
C	-3.73637500	0.63285500	2.12667900
C	-2.67179100	0.61830300	1.21372700
H	-0.96252800	3.32675000	2.40073100
H	-2.84502200	3.33053700	4.00092900
H	-4.63269400	1.60529000	3.82469000
H	-4.51941100	-0.11588200	2.05554100
P	-0.24849900	1.51005000	0.11113600
P	-2.54514800	-0.64245200	-0.13397100
C	1.07024500	0.81911000	1.20900000
C	1.72769100	1.58250300	2.18991300
C	2.67511300	0.99228900	3.02665500
C	2.97100400	-0.36982100	2.90311600
C	2.31707200	-1.13546600	1.93759300
C	1.37628900	-0.54302200	1.09211700
H	1.50849300	2.64058400	2.29419300
H	3.18158200	1.59453400	3.77606900
H	3.71408900	-0.82651200	3.55071800
H	2.54496400	-2.19101900	1.82596000
H	0.88766200	-1.14463300	0.33596900
C	0.26746500	3.24849600	-0.16913300
C	-0.69040700	4.26536200	-0.32020600
C	-0.30140800	5.55565700	-0.68364800
C	1.04509900	5.84745000	-0.91683900
C	2.00255900	4.83817800	-0.78717100
C	1.61850400	3.54762100	-0.41946200
H	-1.74106700	4.04916500	-0.15418200
H	-1.05387400	6.33254200	-0.78713400
H	1.34492500	6.85217200	-1.20101700
H	3.05166100	5.05394100	-0.97038500
H	2.37293700	2.77314100	-0.32056100
C	-1.70533800	-2.06849500	0.67078900
C	-1.50348300	-2.17358800	2.05462400
C	-0.77857700	-3.24523200	2.58148600
C	-0.25510200	-4.22519000	1.73544400
C	-0.46179300	-4.13424200	0.35540800
C	-1.17743200	-3.06025600	-0.17307100
H	-1.89288600	-1.41224000	2.72240800
H	-0.61786400	-3.30857200	3.65402700
H	0.31439300	-5.05342100	2.14752800
H	-0.05510900	-4.89170400	-0.30879300
H	-1.31465700	-2.97904000	-1.24748100
C	-4.27176600	-1.21868300	-0.38102700
C	-4.82792100	-2.30685900	0.30900200
C	-6.14913500	-2.68965000	0.06721900
C	-6.92497300	-1.98960400	-0.86042400
C	-6.37590300	-0.90573200	-1.55189400
C	-5.05389000	-0.52500000	-1.31902300
H	-4.23161500	-2.85495000	1.03233500
H	-6.57182300	-3.53408900	0.60468200
H	-7.95204700	-2.29056400	-1.04734100
H	-6.97395600	-0.36197500	-2.27790400
H	-4.61805100	0.31075800	-1.86094100
C	3.30468400	0.15763400	-1.72125200
C	3.80473400	-1.08826500	-1.29631800
C	3.00222900	-2.22077700	-1.50891500
C	1.74319700	-2.10856000	-2.09404000
C	1.23428800	-0.86184200	-2.49781300
C	2.05236800	0.27016800	-2.30945000

H	3.90876700	1.05028900	-1.58704700
H	3.34851000	-3.19430100	-1.17378200
H	1.13163000	-2.99753500	-2.22037600
H	1.69192200	1.25197500	-2.59971700
C	5.11137400	-1.19231200	-0.60431700
C	5.97352400	-2.27871200	-0.83581000
C	5.50770700	-0.21212400	0.32418600
C	7.19257600	-2.38028800	-0.16490900
H	5.69407600	-3.03688500	-1.56185800
C	6.72724900	-0.31378200	0.99360500
H	4.83978300	0.61455300	0.54568200
C	7.57581900	-1.39775400	0.75209000
H	7.84726900	-3.22424400	-0.36494300
H	7.00969600	0.44967600	1.71352200
H	8.52529400	-1.47711600	1.27410700
Cu	-1.46292000	0.54405400	-1.80701200
C	-0.11186400	-0.78711500	-3.08922400
C	-0.63731400	0.28573300	-3.77182100
H	-0.65673500	-1.72826600	-3.12010200
H	-0.05981400	1.18540100	-3.96482000
H	-1.53651300	0.16340900	-4.36776100
H	-2.38198300	1.79173100	-2.16175400

TS1a

SCF Energy = -2579.647918 a.u.

Gibbs Free Energy = -2579.05611 a.u.

Cu	-1.18621800	0.30342400	-1.63690000
C	-1.66276600	1.61940000	1.30404800
C	-1.69608100	2.58754400	2.31724900
C	-2.79227100	2.68282400	3.17479600
C	-3.87036500	1.80683200	3.02881800
C	-3.84726600	0.83231800	2.03049300
C	-2.74895400	0.72343900	1.16499900
H	-0.86805700	3.28094900	2.42925500
H	-2.80576200	3.44185000	3.95186700
H	-4.72835500	1.88067500	3.69093700
H	-4.68925700	0.15528600	1.92299600
P	-0.22592700	1.43467000	0.14937300
P	-2.66253800	-0.55985700	-0.16612100
C	1.03283000	0.63081100	1.22453100
C	1.71071100	1.30686600	2.25304700
C	2.62481000	0.62434500	3.05573100
C	2.86119300	-0.73957200	2.84938000
C	2.18037400	-1.41826400	1.83794000
C	1.27418000	-0.73422700	1.02521900
H	1.53559900	2.36565800	2.41799600
H	3.15307500	1.15558500	3.84272100
H	3.57905300	-1.26636700	3.47166700
H	2.36320300	-2.47420800	1.66422500
H	0.76758700	-1.25563000	0.22209300
C	0.39060700	3.14072000	-0.12109000
C	-0.51699600	4.19368000	-0.32717100
C	-0.05813700	5.46406600	-0.67740200
C	1.31003900	5.69855300	-0.84076500
C	2.21755300	4.65301000	-0.65463400
C	1.76340800	3.38132300	-0.30028600
H	-1.58305500	4.02246800	-0.20947800
H	-0.77137100	6.27050100	-0.82356800
H	1.66505000	6.68809000	-1.11427200
H	3.28262200	4.82491900	-0.78363200
H	2.47801400	2.57650100	-0.16263000
C	-1.99795100	-2.04567400	0.69565900
C	-2.04663900	-2.22879200	2.08506300
C	-1.45164500	-3.35106500	2.66693800
C	-0.80900700	-4.30043700	1.86905500
C	-0.76121600	-4.12724600	0.48248100
C	-1.34666600	-3.00328000	-0.09948300
H	-2.53375600	-1.49290000	2.71693100
H	-1.48574900	-3.47916000	3.74520200
H	-0.34043100	-5.16753500	2.32592700
H	-0.25424500	-4.85693500	-0.14263000
H	-1.27179500	-2.84414400	-1.17140000
C	-4.41644500	-0.96460200	-0.52827100
C	-5.12626900	-1.98181900	0.12796500
C	-6.46024000	-2.23135000	-0.20231900
C	-7.09577800	-1.46786700	-1.18475100
C	-6.39303000	-0.45517800	-1.84430900
C	-5.05775400	-0.20909800	-1.52355100
H	-4.64019300	-2.58018900	0.89251000
H	-7.00207200	-3.02237600	0.30867600
H	-8.13297400	-1.66549500	-1.44048900

H	-6.88125600	0.13582300	-2.61415000
H	-4.50436700	0.56782700	-2.04605100
C	3.41540000	0.18785000	-1.71435600
C	3.96440000	-1.04095600	-1.29705300
C	3.20105200	-2.19749300	-1.54483400
C	1.94440000	-2.12562800	-2.13271100
C	1.36563200	-0.88947400	-2.51263500
C	2.16501000	0.26544700	-2.31174100
H	3.98563400	1.10175600	-1.56810700
H	3.58071000	-3.16556500	-1.22759800
H	1.37034100	-3.03885800	-2.27312700
C	0.01528500	-0.85141000	-3.04732700
C	-0.59524200	0.27947200	-3.67561000
H	-0.47769100	-1.81241100	-3.17216500
H	1.77555400	1.24122100	-2.58739000
H	0.03403300	1.11299700	-3.97707300
H	-1.38934900	0.06985500	-4.38607900
H	-1.59454700	1.28832700	-2.83812000
C	5.25590500	-1.10688700	-0.57907400
C	6.15862800	-2.16774400	-0.78541400
C	5.60798300	-0.11604000	0.35890300
C	7.36352400	-2.23458600	-0.08532600
H	5.91996900	-2.93500600	-1.51670900
C	6.81570400	-0.17982000	1.05374300
H	4.91289400	0.69211900	0.56588400
C	7.70093200	-1.23979500	0.83693800
H	8.04547000	-3.06102800	-0.26820000
H	7.05963400	0.59388000	1.77728300
H	8.64010300	-1.29115900	1.38072400

IM2a

SCF Energy = -2579.69465 a.u.

Gibbs Free Energy = -2579.09965 a.u.

C	-1.93177600	1.63951500	1.20973300
C	-2.20032900	2.68404300	2.10526100
C	-3.43032600	2.76012200	2.76000300
C	-4.40733200	1.78953500	2.52678100
C	-4.15673500	0.74590500	1.63461800
C	-2.92733900	0.65977000	0.96633400
H	-1.44755700	3.44546200	2.28505700
H	-3.62519200	3.57632800	3.44984900
H	-5.36566100	1.84579400	3.03514900
H	-4.92472500	0.00065700	1.45238000
P	-0.32548200	1.44760900	0.31946600
P	-2.54740100	-0.66749900	-0.26403100
C	0.69560500	0.48119900	1.50347000
C	0.73708600	0.75793500	2.87959300
C	1.51826700	-0.02673600	3.72805100
C	2.26242000	-1.09261300	3.21094200
C	2.22317500	-1.37374400	1.84408400
C	1.44150600	-0.59005000	0.99242800
H	0.15451600	1.57835400	3.28866600
H	1.54442200	0.19039200	4.79236100
H	2.86818900	-1.70380200	3.87422100
H	2.79843200	-2.19876800	1.43640100
H	1.40747000	-0.81173200	-0.06849300
C	0.41473000	3.12337200	0.29979100
C	-0.30929500	4.16924400	-0.30113100
C	0.26666000	5.42956300	-0.45643600
C	1.57926200	5.65926200	-0.03160600
C	2.30870800	4.62237600	0.55374800
C	1.73206600	3.36108400	0.72156800
H	-1.32640700	3.99633700	-0.64365000
H	-0.30696900	6.23083000	-0.91394200
H	2.02997900	6.63930100	-0.15906700
H	3.32945600	4.79291200	0.88466700
H	2.30962900	2.56368400	1.17794600
C	-1.76885900	-2.01339500	0.71445200
C	-1.79464500	-2.06480800	2.11507100
C	-1.10301800	-3.07210300	2.79163000
C	-0.38937100	-4.03730800	2.07761500
C	-0.36487100	-3.99506800	0.68050000
C	-1.04359400	-2.98371000	0.00220300
H	-2.33574000	-1.31164300	2.67912400
H	-1.11551100	-3.09593700	3.87752800
H	0.15405000	-4.81427200	2.60775000
H	0.19689800	-4.73743200	0.12073300
H	-0.99644500	-2.92942700	-1.08251800
C	-4.18834300	-1.31507300	-0.76392200
C	-4.86073900	-2.32683400	-0.06084200
C	-6.11515400	-2.76322000	-0.49185000

C	-6.70750700	-2.19244800	-1.62183900
C	-6.04106800	-1.18702800	-2.32784900
C	-4.78338600	-0.75473000	-1.90533700
H	-4.40555600	-2.77272600	0.81874200
H	-6.62978700	-3.54813400	0.05536600
H	-7.68313700	-2.53474200	-1.95522600
H	-6.49509700	-0.74707400	-3.21123700
H	-4.25500700	0.01490500	-2.46353100
C	3.50005500	0.61513500	-1.54016600
C	3.88846700	-0.73501700	-1.47441200
C	3.04574000	-1.67157800	-2.10797000
C	1.86942800	-1.28059800	-2.73441700
C	1.44360200	0.07353800	-2.77043900
C	2.32726100	1.01072700	-2.17559100
H	4.13574400	1.37518400	-1.09244600
H	3.30164200	-2.72790500	-2.07474800
H	1.23003900	-2.03792900	-3.18481200
H	2.07270000	2.06560900	-2.18550900
C	5.09524500	-1.15874100	-0.73078200
C	5.89680600	-2.22830100	-1.17487700
C	5.46366500	-0.51543800	0.46779600
C	7.01859900	-2.63609400	-0.45257100
H	5.64802700	-2.72952800	-2.10622000
C	6.58934700	-0.91873500	1.18586400
H	4.84204700	0.28738800	0.85293500
C	7.37351000	-1.98269500	0.73114700
H	7.62356900	-3.46073800	-0.82080000
H	6.84638300	-0.40913100	2.11100700
H	8.24825700	-2.29945900	1.29231100
Cu	-0.96576400	0.20804800	-1.63919800
C	0.12538400	0.44701900	-3.31941800
C	-0.01824700	1.88476500	-3.83152100
H	-0.17294600	-0.26685300	-4.09766500
H	0.73741300	2.15491500	-4.59055300
H	-1.00450100	2.03018700	-4.28724900
H	0.06381900	2.62570100	-3.02752800

IM1b

SCF Energy = -2579.66678 a.u.

Gibbs Free Energy = -2579.072976 a.u.

