

Electronic Supplementary Information

Electronic Origins of Stereochemistry in β -Lactam Formation through Staudinger Reaction Catalyzed by a Nucleophile

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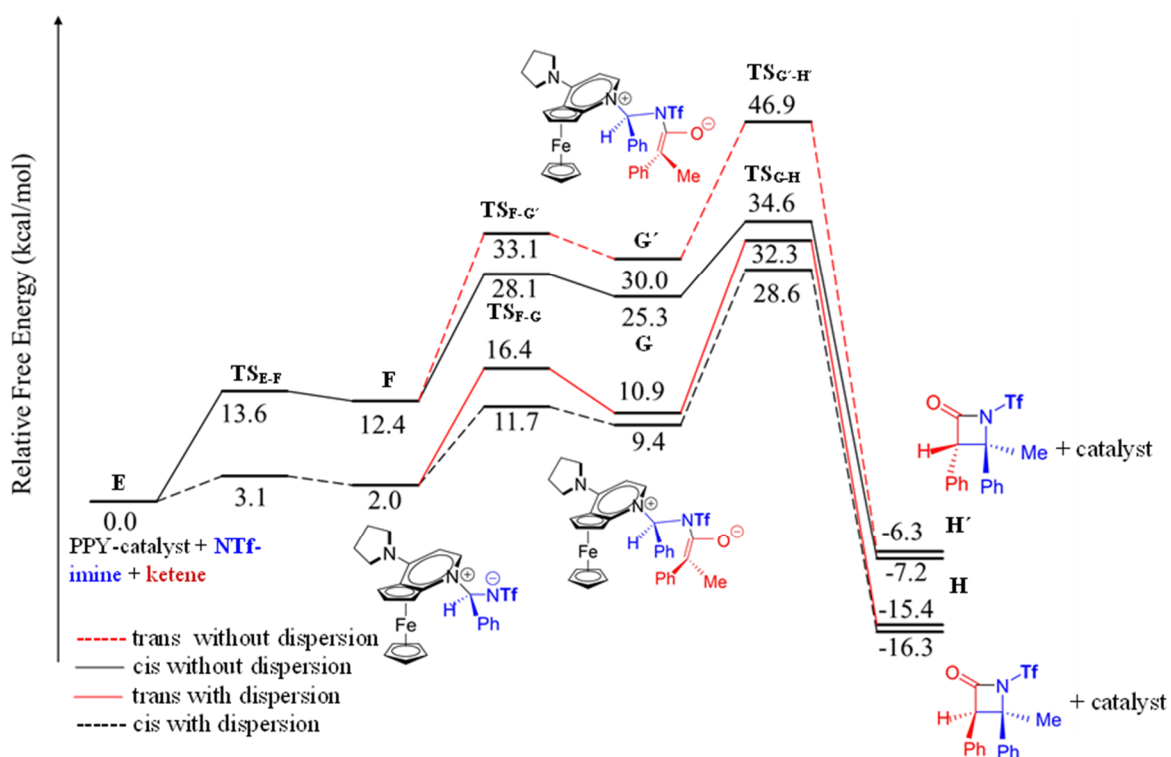


Fig. S1 Gibbs free energy profile for the imine-first mechanism with and without dispersion corrections, comparing cis and trans selectivity of N-Tf imine.

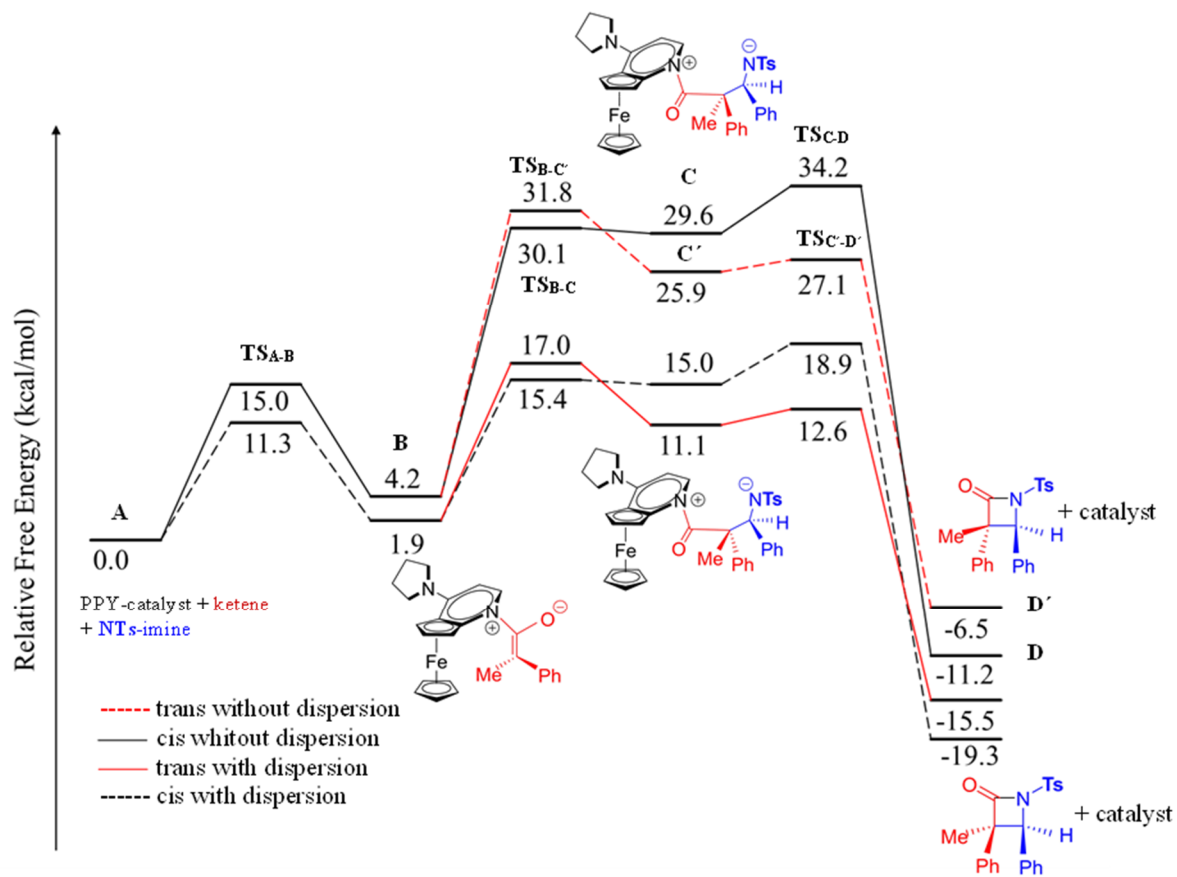


Fig. S2 Gibbs free energy profile for the ketene-first mechanism with and without dispersion corrections, comparing cis and trans selectivity of N-Ts imine.