Cu	0.77004700	-1.52992100	-0.74638200
C	1.16722700	0.21288000	1.98923300
C	0.84841100	0.46782100	3.32893000
C	1.81705300	0.33775300	4.32616100
C	3.11615100	-0.04962600	3.99168300
C	3.44423600	-0.32028200	2.66170400
C	2.47977900	-0.19939900	1.65280200
H	-0.16229300	0.76360800	3.59420200
H	1.55588500	0.53734700	5.36165600
H	3.87270200	-0.15041600	4.76473400
H	4.45176600	-0.63776300	2.41145200
P	-0.04414600	0.38484800	0.60372300
P	2.81567900	-0.63949500	-0.11077600
C	0.17665900	2.16565000	0.16210100
C	0.37394900	3.17064700	1.12421500
C	0.58359600	4.49385100	0.73466300
C	0.60735600	4.83107600	-0.62174500
C	0.41891800	3.83968100	-1.58631700
C	0.20492600	2.51653700	-1.19525300
H	0.37289600	2.91937100	2.18019000
H	0.73488100	5.26032000	1.48983100
H	0.78099500	5.86007500	-0.92393700
H	0.45158000	4.09062300	-2.64260900
H	0.08464700	1.74880600	-1.95072600
C	-1.68901100	0.29742000	1.41891400
C	-2.14740900	-0.98142800	1.78092000
C	-3.40844600	-1.14297900	2.35282200
C	-4.23788200	-0.03496600	2.55106500
C	-3.79627100	1.23547700	2.17845900
C	-2.52715000	1.40435300	1.61857300
H	-1.51684300	-1.84612700	1.59361700
H	-3.75044200	-2.13686800	2.62765700
H	-5.22852500	-0.16428500	2.97628000
H	-4.44013500	2.09925500	2.31949700
H	-2.19963700	2.39836200	1.33248600
C	3.36319000	0.93864000	-0.87996900
C	3.64376200	2.09895400	-0.14369300
C	3.97823000	3.28545200	-0.80014400
C	4.04879700	3.32275500	-2.19423800
C	3.78195900	2.16758100	-2.93506400
C	3.43332900	0.98546900	-2.28255200

H	3.58323300	2.08386900	0.93955000
H	4.17651600	4.18223100	-0.22013800
H	4.30375300	4.24858900	-2.70219800
H	3.83337600	2.19046400	-4.02012900
H	3.20422600	0.09656300	-2.86359800
C	4.33239400	-1.67117600	-0.04282700
C	5.62949100	-1.14459400	-0.14128600
C	6.73683900	-1.99290800	-0.07376300
C	6.55887200	-3.36855200	0.09635000
C	5.26899200	-3.89859900	0.19316400
C	4.15956300	-3.05577300	0.11719100
H	5.77521300	-0.07628700	-0.27022000
H	7.73814000	-1.57841500	-0.15164900
H	7.42230900	-4.02586200	0.14867400
H	5.12623100	-4.96808500	0.32002900
H	3.15343600	-3.46283600	0.18082700
C	-3.61439900	0.02393300	-1.64699500
C	-4.50135500	-0.98418200	-1.22605000
C	-4.04358400	-2.31320100	-1.26795500
C	-2.75475000	-2.61648900	-1.69332300
C	-1.86465100	-1.60790700	-2.09963100
C	-2.32978300	-0.28058700	-2.08061700
H	-3.92282600	1.06382800	-1.60193600
H	-4.70889200	-3.12057400	-0.97669400
H	-2.42228300	-3.65128400	-1.70290300
C	-0.49332800	-1.97628500	-2.50192000
C	0.50320900	-1.11643300	-2.89776600
H	-0.32234200	-3.04446300	-2.61524700
H	-1.67500500	0.52782600	-2.38535500
H	1.40829800	-1.51406000	-3.34653400
H	0.34924600	-0.04826300	-2.99681100
H	0.46125600	-2.80482000	0.16193500
C	-5.86529700	-0.65305100	-0.74718100
C	-6.59146800	0.41341200	-1.30781900
C	-6.46546500	-1.39007000	0.29049500
C	-7.86761800	0.73457300	-0.84475800
H	-6.16219400	0.98182200	-2.12766200
C	-7.74282800	-1.07138200	0.75087100
H	-5.91333500	-2.19823100	0.75944000
C	-8.44997600	-0.00576100	0.18706900
H	-8.41115000	1.55929900	-1.29778500
H	-8.18228600	-1.65018800	1.55881600
H	-9.44404300	0.24426800	0.54701000

TS1b

SCF Energy = -2579.634713 a.u.

Gibbs Free Energy = -2579.042111 a.u.

Cu	0.72536900	-0.97779600	-0.99902000
C	1.14018800	0.45123800	1.89569100
C	0.79477700	0.86788300	3.18750600
C	1.63970700	0.60472800	4.26751500
C	2.84132200	-0.07661900	4.06441000
C	3.19751600	-0.49822300	2.78157500
C	2.35595300	-0.24415900	1.69064700
H	-0.14427700	1.38703400	3.35363800
H	1.35668200	0.92782100	5.26537500
H	3.49924100	-0.28623600	4.90302600
H	4.12950200	-1.03494000	2.63311800
P	0.07278500	0.75466400	0.41469600
P	2.73894700	-0.81129100	-0.02930400
C	0.61375900	2.43413300	-0.11497500
C	0.74921700	3.51208700	0.77513700
C	1.23662700	4.73837600	0.32339500
C	1.59997100	4.89789700	-1.01823900
C	1.47109700	3.82993100	-1.90797500
C	0.97864400	2.60270400	-1.45808500
H	0.48279900	3.39040000	1.82093800
H	1.34077000	5.56706700	1.01833100
H	1.98899900	5.85124400	-1.36503700
H	1.76504100	3.94459800	-2.94726400
H	0.90144700	1.75684800	-2.13621400
C	-1.61373200	0.95688600	1.10786500
C	-2.20101700	-0.16779700	1.71536400
C	-3.52141500	-0.12354500	2.15758400
C	-4.28179400	1.03822700	1.98794900
C	-3.70728000	2.15677300	1.38296500
C	-2.37945100	2.12011100	0.94562400
H	-1.62678400	-1.08432800	1.82164100
H	-3.96528600	-1.00243100	2.61599400
H	-5.31826200	1.06226400	2.31081000
H	-4.29193300	3.06206000	1.24401000

H	-1.94899100	2.99644600	0.47189300
C	3.74833300	0.56203500	-0.72714200
C	4.29875200	1.59035100	0.05068000
C	4.98751200	2.64180300	-0.55952900
C	5.14338400	2.66888700	-1.94673100
C	4.60331400	1.64248000	-2.72797300
C	3.90061000	0.60143000	-2.12297000
H	4.17783100	1.58446600	1.12911700
H	5.39751700	3.44133900	0.05120400
H	5.67481700	3.49030600	-2.41908100
H	4.71365000	1.66288000	-3.80864600
H	3.44033000	-0.17123900	-2.73321800
C	3.92120000	-2.19712400	0.19164600
C	5.30853000	-2.01461200	0.30139700
C	6.14794300	-3.11623700	0.47939000
C	5.61047000	-4.40437500	0.55107600
C	4.22998300	-4.59250300	0.43880700
C	3.38871400	-3.49465400	0.25331100
H	5.73172400	-1.01607400	0.24639900
H	7.22101900	-2.96786700	0.56206600
H	6.26621700	-5.25958700	0.68823400
H	3.80976300	-5.59311300	0.48695800
H	2.31507800	-3.63667300	0.15279500
C	-3.91263300	-0.13377400	-1.51031800
C	-4.77169300	-1.14172800	-1.04251300
C	-4.28103100	-2.45962900	-1.01668300
C	-2.97709100	-2.74592800	-1.41120300
C	-2.11064000	-1.73296400	-1.84876900
C	-2.60930400	-0.42345200	-1.90427500
H	-4.24829300	0.89835900	-1.51191700
H	-4.92934800	-3.26806800	-0.69036700
H	-2.61644500	-3.77120400	-1.36572800
C	-0.68443200	-2.05862000	-2.18010400
C	0.12443800	-1.16359600	-2.98012600
H	-0.52506700	-3.12242000	-2.34358100
H	-1.95896700	0.38859500	-2.21106800
H	0.86403300	-1.62306500	-3.63173600
H	-0.33332300	-0.26169300	-3.37408700
H	-0.22208000	-2.27156600	-0.67430300
C	-6.12910200	-0.81006200	-0.54520000
C	-6.90309400	0.19168200	-1.15775100
C	-6.66194600	-1.46538000	0.58013300
C	-8.16225400	0.52916600	-0.66094900
H	-6.52062200	0.69786900	-2.03933100
C	-7.92207400	-1.12946200	1.07582700
H	-6.07108000	-2.22338300	1.08563900
C	-8.67791100	-0.12870800	0.45885100
H	-8.74432600	1.30320000	-1.15386200
H	-8.30954200	-1.64290800	1.95175200
H	-9.65791700	0.13552700	0.84620500

IM2b

SCF Energy = -2579.684376 a.u.

Gibbs Free Energy = -2579.089389 a.u.

Cu	0.86718700	-1.10756700	-1.04346800
C	1.15416500	0.45490000	1.92668700
C	0.77716000	0.87476200	3.20997600
C	1.68392700	0.81600900	4.26919900
C	2.97893800	0.33614300	4.05659800
C	3.36595400	-0.08870700	2.78499800
C	2.46430700	-0.03612600	1.71286000
H	-0.22993900	1.24192400	3.38258600
H	1.37884700	1.14296800	5.25926100
H	3.68615600	0.28894600	4.87986000
H	4.37133200	-0.46695200	2.62676600
P	0.02165600	0.50549700	0.46482500
P	2.88330000	-0.60355600	0.00647800
C	0.32978800	2.18047200	-0.23023000
C	0.52471900	3.31905800	0.56817100
C	0.81414400	4.54988800	-0.02152200
C	0.92144400	4.65420400	-1.41186400
C	0.73367000	3.52591500	-2.21280600
C	0.43723800	2.29490000	-1.62480700
H	0.46384400	3.24234800	1.64987800
H	0.96616300	5.42548700	0.60348300
H	1.15875100	5.61115000	-1.86810300
H	0.82902700	3.59931700	-3.29225900
H	0.31099300	1.41060500	-2.24440000
C	-1.64740600	0.57244000	1.22396400
C	-2.12826400	-0.61246400	1.80819200
C	-3.39857100	-0.65324600	2.37889100

C	-4.21344700	0.48312000	2.35840300
C	-3.75197000	1.65637100	1.76070700
C	-2.47399200	1.70465700	1.19704500
H	-1.50907600	-1.50620600	1.80690200
H	-3.75878900	-1.57533800	2.82595700
H	-5.21044400	0.44622800	2.78541200
H	-4.38711600	2.53714200	1.72865900
H	-2.12662100	2.62463200	0.73838900
C	3.64158700	0.86597500	-0.79658900
C	3.87692900	2.07548300	-0.12782500
C	4.36460600	3.18224900	-0.82656900
C	4.63309700	3.08927400	-2.19355900
C	4.40898600	1.88383600	-2.86576400
C	3.90688200	0.78155800	-2.17494700
H	3.66629900	2.16178200	0.93298100
H	4.52935700	4.11836400	-0.30058800
H	5.00920300	3.95276300	-2.73494600
H	4.61260300	1.80622900	-3.93015900
H	3.71079900	-0.14620700	-2.70675200
C	4.27279700	-1.77769900	0.24448000
C	5.61893300	-1.38351000	0.29671100
C	6.62140300	-2.33671500	0.48716400
C	6.28946200	-3.68697800	0.62967300
C	4.95124500	-4.08638100	0.57536500
C	3.94769000	-3.13728900	0.37636500
H	5.88326100	-0.33595500	0.18590300
H	7.66147400	-2.02468400	0.52477000
H	7.07203900	-4.42630400	0.77539000
H	4.69004600	-5.13602600	0.67680600
H	2.90747800	-3.44889000	0.31510500
C	-3.71206600	-0.48227400	-1.52775500
C	-4.74343200	-1.22888200	-0.93607400
C	-4.51961400	-2.60502100	-0.74377100
C	-3.32019300	-3.19732000	-1.12917200
C	-2.28919700	-2.45413700	-1.72776400
C	-2.51474900	-1.08445500	-1.91847500
H	-3.82931200	0.59001400	-1.65293400
H	-5.30081300	-3.22103800	-0.30710300
H	-3.18180200	-4.26576100	-0.97403000
C	-1.01281400	-3.15125600	-2.16877800
C	0.19411600	-2.25908300	-2.51809100
H	-1.29432200	-3.80085200	-3.01877000
H	-1.72990300	-0.47356700	-2.35041200
H	0.99105800	-2.92881600	-2.88265400
H	-0.06222800	-1.63945400	-3.39616800
H	-0.72783700	-3.85068400	-1.36959300
C	-6.01640200	-0.58950300	-0.51818800
C	-6.55833600	0.48915800	-1.24041600
C	-6.71299400	-1.03595500	0.62019900
C	-7.74387500	1.10337600	-0.83524200
H	-6.05624000	0.83804800	-2.13792900
C	-7.90156800	-0.42678000	1.02245800
H	-6.30333900	-1.84900100	1.21138700
C	-8.42244600	0.64924200	0.29848400
H	-8.14293100	1.93284500	-1.41296300
H	-8.41579100	-0.78673500	1.90965700
H	-9.34608300	1.12672600	0.61337300

IM1a'

SCF Energy = -2156.732811 a.u.

Gibbs Free Energy = -2156.26578 a.u.

Cu	0.06474900	-1.13972900	1.67292500
C	0.64683200	-0.84809200	-1.47720500
C	1.31698300	-1.26043900	-2.63589200
C	0.59984400	-1.63430400	-3.77370800
C	-0.79607200	-1.59731300	-3.76318300
C	-1.47539000	-1.19592000	-2.61152000
C	-0.76815000	-0.82189100	-1.46107600
H	2.40189800	-1.30057900	-2.64663900
H	1.13148000	-1.95597600	-4.66482500
H	-1.35720000	-1.88692200	-4.64716000
H	-2.56100600	-1.18233700	-2.60570900
P	1.52277500	-0.30244500	0.05956500
P	-1.59749500	-0.35226800	0.12336600
C	1.75484400	1.49579400	-0.29427900
C	2.25933100	1.95643400	-1.52291300
C	2.35247400	3.32390600	-1.78019100
C	1.93742600	4.24955800	-0.81730600
C	1.43167500	3.80190900	0.40374100
C	1.34085400	2.43224100	0.66226100
H	2.57299900	1.24730500	-2.28294500
H	2.74163800	3.66756700	-2.73462300

H	2.00105100	5.31425400	-1.02396300
H	1.09236700	4.51383900	1.15032600
H	0.92032300	2.08921100	1.59892500
C	3.19609200	-1.04664700	-0.08200800
C	3.27979400	-2.44911100	-0.00923200
C	4.51938400	-3.08492000	-0.05133900
C	5.69339600	-2.33002100	-0.14530800
C	5.61871600	-0.93735000	-0.19940500
C	4.37700000	-0.29558000	-0.17071900
H	2.37038900	-3.03572200	0.08851700
H	4.56963900	-4.16916000	-0.00276600
H	6.65964100	-2.82597300	-0.17101100
H	6.52684700	-0.34460600	-0.26756900
H	4.33539600	0.78756700	-0.21842300
C	-1.89586800	1.45474800	-0.04569800
C	-1.67684700	2.17487600	-1.22886700
C	-1.84307200	3.56148100	-1.25068500
C	-2.23993200	4.24141800	-0.09732900
C	-2.46945300	3.53024400	1.08470600
C	-2.29039100	2.14753500	1.11225200
H	-1.36042000	1.65780000	-2.12894000
H	-1.65697100	4.10999600	-2.16981000
H	-2.36520300	5.32033600	-0.11657300
H	-2.77663300	4.05378900	1.98588000
H	-2.45125000	1.60066100	2.03836900
C	-3.27085900	-1.09917300	-0.00816200
C	-4.37463800	-0.44143400	-0.57316700
C	-5.61437200	-1.08111100	-0.63860400
C	-5.76151400	-2.38037700	-0.14503100
C	-4.66682100	-3.03929400	0.42186700
C	-3.42840900	-2.40034300	0.49669400
H	-4.26688500	0.56723300	-0.96096100
H	-6.46427300	-0.56554700	-1.07746000
H	-6.72710300	-2.87568400	-0.19746400
H	-4.77846700	-4.04705000	0.81232100
H	-2.57608300	-2.90273100	0.94772000
C	1.77605000	0.40706100	3.81810200
C	0.30461400	0.27999900	3.52004900
C	-0.43335600	-0.82065600	3.83211100
H	-0.21350900	1.17453100	3.17770000
H	0.01924300	-1.67932900	4.32030800
H	-1.51867000	-0.81354000	3.76984300
H	0.09638200	-2.73666100	1.64400100
H	1.93066200	0.98748000	4.73812800
H	2.23181100	-0.57859400	3.95493800
H	2.31401500	0.92232000	3.01733500

TS1a'

SCF Energy = -2156.700457 a.u.

Gibbs Free Energy = -2156.232745 a.u.

Cu	0.01171000	-0.75453800	1.64781200
C	0.65384400	-0.76448800	-1.53675300
C	1.31405900	-1.07746800	-2.73219100
C	0.58820700	-1.40611200	-3.87836400
C	-0.80780700	-1.41903200	-3.84258800
C	-1.47763700	-1.09977400	-2.66022300
C	-0.76007000	-0.77147000	-1.50222900
H	2.39905300	-1.08114000	-2.76644200
H	1.11369700	-1.65436900	-4.79624400
H	-1.37538700	-1.67719000	-4.73214200
H	-2.56325300	-1.10992500	-2.63789900
P	1.54290700	-0.30763900	0.02499400
P	-1.58581200	-0.34064300	0.09683100
C	1.83657500	1.49437100	-0.24477700
C	2.56138500	1.98891900	-1.34178300
C	2.67840800	3.36375000	-1.54408400
C	2.06572500	4.25834200	-0.65920300
C	1.34017200	3.77386300	0.43009900
C	1.22851400	2.39685400	0.63815500
H	3.03089500	1.30048300	-2.03835800
H	3.24087100	3.73816300	-2.39501900
H	2.15117900	5.32881000	-0.82469700
H	0.85166900	4.46249000	1.11336600
H	0.64576400	2.00867000	1.46859900
C	3.19048300	-1.10126600	-0.13406900
C	3.24904000	-2.48215200	-0.39559700
C	4.47438500	-3.14666800	-0.41593800
C	5.65790400	-2.44744200	-0.15761600
C	5.60671700	-1.08025900	0.11964300
C	4.38158000	-0.40828000	0.13146600
H	2.33358100	-3.03520600	-0.58847000

H	4.50497400	-4.21142000	-0.63002700
H	6.61187500	-2.96690600	-0.17006700
H	6.52113700	-0.53012200	0.32408000
H	4.35867600	0.65580600	0.34392700
C	-2.00507400	1.44288500	-0.10154800
C	-1.81750100	2.16025000	-1.29118600
C	-2.06970800	3.53430600	-1.33301100
C	-2.52208700	4.20191400	-0.19391500
C	-2.71991200	3.49149300	0.99495000
C	-2.45365300	2.12420700	1.04321700
H	-1.45809200	1.65637800	-2.18227900
H	-1.90700700	4.08146700	-2.25745000
H	-2.71428800	5.27063800	-0.22795100
H	-3.06760300	4.00555200	1.88680200
H	-2.57639200	1.58326500	1.97817800
C	-3.20680300	-1.20107000	0.02401000
C	-4.35921400	-0.63267100	-0.54043400
C	-5.55605800	-1.35195800	-0.56351200
C	-5.61164200	-2.64152200	-0.02766000
C	-4.46791900	-3.21162400	0.53881000
C	-3.27248300	-2.49250000	0.57107600
H	-4.32328700	0.36887100	-0.95855800
H	-6.44458400	-0.90487600	-1.00078000
H	-6.54475400	-3.19767900	-0.04615600
H	-4.50874700	-4.21099500	0.96298600
H	-2.38250300	-2.92394900	1.02384900
C	1.56502200	0.59493500	3.92042800
C	0.20986900	-0.00407100	3.59473100
C	0.04738400	-1.43395000	3.65003900
H	-0.65934600	0.58771500	3.87900300
H	0.89047300	-2.02803500	4.00106300
H	-0.90890900	-1.83123300	3.98624500
H	0.02082100	-2.25063000	2.30177800
H	1.77814400	0.62218800	5.00369000
H	2.36946300	0.01250700	3.45297500
H	1.66565700	1.62263700	3.55240700

IM2a'

SCF Energy = -2156.749357 a.u.

Gibbs Free Energy = -2156.279796 a.u.

Cu	-0.00092400	-1.10904100	1.46971400
C	0.65412700	-0.24749200	-1.71252700
C	1.31611800	-0.28307000	-2.94738800
C	0.59057600	-0.35110900	-4.13789300
C	-0.80558000	-0.38767800	-4.10551000
C	-1.47718200	-0.35968300	-2.88215100
C	-0.76094100	-0.29090700	-1.67915400
H	2.40141000	-0.26190300	-2.97857200
H	1.11533000	-0.37942600	-5.08867400
H	-1.37175100	-0.44417600	-5.03086200
H	-2.56208500	-0.39918100	-2.86366600
P	1.52744200	-0.16084200	-0.08619400
P	-1.56777000	-0.29115500	-0.01517500
C	1.68656300	1.64582000	0.20778000
C	1.83844200	2.58995600	-0.82005700
C	1.89318400	3.95182300	-0.52006700
C	1.79125800	4.38335400	0.80567800
C	1.63564300	3.45035900	1.83348800
C	1.58070200	2.08772100	1.53599500
H	1.89844500	2.26313900	-1.85390500
H	2.00648400	4.67667900	-1.32150600
H	1.82377100	5.44473400	1.03526600
H	1.54427400	3.78227600	2.86377400
H	1.43447400	1.35947500	2.32986500
C	3.21963700	-0.76401500	-0.46260600
C	3.41433600	-2.15560200	-0.42424700
C	4.66766500	-2.70174700	-0.69974300
C	5.74538100	-1.86281200	-0.99934200
C	5.56340700	-0.47811500	-1.02444600
C	4.30648700	0.07166100	-0.75978200
H	2.58157000	-2.80804400	-0.17210200
H	4.80616700	-3.77881500	-0.67030700
H	6.72404300	-2.28705800	-1.20524300
H	6.39967000	0.17716500	-1.25212200
H	4.17548900	1.14892300	-0.78395900
C	-1.92953200	1.47627600	0.32998800
C	-1.84892000	2.48778500	-0.63775000
C	-2.08596200	3.81816700	-0.28434000
C	-2.41298700	4.14886700	1.03245100
C	-2.49823100	3.14521800	2.00180300
C	-2.24910700	1.81751100	1.65564300
H	-1.59084400	2.24202300	-1.66292200

H	-2.01138200	4.59572500	-1.03945700
H	-2.59421700	5.18496900	1.30429100
H	-2.74543500	3.39780300	3.02912200
H	-2.29100300	1.04113100	2.41563100
C	-3.20647200	-1.06182200	-0.31666100
C	-4.35141100	-0.33438100	-0.67568700
C	-5.56218500	-0.99564400	-0.89389200
C	-5.63867900	-2.38453800	-0.76009400
C	-4.50215200	-3.11464000	-0.40050900
C	-3.29374000	-2.45592700	-0.17181300
H	-4.29957900	0.74516200	-0.78244000
H	-6.44529500	-0.42531400	-1.16845800
H	-6.58220000	-2.89601100	-0.92879000
H	-4.55918400	-4.19362300	-0.28730600
H	-2.41350400	-3.02079700	0.12632400
C	1.76728500	-1.88906100	3.65878000
C	0.33764400	-2.12731200	3.14487600
C	0.10399800	-3.63288500	2.93423300
H	-0.35154700	-1.80762600	3.94718500
H	0.33539500	-4.23916000	3.83195600
H	-0.93604000	-3.85111300	2.65935300
H	0.73378700	-4.02965300	2.12489100
H	2.00473700	-2.46341500	4.57580300
H	2.51551200	-2.17747800	2.90690900
H	1.94900700	-0.83074300	3.88842100

IM1b'

SCF Energy = -2156.734686 a.u.

Gibbs Free Energy = -2156.267277 a.u.

Cu	0.09535900	-1.18413600	-1.63458100
C	-0.62988800	-0.76245000	1.52213900
C	-1.29995600	-1.13723100	2.69411500
C	-0.58345400	-1.47891400	3.84273200
C	0.81250900	-1.44822400	3.83012600
C	1.49296800	-1.08728800	2.66575500
C	0.78546300	-0.74885600	1.50492400
H	-2.38541500	-1.16570200	2.70799800
H	-1.11567400	-1.76940000	4.74415800
H	1.37322300	-1.71275400	4.72217700
H	2.57861300	-1.08071800	2.65896700
P	-1.50632000	-0.27571000	-0.03296100
P	1.61532600	-0.35177700	-0.09754100
C	-1.78538800	1.52957400	0.23525800
C	-1.96599700	2.10088600	1.50606600
C	-2.12976000	3.47954300	1.64575600
C	-2.11105400	4.30735200	0.51968700
C	-1.93568800	3.74963700	-0.74827900
C	-1.77416500	2.36994400	-0.88843100
H	-1.96721500	1.47182700	2.39052900
H	-2.26492700	3.90817500	2.63502000
H	-2.22866000	5.38153900	0.63138800
H	-1.91607200	4.38697400	-1.62778300
H	-1.62968000	1.94572800	-1.87653600
C	-3.17088300	-1.03705200	0.15021700
C	-3.27636100	-2.40671100	-0.15053400
C	-4.50553400	-3.05809400	-0.05306700
C	-5.64808100	-2.34776900	0.32851000
C	-5.55340000	-0.98453200	0.61588100
C	-4.32117400	-0.33026200	0.53097200
H	-2.39175000	-2.95386500	-0.46616700
H	-4.57278900	-4.11777800	-0.28369400
H	-6.60703800	-2.85391000	0.39659700
H	-6.43823000	-0.42629300	0.90965500
H	-4.26136400	0.72858500	0.76194900
C	1.88846100	1.46627700	-0.03161500
C	1.49433700	2.26179300	1.05350300
C	1.63666200	3.65046300	0.99978300
C	2.18576300	4.25813300	-0.13034100
C	2.59418800	3.47133800	-1.21217600
C	2.43942200	2.08654700	-1.16709600
H	1.06234700	1.80261100	1.93591200
H	1.31339900	4.25514800	1.84224000
H	2.29353600	5.33839200	-0.17076200
H	3.02482200	3.93729600	-2.09423700
H	2.74488300	1.48381700	-2.01792700
C	3.29875300	-1.06778300	0.05751100
C	4.37900900	-0.38190000	0.63488500
C	5.63069700	-0.99410300	0.72414000
C	5.81297500	-2.29316500	0.24130600
C	4.74174900	-2.97987800	-0.33679100
C	3.49067600	-2.36872700	-0.43417900
H	4.24358500	0.62774800	1.01125400

H	6.46268500	-0.45733300	1.17160800
H	6.78833800	-2.76667800	0.31097300
H	4.88131900	-3.98740300	-0.71862300
H	2.65562800	-2.89214500	-0.89361700
C	-0.47024700	-0.77536300	-3.79784200
C	0.38800000	0.20239700	-3.39290700
H	-0.06096800	-1.66241100	-4.27759600
H	1.45723600	0.10707100	-3.56015600
H	0.03492700	1.16699700	-3.04127900
H	-0.05050900	-2.77130100	-1.61853400
C	-1.96861200	-0.63763600	-3.83594100
H	-2.45782900	-1.50955800	-3.39059700
H	-2.30521100	0.25487000	-3.30071300
H	-2.31364900	-0.56498900	-4.87624200

TS1b'

SCF Energy = -2156.705825 a.u.

Gibbs Free Energy = -2156.238003 a.u.

Cu	-0.01882600	-1.07132500	-1.45848100
C	-0.65845300	-0.35338600	1.64411900
C	-1.32485400	-0.42044600	2.87433100
C	-0.60711300	-0.56320500	4.06331900
C	0.78696800	-0.63546300	4.03406300
C	1.46382900	-0.56576600	2.81479500
C	0.75442400	-0.42768900	1.61450400
H	-2.40915300	-0.37598800	2.90474400
H	-1.13748800	-0.62189600	5.00961300
H	1.34791800	-0.75036300	4.95720200
H	2.54774100	-0.62694000	2.79868000
P	-1.53402800	-0.15599500	0.02220700
P	1.58078600	-0.36245200	-0.04060700
C	-1.70047900	1.67795200	-0.08049900
C	-2.22481700	2.45304100	0.96724300
C	-2.24307800	3.84410500	0.87067500
C	-1.73204100	4.47498200	-0.26894000
C	-1.20923500	3.71120700	-1.31374200
C	-1.19500800	2.31739000	-1.22045500
H	-2.61059800	1.97057900	1.86048400
H	-2.64779100	4.43692600	1.68640500
H	-1.73690100	5.55941400	-0.33643600
H	-0.79940800	4.19626300	-2.19480100
H	-0.76532800	1.71481000	-2.01610700
C	-3.22494300	-0.79345700	0.34425300
C	-3.35600700	-2.14004300	0.73049000
C	-4.61778500	-2.70573600	0.90474600
C	-5.76771900	-1.94213700	0.67749400
C	-5.64594500	-0.60978000	0.27977500
C	-4.38244900	-0.03507900	0.11515900
H	-2.46718200	-2.74323000	0.89627100
H	-4.70387500	-3.74448800	1.21131900
H	-6.75090700	-2.38571000	0.80680500
H	-6.53445400	-0.01115200	0.09871000
H	-4.30364800	1.00352600	-0.18939100
C	2.00414100	1.41795600	-0.24765300
C	1.88501100	2.36751400	0.77650500
C	2.13828800	3.71708200	0.51770400
C	2.52621300	4.12746600	-0.75895300
C	2.65475600	3.18430100	-1.78369900
C	2.38410500	1.84012300	-1.53256400
H	1.57711100	2.06215000	1.77114900
H	2.02791400	4.44663500	1.31513300
H	2.71935500	5.17778900	-0.95848500
H	2.94829300	3.49859500	-2.78145300
H	2.44197700	1.11474200	-2.33982600
C	3.19545200	-1.19837300	0.21202500
C	4.34924300	-0.52936500	0.64928000
C	5.54351200	-1.23181700	0.82370200
C	5.59515300	-2.60443000	0.56611900
C	4.45041500	-3.27553600	0.12697300
C	3.25743900	-2.57516300	-0.05637000
H	4.31670600	0.53729100	0.85062500
H	6.43288900	-0.70656200	1.16081200
H	6.52613800	-3.14794400	0.70110400
H	4.48845400	-4.34097200	-0.08221400
H	2.36866000	-3.09079400	-0.41291400
C	-0.43466300	-2.19941800	-3.21992900
C	-0.19056600	-0.81457900	-3.52478400
H	0.34772400	-2.89383400	-3.52282800
H	0.74327100	-0.54531400	-4.01228200
H	-1.04704300	-0.18779100	-3.76596800
H	-0.26202200	-2.66361000	-1.70034600

C	-1.84143600	-2.74672100	-3.39796200
H	-1.96154500	-3.73634600	-2.94547600
H	-2.57326400	-2.07336600	-2.94027800
H	-2.07310700	-2.82048000	-4.46864800

IM2b'

SCF Energy = -2156.754358 a.u.

Gibbs Free Energy = -2156.285528 a.u.

Cu	-0.11859100	-1.14859800	-1.45226800
C	-0.48461900	-0.27675300	1.74236700
C	-1.08312700	-0.31509500	3.00875800
C	-0.30219900	-0.46461800	4.15599500
C	1.08566800	-0.58031700	4.04640600
C	1.69375200	-0.55242000	2.79005700
C	0.92189800	-0.40355300	1.62937900
H	-2.16250100	-0.23423000	3.09828100
H	-0.77714600	-0.49444500	5.13250800
H	1.69512100	-0.69925700	4.93774700
H	2.77193900	-0.65454600	2.71402500
P	-1.43066000	-0.07832200	0.16834400
P	1.63389400	-0.41697700	-0.07732800
C	-1.54390600	1.74434700	-0.03045300
C	-1.69452800	2.63302500	1.04617000
C	-1.71085500	4.01050100	0.82313200
C	-1.56773300	4.51323700	-0.47332400
C	-1.41057800	3.63592300	-1.54880900
C	-1.39777100	2.25773100	-1.32867800
H	-1.78232500	2.25136600	2.05896600
H	-1.82539000	4.69153900	1.66185300
H	-1.56932300	5.58622400	-0.64314400
H	-1.28424300	4.02261000	-2.55585400
H	-1.25127200	1.57328000	-2.16027500
C	-3.11873400	-0.66522800	0.58261500
C	-3.35065000	-2.04371600	0.43517500
C	-4.60289700	-2.58441200	0.72488400
C	-5.64270700	-1.75101300	1.14836400
C	-5.42408600	-0.37789200	1.28248200
C	-4.16745200	0.16551900	1.00307100
H	-2.54819200	-2.68738100	0.08218600
H	-4.77087500	-3.65137600	0.60860500
H	-6.62134000	-2.16984200	1.36531500
H	-6.23162700	0.27329400	1.60558700
H	-4.00877100	1.23399400	1.10866900
C	2.00335400	1.34555900	-0.44253200
C	1.93818000	2.36692300	0.51594000
C	2.15263200	3.69567700	0.14249300
C	2.44424000	4.01537800	-1.18532200
C	2.51791300	3.00161900	-2.14514100
C	2.28949300	1.67560700	-1.77872200
H	1.70496600	2.13047300	1.54923600
H	2.08602400	4.48078900	0.89039700
H	2.60650500	5.05036700	-1.47289300
H	2.73877100	3.24493200	-3.18070100
H	2.32155400	0.89226100	-2.53217700
C	3.27944600	-1.20471700	0.12930600
C	4.44404800	-0.49020600	0.45102300
C	5.66057900	-1.16017100	0.59650000
C	5.72416500	-2.54592400	0.42624800
C	4.56886100	-3.26310500	0.10304800
C	3.35342100	-2.59516100	-0.05223900
H	4.40199400	0.58669500	0.58576000
H	6.55809400	-0.59961900	0.84323000
H	6.67227300	-3.06434000	0.53869900
H	4.61589200	-4.33919400	-0.03858000
H	2.45763600	-3.15017000	-0.32130200
C	-1.87450000	-2.79173900	-3.23137200
C	-0.43399700	-2.26781600	-3.06120200
H	-1.96490000	-3.46715100	-4.10169700
H	0.25517500	-3.13148300	-3.06117100
H	-0.16319700	-1.70605100	-3.97518600
H	-2.15430800	-3.39845500	-2.35714100
C	-2.91096600	-1.67556000	-3.39300400
H	-3.92744300	-2.06865400	-3.52155800
H	-2.90970100	-1.01844800	-2.51577700
H	-2.68084900	-1.05413800	-4.26874800

TS2

SCF Energy = -3634.366404 a.u.

Gibbs Free Energy = -3633.590068 a.u.

C	0.87263400	0.26254900	2.13199900
C	0.71978000	0.39307000	3.51906400

C	1.83658100	0.46135400	4.35330000	H	1.00666200	3.80593000	-3.18719600
C	3.12078400	0.39843300	3.80813100	H	1.07524500	1.43920900	-2.43831600
C	3.28862500	0.27394200	2.42792700	C	4.00462800	-0.65992600	-0.50978600
C	2.17649500	0.21067200	1.57796300	C	5.14517900	0.07740100	-0.85857500
H	-0.27671300	0.43480700	3.94841800	C	6.37030300	-0.57121400	-1.03658400
H	1.70271600	0.55876300	5.42677800	C	6.46721400	-1.95359200	-0.86364800
H	3.99192700	0.44355800	4.45535600	C	5.33162700	-2.69430600	-0.52104200
H	4.28961000	0.21916200	2.01080700	C	4.10494900	-2.05380800	-0.35270800
P	-0.56885400	0.11490300	0.98956100	H	5.08310500	1.15216100	-0.99514400
P	2.34307800	0.07096300	-0.26092200	H	7.24892100	0.00710300	-1.30847500
C	-0.98087100	1.84569600	0.53048700	H	7.42150200	-2.45385300	-1.00226200
C	-0.32683000	2.96086500	1.07230300	H	5.39845100	-3.77133000	-0.39527700
C	-0.63180200	4.24416900	0.61220500	H	3.21631700	-2.63364100	-0.11569900
C	-1.60014600	4.42609500	-0.37754200	C	-2.61795500	-2.75438300	-0.94841600
C	-2.26357800	3.31816900	-0.91357800	C	-2.77026300	-1.57933300	-1.74735000
C	-1.94854600	2.03403900	-0.47163600	C	-1.66123600	-1.23687900	-2.54597400
H	0.42965000	2.83247600	1.83936300	C	-1.45421800	-3.47882000	-0.88780800
H	-0.10857100	5.10066700	1.02750700	H	-3.46971200	-3.10380700	-0.36954900
H	-1.83450800	5.42595300	-0.73203500	H	-1.71926000	-0.37484000	-3.20602300
H	-3.02139400	3.44755100	-1.68111300	C	1.20495900	-4.90898300	-0.57599200
H	-2.45701800	1.17803900	-0.90212800	H	-1.42492100	-4.38231200	-0.28542000
C	-1.96295400	-0.45213000	2.03277300	H	0.71280200	-5.83956800	-0.90956900
C	-2.05433300	-1.82860300	2.29983500	H	2.27486600	-5.13442800	-0.50025300
C	-3.12058500	-2.33095500	3.04516100	H	0.84346700	-4.73074900	0.44852900
C	-4.11353600	-1.46698500	3.51805500	C	-3.96599800	-0.73152300	-1.66237900
C	-4.03092300	-0.09828300	3.25082600	C	-4.37477800	0.10182800	-2.73065100
C	-2.95984200	0.40996100	2.51270800	C	-4.72998200	-0.66523900	-0.47245500
H	-1.30481500	-2.50623800	1.90191100	C	-5.46742300	0.95878200	-2.60981300
H	-3.18450800	-3.39705100	3.24375000	H	-3.83556400	0.06442400	-3.67302500
H	-4.95054600	-1.86070100	4.08772300	C	-5.82898900	0.18396500	-0.35925400
H	-4.80154100	0.57619000	3.61333400	H	-4.42801500	-1.25173000	0.38949200
H	-2.90934800	1.47292600	2.30029800	C	-6.20790000	1.00846800	-1.42344900
C	2.42199100	1.82424100	-0.80005700	H	-5.75117600	1.58315000	-3.45385300
C	3.14034500	2.80682100	-0.09982400	H	-6.37925000	0.21731800	0.57807400
C	3.10115900	4.13633600	-0.52084900	H	-7.05947800	1.67654600	-1.33086900
C	2.33672400	4.49764700	-1.63442200	Cu	0.38626000	-0.92058300	-0.84438500
C	1.61404800	3.52671400	-2.33135100	C	-0.25365500	-3.09742200	-1.62696000
C	1.65730500	2.19480200	-1.91635000	C	-0.44764000	-1.94266000	-2.51927900
H	3.71535500	2.53844400	0.78144700	H	0.29925300	-1.74207800	-3.28666500
H	3.65740100	4.89209500	0.02650400	C	0.96674700	-3.73515900	-1.48786900
H	2.29725300	5.53589800	-1.95141100	H	1.78837700	-3.40603900	-2.12023500

IM3

SCF Energy = -3634.432335 a.u.

Gibbs Free Energy = -3633.654731 a.u.

Cu	0.26391700	-0.87224600	-1.57038500
C	-2.11009100	-2.73665300	0.90920700
C	-3.20702100	-3.51480200	1.31749700
C	-3.06281800	-4.86457400	1.63320700
C	-1.80873600	-5.46975900	1.53511900
C	-0.70952300	-4.72073400	1.12044100
C	-0.84410500	-3.35845800	0.80505300
H	-4.18904700	-3.05707600	1.38234900
H	-3.92756300	-5.44171600	1.94828200
H	-1.68536800	-6.52231500	1.77326500
H	0.25821400	-5.20359900	1.03451400
P	-2.32190700	-0.94570700	0.45761100
P	0.63735500	-2.40882900	0.25781000
C	-2.60316800	-0.09346900	2.06799600
C	-2.89296500	-0.72326400	3.28817200
C	-3.05659500	0.03069300	4.45299800
C	-2.95051100	1.42325800	4.41107200
C	-2.67061200	2.06111600	3.19956400
C	-2.48481400	1.30781000	2.03986700
H	-2.98602600	-1.80340600	3.33591700
H	-3.27204900	-0.47149000	5.39240400
H	-3.08168300	2.00708500	5.31795300
H	-2.58508800	3.14345300	3.15780200
H	-2.24310900	1.80880500	1.10625700
C	-4.01181100	-1.00707900	-0.28253000
C	-4.11721300	-1.56519900	-1.56995000
C	-5.35101700	-1.61598900	-2.21720800
C	-6.49489500	-1.10141600	-1.59625800
C	-6.39708600	-0.54684600	-0.31870300
C	-5.16238400	-0.50135000	0.33804000
H	-3.22118400	-1.93862000	-2.05870500
H	-5.41951800	-2.04893000	-3.21172100
H	-7.45423900	-1.13382200	-2.10521100
H	-7.28084500	-0.14734400	0.17182500
H	-5.10010300	-0.06466700	1.32974100
C	1.39027300	-1.77115400	1.80027200
C	0.62676500	-1.59729800	2.96543100
C	1.17520700	-0.95923000	4.07893700
C	2.48979400	-0.48857100	4.04490300
C	3.26283900	-0.66704800	2.89421300
C	2.71685800	-1.30545000	1.78103300
H	-0.39842700	-1.94563900	3.00708800
H	0.56565900	-0.82174600	4.96763400
H	2.90890200	0.02143300	4.90774000
H	4.27340300	-0.27352700	2.83439900
H	3.32105000	-1.41872600	0.88707700
C	1.80090900	-3.65788100	-0.41022900
C	2.78448800	-4.29610600	0.36077500
C	3.64266000	-5.22561000	-0.23039800
C	3.52319200	-5.52828100	-1.58909800
C	2.54054200	-4.90092800	-2.36006200
C	1.68397100	-3.96696300	-1.77726900
H	2.88627300	-4.06638800	1.41645800
H	4.40395500	-5.71292800	0.37212200
H	4.19480800	-6.24971900	-2.04584200
H	2.44408000	-5.13343300	-3.41683300
H	0.91632100	-3.47645100	-2.37097200
C	-3.38230900	1.80804300	-2.25568700
C	-3.08768800	2.95207000	-1.49159500
C	-1.73175200	3.29910800	-1.32388400
C	-0.72324500	2.52084200	-1.87139700
C	-1.01495800	1.35464900	-2.61052800
C	-2.37068800	1.02688800	-2.80352000
H	-4.41657900	1.52294300	-2.42087700
H	-1.46941200	4.16761100	-0.72721900
H	0.31501400	2.79320700	-1.70614400
C	0.09007900	0.51868200	-3.10959700
C	-0.08996800	-0.32999100	-4.34796000
H	1.02390400	1.07387500	-3.13939800
H	-2.63396800	0.13882700	-3.36549600
H	-0.23552100	0.33172700	-5.21485900
H	0.80686600	-0.92918100	-4.53023500
C	-4.15982100	3.75485000	-0.85620700
C	-4.04647500	5.15185200	-0.73136700
C	-5.31079800	3.13182400	-0.34026500
C	-5.04832400	5.89809500	-0.11088700
H	-3.17859500	5.65910400	-1.14262600
C	-6.31117200	3.87882100	0.28074700

H	-5.40827000	2.05363500	-0.40289600
C	-6.18518500	5.26542500	0.39961100
H	-4.94383300	6.97685400	-0.03240500
H	-7.18631400	3.37406400	0.68119600
H	-6.96409400	5.84717300	0.88450800
H	-0.93855200	-1.00764100	-4.27012900
C	1.68236100	1.06889100	0.05464500
C	2.81547600	1.68997800	0.56976100
C	4.07364600	1.45822800	0.02416800
C	4.14773700	0.58770400	-1.06007300
C	3.00435100	-0.02042400	-1.56576500
C	1.74792900	0.18412900	-1.01203500
O	5.80328100	1.32967600	1.64079900
F	2.69912600	2.50358600	1.63999300
F	0.50098600	1.29863800	0.67590100
F	3.14327800	-0.86260900	-2.62425200
F	5.34866300	0.33205300	-1.62814000
F	-0.97400600	-2.05513500	-2.28914300
C	5.32074400	1.97619500	0.70658400
N	5.84737900	3.13260400	0.24145200
C	7.06139500	3.65448400	0.88395000
C	5.26433900	3.92120800	-0.85174700
H	5.38122300	4.97783200	-0.58912400
H	4.19135200	3.72468800	-0.89740300
H	7.67085800	2.80391700	1.19601500
H	7.62242900	4.21139600	0.12806400
C	5.91794600	3.62697600	-2.20245600
C	6.73624900	4.54366800	2.08433900
H	6.20030400	3.97039600	2.84653000
H	7.65776200	4.93373700	2.52982500
H	6.11324000	5.39528400	1.79020100
H	6.99229000	3.83762200	-2.17566500
H	5.78429800	2.57625000	-2.47350300
H	5.46954300	4.25042000	-2.98339200

TS3

SCF Energy = -2579.672331 a.u.

Gibbs Free Energy = -2579.07607 a.u.

C	0.87263400	0.26254900	2.13199900
C	0.71978000	0.39307000	3.51906400
C	1.83658100	0.46135400	4.35330000
C	3.12078400	0.39843300	3.80813100
C	3.28862500	0.27394200	2.42792700
C	2.17649500	0.21067200	1.57796300
H	-0.27671300	0.43480700	3.94841800
H	1.70271600	0.55876300	5.42677800
H	3.99192700	0.44355800	4.45535600
H	4.28961000	0.21916200	2.01080700
P	-0.56885400	0.11490300	0.98956100
P	2.34307800	0.07096300	-0.26092200
C	-0.98087100	1.84569600	0.53048700
C	-0.32683000	2.96086500	1.07230300
C	-0.63180200	4.24416900	0.61220500
C	-1.60014600	4.42609500	-0.37754200
C	-2.26357800	3.31816900	-0.91357800
C	-1.94854600	2.03403900	-0.47163600
H	0.42965000	2.83247600	1.83936300
H	-0.10857100	5.10066700	1.02750700
H	-1.83450800	5.42595300	-0.73203500
H	-3.02139400	3.44755100	-1.68111300
H	-2.45701800	1.17803900	-0.90212800
C	-1.96295400	-0.45213000	2.03277300
C	-2.05433300	-1.82860300	2.29983500
C	-3.12058500	-2.33095500	3.04516100
C	-4.11353600	-1.46698500	3.51805500
C	-4.03092300	-0.09828300	3.25082600
C	-2.95984200	0.40996100	2.51270800
H	-1.30481500	-2.50623800	1.90191100
H	-3.18450800	-3.39705100	3.24375000
H	-4.95054600	-1.86070100	4.08772300
H	-4.80154100	0.57619000	3.61333400
H	-2.90934800	1.47292600	2.30029800
C	2.42199100	1.82424100	-0.80005700
C	3.14034500	2.80682100	-0.09982400
C	3.10115900	4.13633600	-0.52084900
C	2.33672400	4.49764700	-1.63442200
C	1.61404800	3.52671400	-2.33135100
C	1.65730500	2.19480200	-1.91635000
H	3.71535500	2.53844400	0.78144700
H	3.65740100	4.89209500	0.02650400
H	2.29725300	5.53589800	-1.95141100

H	1.00666200	3.80593000	-3.18719600
H	1.07524500	1.43920900	-2.43831600
C	4.00462800	-0.65992600	-0.50978600
C	5.14517900	0.07740100	-0.85857500
C	6.37030300	-0.57121400	-1.03658400
C	6.46721400	-1.95359200	-0.86364800
C	5.33162700	-2.69430600	-0.52104200
C	4.10494900	-2.05380800	-0.35270800
H	5.08310500	1.15216100	-0.99514400
H	7.24892100	0.00710300	-1.30847500
H	7.42150200	-2.45385300	-1.00226200
H	5.39845100	-3.77133000	-0.39527700
H	3.21631700	-2.63364100	-0.11569900
C	-2.61795500	-2.75438300	-0.94841600
C	-2.77026300	-1.57933300	-1.74735000
C	-1.66123600	-1.23687900	-2.54597400
C	-1.45421800	-3.47882000	-0.88780800
H	-3.46971200	-3.10380700	-0.36954900
H	-1.71926000	-0.37484000	-3.20602300
C	1.20495900	-4.90898300	-0.57599200
H	-1.42492100	-4.38231200	-0.28542000
H	0.71280200	-5.83956800	-0.90956900
H	2.27486600	-5.13442800	-0.50025300
H	0.84346700	-4.73074900	0.44852900
C	-3.96599800	-0.73152300	-1.66237900
C	-4.37477800	0.10182800	-2.73065100
C	-4.72998200	-0.66523900	-0.47245500
C	-5.46742300	0.95878200	-2.60981300
H	-3.83556400	0.06442400	-3.67302500
C	-5.82898900	0.18396500	-0.35925400
H	-4.42801500	-1.25173000	0.38949200
C	-6.20790000	1.00846800	-1.42344900
H	-5.75117600	1.58315000	-3.45385300
H	-6.37925000	0.21731800	0.57807400
H	-7.05947800	1.67654600	-1.33086900
Cu	0.38626000	-0.92058300	-0.84438500
C	-0.25365500	-3.09742200	-1.62696000
C	-0.44764000	-1.94266000	-2.51927900
H	0.29925300	-1.74207800	-3.28666500
C	0.96674700	-3.73515900	-1.48786900
H	1.78837700	-3.40603900	-2.12023500

IM4

SCF Energy = -2579.674361 a.u.

Gibbs Free Energy = -2579.080484 a.u.

C	-0.72696100	-0.64508800	2.11220200
C	-0.52263000	-0.94181700	3.46676600
C	-1.60647100	-1.08259100	4.33421800
C	-2.90934700	-0.92220700	3.85695800
C	-3.12906700	-0.63003600	2.51002000
C	-2.05054400	-0.49770200	1.62504400
H	0.48842400	-1.05315100	3.84701700
H	-1.43261100	-1.31003200	5.38195400
H	-3.75437900	-1.02125100	4.53216200
H	-4.14380900	-0.49780100	2.14727400
P	0.67684600	-0.38549300	0.94200300
P	-2.27313500	-0.13309400	-0.17202600
C	1.08580500	-2.05569000	0.30219200
C	0.37141400	-3.20661700	0.66254900
C	0.66360300	-4.43176100	0.05793300
C	1.67837000	-4.52108800	-0.89696400
C	2.40297600	-3.37843000	-1.25068000
C	2.10388900	-2.14974400	-0.66382600
H	-0.42253000	-3.14848900	1.39955700
H	0.09297400	-5.31420200	0.33270200
H	1.90218800	-5.47514500	-1.36591500
H	3.19774300	-3.43658500	-1.98900200
H	2.66468700	-1.26688500	-0.95419100
C	2.09233200	0.10250000	1.99537500
C	2.17747000	1.45283900	2.37281600
C	3.25377700	1.90245100	3.13739500
C	4.26172400	1.01193200	3.51981700
C	4.18339200	-0.33162400	3.14441900
C	3.10229100	-0.78802800	2.38747000
H	1.41681400	2.15478200	2.04353000
H	3.31375100	2.94975000	3.41957100
H	5.10669500	1.36520700	4.10407500
H	4.96502600	-1.02650700	3.43825300
H	3.05602800	-1.83124200	2.09183800
C	-2.41651300	-1.79819500	-0.93065400
C	-3.06273700	-2.87733400	-0.30701600

C	-3.08070000	-4.13161800	-0.91810400
C	-2.44534900	-4.32243000	-2.14863100
C	-1.79259200	-3.25578400	-2.77089100
C	-1.77736900	-1.99913000	-2.16413700
H	-3.53506000	-2.74516900	0.66173800
H	-3.58129500	-4.96232100	-0.42874200
H	-2.45101900	-5.30297600	-2.61598700
H	-1.28567200	-3.40339600	-3.72003600
H	-1.24971400	-1.17220700	-2.63375300
C	-3.90807100	0.67963900	-0.29986500
C	-5.12314100	-0.00854900	-0.43732600
C	-6.32295900	0.70150500	-0.51867200
C	-6.31919900	2.09788700	-0.46181900
C	-5.11084300	2.78841400	-0.33400500
C	-3.90845400	2.08463500	-0.26085100
H	-5.13592700	-1.09280700	-0.48702800
H	-7.26035000	0.16321100	-0.62742900
H	-7.25479100	2.64616800	-0.52714500
H	-5.10104500	3.87435200	-0.30372700
H	-2.96748200	2.62733800	-0.19060700
C	2.40279900	3.06382800	-0.64470500
C	2.49167400	1.97305200	-1.56071600
C	1.31134800	1.70041300	-2.29276300
C	1.26712100	3.82223300	-0.47736700
H	3.27987800	3.32205700	-0.05565600
H	1.30674000	0.88954900	-3.01838700
C	-1.17407300	5.60586400	-0.26081400
H	1.29964500	4.66559200	0.20739400
H	-0.42722200	6.39054800	-0.46873000
H	-2.15805900	6.07882200	-0.35474600
H	-1.04757600	5.35018300	0.80455900
C	3.65515900	1.08253400	-1.62411000
C	3.94519400	0.31150100	-2.77662000
C	4.51251300	0.90529200	-0.51105300
C	5.00109300	-0.59758600	-2.80162500
H	3.33946500	0.43680700	-3.66977100
C	5.57396800	0.00313600	-0.54308500
H	4.31249300	1.44380500	0.40925400
C	5.82733700	-0.76458200	-1.68437400
H	5.18816200	-1.17187400	-3.70613400
H	6.19282500	-0.11697000	0.34285000
H	6.64859500	-1.47537400	-1.70429400
Cu	-0.29475200	0.87367300	-0.74110300
C	0.04895500	3.60532900	-1.25152100
C	0.11815600	2.43294800	-2.13603700
H	-0.67846800	2.29719800	-2.86728400
C	-1.05969100	4.41394300	-1.17575700
H	-1.90690200	4.18585500	-1.81995300

$TS5_p$

SCF Energy = -3634.377966 a.u.

Gibbs Free Energy = -3633.60312 a.u.

Cu	0.97682400	0.37169500	-0.08968900
C	3.87337300	-0.51334600	-1.26131100
C	4.79397700	-1.09817800	-2.14176900
C	5.93695700	-0.40265600	-2.53828200
C	6.16894300	0.88970700	-2.06231100
C	5.26362900	1.48365900	-1.18140800
C	4.11730300	0.79319200	-0.76622900
H	4.61101500	-2.09721700	-2.52614600
H	6.64052500	-0.86688400	-3.22314100
H	7.05285000	1.43712700	-2.37656700
H	5.44762700	2.49045600	-0.81853000
P	2.31324000	-1.36619100	-0.76982000
P	2.90008200	1.51105000	0.42356300
C	2.73984500	-2.40370200	0.67991500
C	4.03258500	-2.47581100	1.21631900
C	4.26432400	-3.19946000	2.38882600
C	3.21434400	-3.86531800	3.02426700
C	1.92467200	-3.80566900	2.48651400
C	1.68388200	-3.07089100	1.32684700
H	4.85494100	-1.95851200	0.73318400
H	5.26670200	-3.23735900	2.80542300
H	3.39836200	-4.42532500	3.93679100
H	1.10123100	-4.32128700	2.97239300
H	0.67647900	-3.01549700	0.92572200
C	1.94241500	-2.52502200	-2.13480700
C	1.26743000	-2.00513700	-3.25154500
C	0.91156100	-2.84147100	-4.30927900
C	1.21244700	-4.20601400	-4.25337600
C	1.87926500	-4.72876000	-3.14220800

C	2.24699500	-3.89274600	-2.08568100	H	-2.07690800	3.05025100	-3.67979800
H	0.99908900	-0.95281400	-3.27844100	H	-1.44654800	4.57250200	-3.06971600
H	0.38575400	-2.43210900	-5.16709000	H	-0.33064200	3.30757000	-3.59858800
H	0.92318500	-4.86003100	-5.07103400	C	-1.68570000	-2.63098800	-0.22787600
H	2.11278200	-5.78865400	-3.09556200	C	-2.11754000	-3.02018500	1.05821000
H	2.75631500	-4.30760800	-1.22161700	C	-1.28003300	-3.64599300	-1.11930400
C	3.54658800	0.97497800	2.05472200	C	-2.12541200	-4.36342300	1.43578300
C	4.91685200	0.86722500	2.34085400	H	-2.48131300	-2.26551200	1.74783700
C	5.33746000	0.38646300	3.58145800	C	-1.29251200	-4.98756700	-0.73830500
C	4.39667600	0.00029100	4.54057600	H	-0.90989800	-3.38050600	-2.10372900
C	3.03169700	0.10053400	4.26130900	C	-1.70897000	-5.35672100	0.54361300
C	2.60788800	0.58541100	3.02324400	H	-2.46976100	-4.63549600	2.43047000
H	5.65380400	1.13969400	1.59147300	H	-0.95420000	-5.74346600	-1.44217700
H	6.39925900	0.30368800	3.79568500	H	-1.71045500	-6.40128400	0.84242400
H	4.72767800	-0.38517300	5.50069100	C	-3.41772900	3.26539100	0.44357000
H	2.29807700	-0.20909400	4.99981000	C	-3.81420700	2.19030700	1.20870600
H	1.54613800	0.64406000	2.79593200	C	-4.45343800	1.06011500	0.66361600
C	3.10549400	3.32435300	0.31030300	C	-4.57867700	1.07636400	-0.73968400
C	4.02619300	4.05893300	1.07265100	C	-4.20861300	2.15039400	-1.51875200
C	4.10642800	5.44531000	0.92449900	C	-3.48591100	3.23724100	-0.96908500
C	3.27316800	6.10559300	0.01754200	O	-3.79529500	-0.51884300	2.29868000
C	2.34928500	5.37929400	-0.73927000	F	-3.59837900	2.26672000	2.53877800
C	2.25973600	3.99541100	-0.58945000	F	-2.77595100	4.30852100	1.02737900
H	4.67205700	3.55584800	1.78551300	F	-4.32540600	2.07937200	-2.87069300
H	4.81923100	6.00913800	1.51962600	F	-5.07241800	-0.01218000	-1.37596500
H	3.33682300	7.18446100	-0.09199100	F	-3.55380700	4.44339500	-1.62029600
H	1.68942700	5.88905800	-1.43545300	C	-4.67473500	-0.15297100	1.50383900
H	1.52089200	3.43658700	-1.15870700	N	-5.84540100	-0.84690000	1.34203200
C	-1.72861000	-0.76916600	-1.94036700	C	-5.97963700	-2.16001300	1.98517300
C	-1.59346700	-1.20628400	-0.60619500	C	-7.08297600	-0.25792500	0.81343900
C	-1.23966100	-0.22143500	0.34892900	H	-7.69459400	-1.07944400	0.42784900
C	-1.03675800	1.12580700	-0.00499100	H	-6.86583700	0.38470900	-0.03684400
C	-1.22157400	1.57851800	-1.36542800	H	-5.19637400	-2.24547100	2.73865100
C	-1.53675300	0.55368500	-2.31286500	H	-6.94450400	-2.19846700	2.50307500
H	-2.00838900	-1.48741700	-2.70611500	C	-7.85001400	0.52621200	1.88017800
H	-1.17721100	-0.49154100	1.39775800	C	-5.87086700	-3.29791300	0.96806800
H	-0.94712300	1.87266400	0.78054800	H	-4.90048200	-3.26756900	0.46449400
C	-1.28805900	2.95659300	-1.65871200	H	-5.96873300	-4.26806200	1.46850000
C	-1.28112200	3.49149700	-3.06982200	H	-6.65506100	-3.23013800	0.20603500
H	-0.90443700	3.62816000	-0.89265800	H	-8.09083600	-0.10314200	2.74362100
H	-1.69865000	0.82942600	-3.35004100	H	-7.25355000	1.37475000	2.23159800

H	-8.78925400	0.91319900	1.46924200

IM5

SCF Energy = -3634.410566 a.u.

Gibbs Free Energy = -3633.633347 a.u.

Cu	1.00004100	0.25277100	-0.15572200
C	4.02397700	-0.45536900	-1.08474500
C	5.05702200	-1.02866100	-1.83874000
C	6.17077600	-0.27239300	-2.20524000
C	6.25966600	1.06926400	-1.82703100
C	5.24015100	1.65295000	-1.07339700
C	4.12150600	0.90220100	-0.68740500
H	4.98435000	-2.06666400	-2.14971700
H	6.96325100	-0.72840800	-2.79131600
H	7.12097600	1.66294500	-2.11916400
H	5.31219200	2.69821600	-0.78823100
P	2.50480600	-1.40373400	-0.64674300
P	2.76311300	1.61814400	0.33962000
C	2.89642000	-2.32448900	0.88665000
C	4.07858100	-2.11282200	1.60918600
C	4.26036500	-2.73069300	2.84917500
C	3.27350500	-3.57086500	3.36825300
C	2.09646200	-3.79343900	2.64572400
C	1.90128300	-3.16659300	1.41627700
H	4.84838000	-1.45595300	1.21829300
H	5.17340700	-2.54925600	3.40865400
H	3.41790800	-4.04920800	4.33280500
H	1.32358400	-4.44650600	3.04088400
H	0.97855500	-3.33322800	0.86826000
C	2.28272600	-2.63716200	-1.97417300
C	1.61412400	-2.20575300	-3.13242500
C	1.35759000	-3.10130600	-4.17009000
C	1.75127400	-4.43805100	-4.05160700
C	2.41284300	-4.87248200	-2.89992200
C	2.68283500	-3.97642100	-1.86336900
H	1.27811900	-1.17471100	-3.20912700
H	0.83671100	-2.76175000	-5.06063100
H	1.53836100	-5.13957500	-4.85296200
H	2.71873000	-5.91056800	-2.80651500
H	3.18803000	-4.32353900	-0.96762200
C	3.32893300	1.33895700	2.06074400
C	4.67865500	1.39600100	2.44222200
C	5.04667900	1.10716900	3.75695200
C	4.07433500	0.75236900	4.69682200
C	2.72966100	0.69206400	4.32333100
C	2.35791700	0.98294000	3.01011700
H	5.44252400	1.64718500	1.71277200
H	6.09311400	1.15042000	4.04517500
H	4.36538900	0.51744600	5.71660000
H	1.97217300	0.40985900	5.04854400
H	1.31370800	0.92010900	2.71449100
C	2.79069800	3.41570100	0.01706500
C	3.49506000	4.34229700	0.79905300
C	3.43176200	5.70350900	0.49104200
C	2.67023100	6.14591400	-0.59357200
C	1.96315800	5.22605400	-1.37392000
C	2.01753400	3.86746700	-1.06628700
H	4.08283400	4.00780200	1.64841800
H	3.97577200	6.41836800	1.10180700
H	2.62011900	7.20592100	-0.82521000
H	1.35904200	5.56518900	-2.21036400
H	1.45088500	3.15548800	-1.66055800
C	-1.62597900	-1.06152900	-1.95247700
C	-1.42749500	-1.49433800	-0.63921300
C	-1.12080100	-0.51756200	0.34015800
C	-1.08440400	0.84995500	0.01291200
C	-1.33657600	1.28066900	-1.31637700
C	-1.57360900	0.30008500	-2.28481800
H	-1.86177300	-1.78687700	-2.72517800
H	-0.99938300	-0.81625600	1.37613800
H	-1.00260900	1.58726300	0.80445300
C	-1.56813900	2.76084400	-1.56156100
C	-1.32239400	3.23804700	-2.99522300
H	-0.89898700	3.32550400	-0.90462600
H	-1.79454700	0.59573700	-3.30423000
H	-2.03460500	2.80794200	-3.70086900
H	-1.43066800	4.32323400	-3.03960700
H	-0.30883400	2.97775200	-3.32226100
C	-1.49185600	-2.92158400	-0.25021100
C	-2.07553800	-3.29274700	0.97583600
C	-0.93046600	-3.91999100	-1.06488500
C	-2.07408700	-4.62786100	1.38147100

H	-2.56335500	-2.53544400	1.58466800
C	-0.92770600	-5.25308600	-0.65220700
H	-0.46214300	-3.64674600	-2.00444500
C	-1.49236800	-5.61109100	0.57483200
H	-2.53632300	-4.90157600	2.32595100
H	-0.46962100	-6.00774400	-1.28534400
H	-1.48592000	-6.64855600	0.89717900
C	-3.10148800	3.00860800	0.44790900
C	-3.75276500	2.04957400	1.16902400
C	-4.64185900	1.09874200	0.61151000
C	-4.71683100	1.20581900	-0.80018500
C	-4.06791400	2.14813700	-1.54791300
C	-3.03103500	3.04838200	-1.02104500
O	-4.14484200	-0.69697900	2.08670600
F	-3.52457900	2.03034100	2.50618200
F	-2.14735000	3.76530500	1.09990900
F	-4.09723100	2.00704300	-2.92106100
F	-5.43942900	0.27762700	-1.48741900
F	-3.28555500	4.43833700	-1.47264300
C	-4.97694100	-0.14114400	1.34500500
N	-6.21980600	-0.70373900	1.15235300
C	-6.43869500	-2.06378800	1.65605000
C	-7.39636600	0.02516700	0.67316100
H	-7.98320000	-0.65130500	0.04054500
H	-7.07862000	0.84871900	0.03873300
H	-5.90981500	-2.17932700	2.60490200
H	-7.50767200	-2.18561200	1.85339700
C	-8.25470800	0.56796700	1.81921500
C	-5.96339400	-3.12037000	0.65599300
H	-4.89070100	-3.01417200	0.47043800
H	-6.14440200	-4.13061300	1.04169400
H	-6.48814600	-3.01880700	-0.30046100
H	-8.59569800	-0.23153100	2.48569900
H	-7.67993600	1.28527400	2.41487900
H	-9.14034800	1.07961100	1.42512400

IM6

SCF Energy = -3634.491155 a.u.

Gibbs Free Energy = -3633.709336 a.u.

Cu	-0.26249900	-0.08560900	-0.98810600
C	0.94501100	1.35534900	1.81096400
C	1.02175300	1.10934100	3.18871800
C	2.20248300	1.34569300	3.89127000
C	3.32534400	1.83246800	3.22130100
C	3.25208300	2.09577300	1.85387600
C	2.07148700	1.86896900	1.13111200
H	0.16083200	0.71621500	3.71798300
H	2.24348200	1.14450200	4.95807600
H	4.25184900	2.01287700	3.75916500
H	4.12527000	2.48810900	1.34288200
P	-0.60360500	0.97383400	0.87434200
P	1.96843400	2.26630400	-0.68457100
C	-1.38989200	2.61174300	0.63187300
C	-1.27431300	3.63696000	1.58329800
C	-1.90209500	4.86465700	1.36796000
C	-2.64622800	5.07675800	0.20398000
C	-2.76262800	4.05994300	-0.74670300
C	-2.13652300	2.83133300	-0.53481700
H	-0.69384100	3.47767300	2.48739500
H	-1.80684400	5.65560800	2.10657800
H	-3.13221300	6.03393400	0.03721200
H	-3.34437500	4.21790100	-1.64871400
H	-2.22004100	2.03925400	-1.27355400
C	-1.67969900	0.08729900	2.06677300
C	-1.30893300	-1.22727600	2.39378200
C	-2.13261400	-2.01448400	3.19493200
C	-3.33411800	-1.49105200	3.68475200
C	-3.69650500	-0.17757400	3.38038900
C	-2.87426900	0.61385900	2.57170100
H	-0.36038800	-1.60940000	2.03520900
H	-1.83869600	-3.03360500	3.42326700
H	-3.98293300	-2.10430800	4.30396400
H	-4.62427700	0.23531900	3.76709500
H	-3.17565600	1.62607500	2.32493200
C	2.41623300	4.05537700	-0.70461800
C	2.13040500	4.90684100	0.37595500
C	2.34816800	6.28279100	0.27474600
C	2.85682700	6.83250200	-0.90362500
C	3.13660600	5.99602700	-1.98837800
C	2.91009000	4.62292200	-1.89402200
H	1.73843200	4.49841300	1.30154400

H	2.12363000	6.92393200	1.12307800
H	3.03143700	7.90212600	-0.97857600
H	3.53052500	6.41307000	-2.91133600
H	3.12860300	3.98689200	-2.74778700
C	3.46743400	1.41838200	-1.35890300
C	4.77115500	1.93840300	-1.28284600
C	5.85023500	1.22565500	-1.80763200
C	5.64276300	-0.01797300	-2.41211400
C	4.35156800	-0.54261300	-2.49202700
C	3.26605800	0.17223500	-1.97889700
H	4.94370100	2.90998200	-0.82992100
H	6.85217500	1.64199900	-1.74561400
H	6.48402100	-0.57144600	-2.82056100
H	4.18033300	-1.50659200	-2.96123200
H	2.26367800	-0.23488100	-2.08778500
C	-4.80027800	-1.58455400	-0.39191000
C	-4.47822700	-0.44440300	-1.14782800
C	-3.48248500	-0.57430900	-2.13204900
C	-2.84851400	-1.79274300	-2.35446700
C	-3.18019200	-2.93057200	-1.60497500
C	-4.16054200	-2.80575000	-0.61326400
H	-5.57226500	-1.52304900	0.36947600
H	-3.17385100	0.29179600	-2.70941600
H	-2.03796200	-1.84070900	-3.07448700
C	-2.38333700	-4.21584300	-1.84867000
C	-3.11558600	-5.52425400	-1.51684900
H	-2.14945700	-4.24155800	-2.91596800
H	-4.43677200	-3.66129400	-0.00624100
H	-4.04557400	-5.58378600	-2.09066000
H	-2.49073700	-6.37984400	-1.79124000
C	-5.14635500	0.86072300	-0.91429300
C	-5.41220300	1.73782500	-1.98160200
C	-5.51297600	1.26388500	0.38196100
C	-6.01483400	2.97617000	-1.75864400
H	-5.16231700	1.44032300	-2.99569500
C	-6.10992200	2.50453700	0.60541200
H	-5.30004500	0.61170400	1.22141900
C	-6.36202800	3.36848400	-0.46318800
H	-6.21559300	3.63421400	-2.59979100
H	-6.36989700	2.80010300	1.61834600
H	-6.82438800	4.33588500	-0.28884200
H	-3.35960000	-5.61591000	-0.45797000
C	0.09210300	-3.65496100	-1.82729300
C	1.26042600	-3.27292800	-1.17559500
C	1.36023200	-3.30633900	0.20979900
C	0.25605800	-3.79305900	0.90686300
C	-0.92377900	-4.12651700	0.26130000
C	-1.04901900	-4.05155300	-1.12860800
O	2.06152500	-1.53896300	1.57955300
F	2.30386100	-2.83408900	-1.90703900
F	0.06294300	-3.58456900	-3.17058300
F	-1.97954500	-4.47998300	1.02544800
F	0.30369100	-3.87235600	2.25420800
F	0.15193800	-0.79064400	-2.62298100
C	2.42484000	-2.55731200	0.98132000
N	3.69217900	-3.01825000	0.99302500
C	4.68162400	-2.27840300	1.79391000
C	4.11235000	-4.27039700	0.35247100
H	5.15888400	-4.14594600	0.05899000
H	3.54962800	-4.41157900	-0.57079000
H	4.16967700	-1.87008900	2.66815200
H	5.42475000	-3.00106000	2.14318300
C	3.94612200	-5.47529700	1.27801800
C	5.34182100	-1.15354200	0.99948600
H	4.59251300	-0.43401700	0.66153700
H	6.06893500	-0.62585200	1.62659300
H	5.86558300	-1.54310200	0.12193800
H	4.53216800	-5.35154800	2.19454000
H	2.89464300	-5.59756800	1.55937600
H	4.28045800	-6.39111100	0.77900800

IM7

SCF Energy = -2138.116554 a.u.

Gibbs Free Energy = -2137.733784 a.u.

Cu	-0.01865800	-0.73046200	-1.90578700
C	-0.75071600	-0.88089000	1.25065800
C	-1.45650800	-1.30175700	2.38577900
C	-0.77519300	-1.71535500	3.53161200
C	0.62117400	-1.71554400	3.55243000
C	1.33683300	-1.30759100	2.42573200
C	0.66651900	-0.88886800	1.26811700

H	-2.54221600	-1.30956900	2.37477400	C	5.53281800	-1.12705800	0.60634100
H	-1.33487000	-2.03862800	4.40466500	C	5.69963900	-2.41392200	0.08755700
H	1.15442000	-2.03769400	4.44223600	C	4.62849700	-3.05964900	-0.53650800
H	2.42218400	-1.32066300	2.44632900	C	3.39347000	-2.41907800	-0.64228900
P	-1.58145900	-0.30571300	-0.29559900	H	4.17300800	0.51334200	0.91655000
P	1.54996900	-0.37984200	-0.27215300	H	6.36543800	-0.62125900	1.08731600
C	-1.77500800	1.50030200	-0.02182500	H	6.66336700	-2.90961100	0.16320900
C	-1.99860600	2.06767200	1.24253000	H	4.75712400	-4.05623300	-0.94931200
C	-2.09111100	3.45296700	1.38267900	H	2.56464600	-2.91328100	-1.14384800
C	-1.95317200	4.28219100	0.26595000	F	-0.00664000	-1.22545200	-3.69156800
C	-1.72521200	3.72480700	-0.99434400	**P_1**			
C	-1.63509500	2.33948600	-1.13793100	SCF Energy = -1496.352402 a.u.			
H	-2.08284100	1.43113500	2.11808400	Gibbs Free Energy = -1495.9869 a.u.			
H	-2.26012800	3.88561700	2.36477700				
H	-2.01381100	5.36079100	0.38007700	C	-3.68387300	-0.88016300	-0.93550600
H	-1.60442200	4.36640800	-1.86232000	C	-4.01320300	-0.09811700	0.18381800
H	-1.43604400	1.90274100	-2.11363100	C	-3.20283000	-0.21870500	1.32757600
C	-3.26314700	-1.03096500	-0.20678800	C	-2.11313900	-1.08425600	1.34319900
C	-3.42191400	-2.31955700	-0.74380500	C	-1.78859800	-1.86382800	0.22316100
C	-4.66462300	-2.95158400	-0.70403000	C	-2.59103900	-1.74703700	-0.91707400
C	-5.76448700	-2.29594300	-0.14295800	H	-4.27396300	-0.79345700	-1.84324000
C	-5.61732900	-1.00782400	0.37751800	H	-3.44447100	0.35061300	2.22039000
C	-4.37218300	-0.37552400	0.34868400	H	-1.50270000	-1.16410200	2.24005000
H	-2.57054400	-2.82056800	-1.19902900	C	-0.56056100	-2.77090100	0.29006500
H	-4.77671100	-3.94895000	-1.11970000	C	-0.58334300	-3.97286200	-0.66940800
H	-6.73449200	-2.78445400	-0.11929600	H	-0.52164500	-3.16984600	1.30699400
H	-6.47191800	-0.49323900	0.80799500	H	-2.36431100	-2.32484100	-1.80624200
H	-4.26803500	0.62525000	0.75591000	H	-0.53460700	-3.66736800	-1.71645700
C	1.82019500	1.42688900	-0.07876000	H	0.27324900	-4.62329200	-0.46902800
C	1.68120900	2.10533400	1.14008600	H	-1.49805500	-4.55471900	-0.52021300
C	1.85926900	3.48955000	1.19574800	C	-5.17402300	0.82785300	0.16010100
C	2.18410800	4.20387900	0.04038600	C	-5.11645900	2.07290800	0.81225000
C	2.32620200	3.53291500	-1.17768800	C	-6.35731800	0.48861500	-0.52051600
C	2.13669100	2.15280000	-1.23932100	C	-6.20409600	2.94607300	0.78663800
H	1.42342800	1.55816800	2.04140300	H	-4.20453300	2.36853800	1.32273800
H	1.73857200	4.00935600	2.14200200	C	-7.44393400	1.36314000	-0.54818600
H	2.31780700	5.28097700	0.08656100	H	-6.43436900	-0.47671300	-1.01219500
H	2.56992700	4.08548000	-2.08069400	C	-7.37278700	2.59608700	0.10537200
H	2.21990300	1.63444400	-2.19162700	H	-6.13442600	3.90582500	1.29137000
C	3.21508000	-1.13198800	-0.11003300	H	-8.35015600	1.07726100	-1.07520500
C	4.29583300	-0.48632100	0.51043700	H	-8.21881200	3.27722200	0.08388400

C	1.02099800	-1.29772300	-1.08437500
C	2.16937800	-0.52779500	-1.22465200
C	3.04870600	-0.33952300	-0.16407500
C	2.73878300	-0.96380500	1.03803800
C	1.58875200	-1.73463400	1.17527400
C	0.70185800	-1.93516800	0.11675200
O	5.36035600	-0.24285900	-0.67112000
F	2.41602000	0.06746200	-2.41006000
F	0.20226600	-1.41955800	-2.14944900
F	1.33493200	-2.28743000	2.38036700
F	3.54784800	-0.79675900	2.10208500
C	4.36096400	0.39837700	-0.34604000
N	4.34662700	1.73666700	-0.14177800
C	5.60067300	2.48054500	-0.32470500
C	3.15902100	2.49742200	0.26792400
H	3.49242300	3.26767900	0.97123600
H	2.48726600	1.83879300	0.82188000
H	6.16683700	1.99663400	-1.12316800
H	5.34023700	3.48851000	-0.65993800
C	2.42860300	3.13039100	-0.91719700
C	6.42913700	2.53326500	0.95901500
H	6.71150000	1.52361000	1.27135300
H	7.34407100	3.11331100	0.79690800
H	5.86820200	3.00376900	1.77358000
H	3.08308400	3.81877500	-1.46210500
H	2.08845700	2.36065500	-1.61507800
H	1.55785800	3.69495400	-0.56729700

S2

SCF Energy = -1054.695364 a.u.

Gibbs Free Energy = -1054.540986 a.u.

C	2.17445900	-1.06961700	-0.26408000
C	0.80771700	-1.05199100	-0.52360300
C	0.05551300	0.11131100	-0.40226000
C	0.71667600	1.27709200	-0.02832100
C	2.08215300	1.28844700	0.23706600
C	2.81302800	0.10934100	0.11208200
O	-1.68627900	0.45953900	-1.96891700
F	0.20850300	-2.20264000	-0.88168400
F	2.87706000	-2.20414000	-0.37937500
F	2.69677700	2.41888200	0.60921700
F	0.02369000	2.42002200	0.10985000
F	4.12703300	0.10873800	0.36053300
C	-1.40615000	0.15027900	-0.81112800
N	-2.31788900	-0.16737700	0.13670400
C	-3.73969600	-0.14197600	-0.23576400
C	-1.98516300	-0.50340500	1.52719800
H	-2.74526600	-0.04002200	2.16496600
H	-1.03241300	-0.03814700	1.78706200
H	-3.82221200	-0.46593300	-1.27528200
H	-4.25736400	-0.87611100	0.38790000
C	-1.92662400	-2.01184900	1.77049100
C	-4.35209300	1.24789600	-0.06153600
H	-3.84782800	1.96920700	-0.71117100
H	-5.41521800	1.22992900	-0.32470400
H	-4.26387900	1.59300100	0.97424500
H	-2.88688200	-2.48608900	1.54272700
H	-1.16170400	-2.47491600	1.14127000
H	-1.68828500	-2.21652100	2.81964900

$TS4_p$

SCF Energy = -3634.376217 a.u.

Gibbs Free Energy = -3633.598863 a.u.

Cu	1.15719700	0.00195300	-0.68086300
C	0.79981100	2.00643100	1.86761800
C	0.36331900	3.08502000	2.65009600
C	0.25024400	2.96046600	4.03343600
C	0.58154000	1.75222600	4.65147600
C	1.02148600	0.67346900	3.88552100
C	1.13355400	0.78043500	2.49015800
H	0.09927200	4.02319100	2.17169900
H	-0.09415500	3.80266200	4.62647700
H	0.49861000	1.64867600	5.72946200
H	1.27394400	-0.26068800	4.37676400
P	0.98857500	2.16068200	0.03799400
P	1.73533900	-0.63586100	1.46070200
C	2.52353500	3.14628600	-0.14795300
C	2.58635100	4.53294000	0.06012200
C	3.80993900	5.19728000	-0.03226400
C	4.97931100	4.48472200	-0.31885600

C	4.92404200	3.10408800	-0.52161400	C	2.61955400	-1.77388700	-2.63540800
C	3.69933700	2.43882700	-0.44440800	C	1.87954200	-2.95049900	-2.31483400
H	1.68355100	5.09229500	0.28725000	C	0.50652700	-2.95561300	-2.19307200
H	3.85223100	6.27127900	0.12579400	C	-0.29797800	-1.77901800	-2.38344300
H	5.92985300	5.00667200	-0.38331900	C	0.45010200	-0.58127900	-2.67419200
H	5.82748100	2.54128700	-0.73776800	H	2.33019700	0.31108400	-3.15551500
H	3.65823800	1.36438300	-0.59729300	H	2.40874000	-3.88228300	-2.13886800
C	-0.40936700	3.19282300	-0.52874400	H	-0.00006700	-3.88564700	-1.94862400
C	-1.68476700	2.99155800	0.02541500	C	-1.70618300	-1.80282500	-2.29216400
C	-2.80234800	3.61398700	-0.53143000	C	-2.53579900	-0.60632600	-2.67274700
C	-2.66285300	4.44358400	-1.64707400	H	-2.15937000	-2.77892000	-2.44534900
C	-1.39740000	4.64729900	-2.20433400	H	-0.08142100	0.31542800	-2.98045800
C	-0.27588400	4.02295800	-1.65498500	H	-2.45679300	-0.33260300	-3.73734200
H	-1.81162500	2.34069300	0.88071100	H	-3.59406800	-0.79393800	-2.46804200
H	-3.77979700	3.43777100	-0.09347000	C	4.08796500	-1.76232200	-2.77276100
H	-3.53422600	4.92456600	-2.08207500	C	4.83186400	-2.95573600	-2.90670900
H	-1.28038900	5.29175400	-3.07105100	C	4.82235700	-0.55349700	-2.75323900
H	0.69996100	4.18410600	-2.10377000	C	6.22259500	-2.94106500	-3.01012800
C	3.56756000	-0.54370200	1.58805600	H	4.31945900	-3.91131400	-2.94877900
C	4.24538300	0.27652900	2.50196400	C	6.20988700	-0.53964100	-2.87125100
C	5.64003500	0.34427800	2.47968800	H	4.30809700	0.39157500	-2.61759500
C	6.36920700	-0.41116800	1.55732000	C	6.92661400	-1.73355600	-2.99619200
C	5.70076700	-1.23676400	0.64956700	H	6.75756100	-3.88172700	-3.11354200
C	4.30679400	-1.29345800	0.65843900	H	6.73629200	0.41125500	-2.84906300
H	3.69240700	0.87148200	3.22127100	H	8.00943000	-1.72327000	-3.08048600
H	6.15630500	0.99107400	3.18353500	H	-2.25281300	0.28532800	-2.09593000
H	7.45381000	-0.35118300	1.54161800	C	-3.65060900	-2.70264900	-0.31518900
H	6.25533400	-1.81552600	-0.08247100	C	-4.86200200	-2.05878600	-0.17566600
H	3.78934900	-1.90816200	-0.07103600	C	-4.97066200	-0.76212300	0.34012800
C	1.25389200	-2.12911900	2.42074300	C	-3.77061900	-0.14110600	0.68253800
C	2.15465700	-3.17939400	2.65357700	C	-2.54410400	-0.75352700	0.51177900
C	1.72964600	-4.34108500	3.30231700	C	-2.42364100	-2.02644600	-0.09415300
C	0.40593200	-4.46650300	3.72829900	O	-6.70652700	0.06585500	1.74174800
C	-0.49578800	-3.42311300	3.50077700	F	-5.98874600	-2.70206600	-0.56155700
C	-0.07929300	-2.26516800	2.84637000	F	-3.60223900	-3.94754700	-0.84446600
H	3.18902100	-3.09631600	2.33622800	F	-1.41325400	-0.07822100	0.85513000
H	2.43875400	-5.14500800	3.47896700	F	-3.80322000	1.11533900	1.18797900
H	0.07824800	-5.37030100	4.23408200	F	-1.33439300	-2.78760300	0.23883100
H	-1.52842900	-3.51110200	3.82653400	C	-6.28967500	-0.07638000	0.58998600
H	-0.78845000	-1.46469200	2.67225100	N	-6.95813100	0.37820200	-0.50528900
C	1.85205400	-0.60323000	-2.81543500	C	-8.23946400	1.06694000	-0.30557900

C	-6.42961400	0.31859100	-1.87495100
H	-7.29051500	0.29860700	-2.55016700
H	-5.90229800	-0.62407500	-2.02569600
H	-8.20890800	1.56430300	0.66586200
H	-8.32664500	1.83917700	-1.07643500
C	-5.51880900	1.50300100	-2.20120400
C	-9.42501100	0.10404900	-0.37052400
H	-9.34819900	-0.64704100	0.42156800
H	-10.36771000	0.64719900	-0.24078300
H	-9.46090000	-0.41512600	-1.33446400
H	-6.04959800	2.45262300	-2.07151600
H	-4.64338800	1.50940800	-1.54654100
H	-5.16923400	1.44591800	-3.23762500

TS5$_o$

SCF Energy = -3634.372197 a.u.

Gibbs Free Energy = -3633.600775 a.u.

Cu	-1.05629200	0.32247100	-0.22130900
C	-3.46045100	0.53878800	1.94875700
C	-4.16219400	0.30081200	3.13843100
C	-4.76503900	1.35311500	3.82837500
C	-4.66611300	2.65714700	3.33812300
C	-3.97261500	2.90880600	2.15314400
C	-3.37233100	1.86060900	1.44274900
H	-4.22837300	-0.70966000	3.53077300
H	-5.30448500	1.15536100	4.75010500
H	-5.12615700	3.47972200	3.87794900
H	-3.89399300	3.92671200	1.78343500
P	-2.58984700	-0.81162500	1.04652700
P	-2.46836700	2.12616900	-0.14771000
C	-3.82574400	-1.54263900	-0.09353700
C	-5.14575200	-1.08122900	-0.18530200
C	-6.00178300	-1.59769900	-1.16127500
C	-5.55235700	-2.58553900	-2.03987200
C	-4.23884300	-3.05715100	-1.94552600
C	-3.37449900	-2.53210400	-0.98619900
H	-5.50297600	-0.31037200	0.48963000
H	-7.01857900	-1.22302600	-1.23503300
H	-6.22058800	-2.98404000	-2.79801000
H	-3.88044600	-3.82643100	-2.62369700
H	-2.35075100	-2.89052600	-0.93022700
C	-2.22856900	-2.09157300	2.30103200
C	-1.09542000	-1.89689000	3.10869200
C	-0.72369900	-2.86366300	4.04244100
C	-1.47079000	-4.03924100	4.16712300
C	-2.59763400	-4.23824500	3.36536800
C	-2.98000500	-3.26790800	2.43653800
H	-0.49163100	-1.00219200	2.98692100
H	0.15788000	-2.70776300	4.65752300
H	-1.17173000	-4.79958500	4.88290300
H	-3.17932000	-5.15084100	3.45987800
H	-3.84996700	-3.43599500	1.80963300
C	-3.78872100	1.98976700	-1.41384300
C	-5.09865700	2.45392900	-1.21532000
C	-6.07161500	2.24592600	-2.19373700
C	-5.74892600	1.56647600	-3.37201400
C	-4.44853200	1.09866300	-3.57523500
C	-3.47266700	1.30815300	-2.59992200
H	-5.36491500	2.96026600	-0.29274100
H	-7.08389800	2.60525700	-2.03188900
H	-6.51170600	1.39603600	-4.12634300
H	-4.19661900	0.56065400	-4.48440400
H	-2.46558300	0.92448400	-2.74533900
C	-1.89707400	3.86208100	-0.10150600
C	-2.65601300	4.95404000	-0.54794200
C	-2.13046900	6.24585700	-0.47228200
C	-0.85018200	6.45554100	0.04750900
C	-0.08670600	5.36976000	0.48588700
C	-0.60442200	4.07708400	0.40659900
H	-3.64866100	4.79948200	-0.95951900
H	-2.72136500	7.08817600	-0.82082100
H	-0.44498600	7.46195500	0.10177000
H	0.91468600	5.52481600	0.87719400
H	0.00123100	3.23136100	0.72170900
C	1.46169500	-1.79960300	0.79290600
C	0.78103700	-2.12282800	-0.39913300
C	0.50885800	-1.05539000	-1.28732700
C	0.94015400	0.25786600	-1.02310500
C	1.69045900	0.57248500	0.16874800
C	1.88336200	-0.50899900	1.08188300
H	1.69507500	-2.59347600	1.49696000

H	-0.00072800	-1.25317400	-2.22689200	H	8.04428700	2.32710700	3.75399500
H	0.88507000	1.00403100	-1.81232200	H	7.80999300	2.97743900	2.11929600
C	2.37665500	1.81226600	0.26077100	H	9.03687700	-0.71931500	-0.03108100
C	2.85861500	2.39007000	1.56929000	H	7.57757500	-1.17251100	-0.92617700
H	2.05728400	2.55966600	-0.46524500	H	8.81713900	-0.15917200	-1.69968100
H	2.48440900	-0.34300500	1.96842700	F	3.91662100	-2.63507700	-2.53758800
H	3.39848500	1.65558500	2.17138000	F	5.29658900	-2.23744000	-0.20034700
H	3.54593700	3.22171500	1.38321400				
H	2.03309800	2.78370200	2.18589300	**TS5$_m$**			
C	0.26791900	-3.47907800	-0.67653400	SCF Energy = -3634.371398 a.u.			
C	0.17885500	-3.96781200	-1.99585500	Gibbs Free Energy = -3633.598967 a.u.			
C	-0.20453800	-4.30368200	0.36441300				
C	-0.38362300	-5.21527000	-2.26430800	Cu	1.20127000	0.40348100	0.00852300
H	0.57595500	-3.37216700	-2.81298000	C	3.75128400	-0.59137000	-1.74389300
C	-0.75961800	-5.55425200	0.09442000	C	4.46159400	-1.26188600	-2.74897200
H	-0.17493800	-3.94448600	1.38750600	C	5.47610500	-0.61311500	-3.45393100
C	-0.86038400	-6.01553300	-1.22098200	C	5.78673500	0.71746700	-3.16528200
H	-0.43849400	-5.56884400	-3.29062600	C	5.09121800	1.39707500	-2.16376600
H	-1.13226300	-6.15998300	0.91614400	C	4.07865000	0.75488000	-1.43886000
H	-1.30061900	-6.98625300	-1.43112800	H	4.21270500	-2.29145900	-2.98857600
C	3.67800400	0.99184100	-2.15404400	H	6.01657800	-1.14376000	-4.23234800
C	3.51537500	-0.27798500	-2.66149100	H	6.56881300	1.22825900	-3.71951000
C	4.04133600	-1.39456900	-2.00194700	H	5.33507900	2.43319900	-1.94962700
C	4.70471500	-1.17435500	-0.80081300	P	2.35110400	-1.38619100	-0.84406600
C	4.84486000	0.08388300	-0.23585100	P	3.15194300	1.58431900	-0.07152900
C	4.18274300	1.20228000	-0.83883200	C	3.10159200	-2.27799200	0.57141900
O	5.02559900	-0.02869600	2.15527000	C	4.47582500	-2.25450800	0.84468000
F	2.80433500	-0.46195400	-3.79406500	C	4.96880100	-2.85113600	2.00801200
F	3.05566300	2.03254000	-2.77596400	C	4.09869000	-3.48572600	2.89668600
F	4.79447300	2.43694400	-0.62194000	C	2.72738900	-3.52189000	2.62292600
C	5.57654200	0.22728700	1.07735500	C	2.22760100	-2.91231900	1.47343100
N	6.86870500	0.64544800	1.00797800	H	5.16000300	-1.75980300	0.16327600
C	7.62024900	0.81204300	2.25714100	H	6.03367200	-2.81506300	2.21890900
C	7.58335700	0.88799200	-0.25066300	H	4.48576500	-3.94745400	3.80059300
H	8.30284300	1.69311200	-0.06738900	H	2.04245200	-4.01505700	3.30690700
H	6.87876200	1.25975600	-0.99403900	H	1.15979400	-2.93140300	1.27619600
H	7.26040400	0.06966700	2.97251500	C	1.70017300	-2.67157800	-1.96888700
H	8.67201300	0.59464400	2.04695000	C	0.77896800	-2.26078100	-2.94679800
C	8.29721600	-0.36564200	-0.75774600	C	0.19883900	-3.19719000	-3.80215900
C	7.46297000	2.22073000	2.83130000	C	0.52164200	-4.55220300	-3.67781200
H	6.41164200	2.42010600	3.05963700	C	1.43524800	-4.96604300	-2.70495100

C	2.02691400	-4.03053100	-1.85362900	H	-2.72017800	2.82184300	-2.57574300
H	0.50092000	-1.21301900	-3.02016400	H	-2.35637400	4.42011500	-1.94219500
H	-0.51693700	-2.87239400	-4.55172100	H	-1.08228700	3.47265500	-2.72401000
H	0.05791800	-5.28328100	-4.33384000	C	-1.45463300	-2.72014300	0.73515600
H	1.68700200	-6.01813200	-2.60587400	C	-1.75101100	-3.01717800	2.08017500
H	2.72803000	-4.36060500	-1.09366700	C	-1.20566500	-3.79128700	-0.14376600
C	4.18861100	1.24618900	1.40414100	C	-1.76725200	-4.33570000	2.53434500
C	5.58967300	1.17348100	1.36121600	H	-2.00113700	-2.20593800	2.75832900
C	6.30969100	0.84552100	2.51072800	C	-1.22836400	-5.10943900	0.31171900
C	5.63868900	0.57978400	3.70781500	H	-0.96016300	-3.58580100	-1.18024200
C	4.24423400	0.64684300	3.75712700	C	-1.50061500	-5.38915800	1.65382300
C	3.52167200	0.97732600	2.60995400	H	-2.00248300	-4.54250400	3.57510500
H	6.11710200	1.35235400	0.42926700	H	-1.01600300	-5.91787300	-0.38281400
H	7.39372400	0.78846800	2.46947700	H	-1.51177900	-6.41591900	2.00880100
H	6.20159200	0.31417500	4.59808100	C	-3.12645000	2.42068300	1.74348200
H	3.71841800	0.43138200	4.68271700	C	-3.44037400	1.15797400	2.21472800
H	2.43520700	1.00764300	2.64000700	C	-4.25640200	0.30521700	1.47916100
C	3.23202200	3.37812000	-0.41254900	C	-4.76378700	0.73628800	0.24870300
C	4.31923900	4.19462200	-0.06609300	C	-4.41017700	1.99034600	-0.20934600
C	4.28959700	5.55849300	-0.36330400	C	-3.44314800	2.83493200	0.41656600
C	3.17823300	6.11487000	-1.00320400	O	-5.07069600	-1.05769200	-1.29122300
C	2.08789700	5.30818000	-1.34031700	F	-2.90434000	0.72948600	3.38145200
C	2.11046900	3.94568200	-1.04089700	F	-2.22947200	3.17709900	2.44078100
H	5.18074000	3.77152400	0.44147200	F	-4.88137100	2.40575300	-1.42744400
H	5.13324800	6.18694900	-0.09229100	F	-3.62601900	4.20748100	0.23234300
H	3.15831900	7.17715900	-1.22943000	C	-5.60755500	-0.19711800	-0.59034700
H	1.21569600	5.73910200	-1.82344500	N	-6.95553400	-0.03210600	-0.52502800
H	1.25068100	3.32359500	-1.27815500	C	-7.80113100	-0.92476100	-1.32598900
C	-1.79730600	-0.90905000	-0.99670200	C	-7.62840400	0.93454400	0.34947200
C	-1.36850200	-1.31823700	0.28041800	H	-6.96028000	1.18702400	1.17448300
C	-0.77487800	-0.33747300	1.10722900	H	-8.49883700	0.43316300	0.78773600
C	-0.71968700	1.01567800	0.72294400	H	-8.73394100	-0.39522700	-1.54097900
C	-1.28288800	1.45246200	-0.52892700	H	-7.29450200	-1.11113100	-2.27563300
C	-1.73209600	0.41786600	-1.40236100	C	-8.05708600	2.20213400	-0.39111300
H	-2.25043900	-1.63712600	-1.66039900	C	-8.08147500	-2.24624200	-0.60968500
H	-0.40990000	-0.61394000	2.09215300	H	-8.58005700	-2.07758100	0.35110100
H	-0.45983500	1.76606900	1.46516300	H	-8.72840900	-2.88461600	-1.22171700
C	-1.61661600	2.82803800	-0.70176800	H	-7.14452500	-2.77944600	-0.42477100
C	-1.95657300	3.40822100	-2.05600700	H	-7.18602500	2.71107200	-0.81156000
H	-1.07603900	3.51187700	-0.04650200	H	-8.74520500	1.96900300	-1.21099100
H	-2.14271100	0.68427400	-2.37084700	H	-8.56736800	2.88780000	0.29408400

F	-4.58630500	-0.91758800	1.98136700

HSi(OMe)$_2$Me

SCF Energy = -560.4833973 a.u.

Gibbs Free Energy = -560.3860023 a.u.

Si	-0.54739300	-0.00018400	0.31253500
H	-0.28561100	-0.00058900	1.78264100
C	-2.35116900	-0.00134200	-0.13591300
H	-2.85291300	-0.88927600	0.26352400
H	-2.48378000	0.00025900	-1.22338400
H	-2.85510800	0.88400100	0.26647600
O	0.12126200	1.38775500	-0.31128500
O	0.12318900	-1.38673500	-0.31224300
C	1.45294700	-1.79960100	-0.00637900
C	1.45139700	1.80049700	-0.00679600
H	1.52457500	-2.88229600	-0.15474200
H	2.18030100	-1.31375800	-0.66958000
H	1.73045800	-1.57928800	1.03447200
H	1.73016600	1.57965600	1.03361300
H	2.17795700	1.31508400	-0.67117100
H	1.52279400	2.88328600	-0.15459400

TS6

SCF Energy = -2698.602733 a.u.

Gibbs Free Energy = -2698.097422 a.u.

Si	1.98598700	3.28448400	0.18151600
Cu	0.13745900	0.94838900	-0.83195900
H	0.74990300	2.61264500	0.72773100
C	-1.70114500	-1.68788800	-0.69632900
C	-2.79594500	-2.50402200	-1.01060200
C	-2.61515200	-3.86121200	-1.28114600
C	-1.33479300	-4.41713500	-1.23956000
C	-0.23429400	-3.61425100	-0.93679100
C	-0.39922100	-2.24833300	-0.66762200
H	-3.79364700	-2.07731300	-1.04776900
H	-3.47296400	-4.48113900	-1.52536400
H	-1.19033600	-5.47319700	-1.44837600
H	0.75957800	-4.05055800	-0.91785700
P	-1.88962000	0.10542700	-0.28350400
P	1.02988700	-1.12664500	-0.34250800
C	-2.15463200	0.07043500	1.53435000
C	-2.91745700	-0.92337600	2.16925300
C	-3.03637100	-0.93497900	3.55914300
C	-2.38649000	0.03582900	4.32716200
C	-1.62075400	1.02240000	3.70248600
C	-1.50609500	1.04137000	2.31147100
H	-3.40537100	-1.69580300	1.58289500
H	-3.62707100	-1.70779900	4.04289000
H	-2.46961500	0.01640200	5.41013900
H	-1.10127500	1.76976900	4.29492800
H	-0.89018600	1.79323200	1.82658700
C	-3.48195600	0.58469700	-1.05472600
C	-3.44292300	0.92288700	-2.41837400
C	-4.61022700	1.28727200	-3.08815100
C	-5.82558200	1.33569900	-2.39848100
C	-5.86812100	1.01788900	-1.03923100
C	-4.70274700	0.64116700	-0.36675200
H	-2.49523700	0.90430100	-2.95193800
H	-4.57009000	1.54306500	-4.14313200
H	-6.73394900	1.62738100	-2.91792500
H	-6.80939000	1.06136500	-0.49854200
H	-4.74853300	0.39617400	0.68928800
C	1.28261700	-1.15854600	1.47477400
C	0.56357100	-1.99732800	2.33704200
C	0.73980900	-1.89680200	3.71900100
C	1.64159400	-0.97031700	4.24680400
C	2.36860300	-0.13812100	3.38987000
C	2.18480500	-0.22156500	2.00999400
H	-0.14455500	-2.71468900	1.93531200
H	0.16694100	-2.53923300	4.38147800
H	1.77319800	-0.89179700	5.32231200
H	3.06778800	0.58755700	3.79582100
H	2.72826700	0.45155300	1.35072800
C	2.47601100	-2.00373000	-1.04771300
C	3.32858000	-2.81323200	-0.28269800
C	4.42213200	-3.44194000	-0.88257500
C	4.66905000	-3.27229600	-2.24705700
C	3.82232200	-2.46708400	-3.01493200
C	2.73504400	-1.83005700	-2.41743100
H	3.14199400	-2.95066500	0.77798100
H	5.07951200	-4.06527700	-0.28287100

H	5.52164300	-3.76074200	-2.71029400
H	4.01519900	-2.32681200	-4.07472700
H	2.08858400	-1.18859400	-3.01174800
C	2.64994600	3.92060400	1.85426100
H	1.91543700	4.57761400	2.33850200
H	3.58701300	4.48234500	1.75613900
H	2.83570400	3.08006700	2.53593000
O	3.32698200	2.32177000	-0.16483300
O	1.83295000	4.79031600	-0.54672800
C	1.26904900	5.13648000	-1.79844300
C	3.66539900	1.62046500	-1.34798400
H	1.31169300	6.22886000	-1.89476200
H	1.81960600	4.69778800	-2.63978800
H	0.22056700	4.82461500	-1.88206000
H	2.87456700	0.93831500	-1.66986200
H	3.88510700	2.30510500	-2.17888400
H	4.56916400	1.03235500	-1.14580100
F	1.11771300	2.50208200	-1.50586900

$FSi(OMe)_2Me$

SCF Energy = -659.8345738 a.u.

Gibbs Free Energy = -659.7442468 a.u.

Si	-0.53147800	-0.00835200	0.03009400
C	-2.25791600	-0.06304700	-0.62098200
H	-2.71911100	-1.03657200	-0.42685800
H	-2.26456100	0.10727900	-1.70258800
H	-2.87592600	0.70979200	-0.15258300
O	0.07331900	1.50968300	-0.17523300
O	0.38779200	-1.16718300	-0.69335100
C	1.60943300	-1.68752800	-0.16244100
C	1.46919300	1.81447300	-0.11654400
H	1.80115200	-2.65637600	-0.63349400
H	2.45147700	-1.02083300	-0.38390600
H	1.55171500	-1.83475000	0.92256900
H	1.92928500	1.45869900	0.81409300
H	2.00517300	1.37869400	-0.96835600
H	1.58149900	2.90192700	-0.15714600
F	-0.51479500	-0.33492400	1.62393600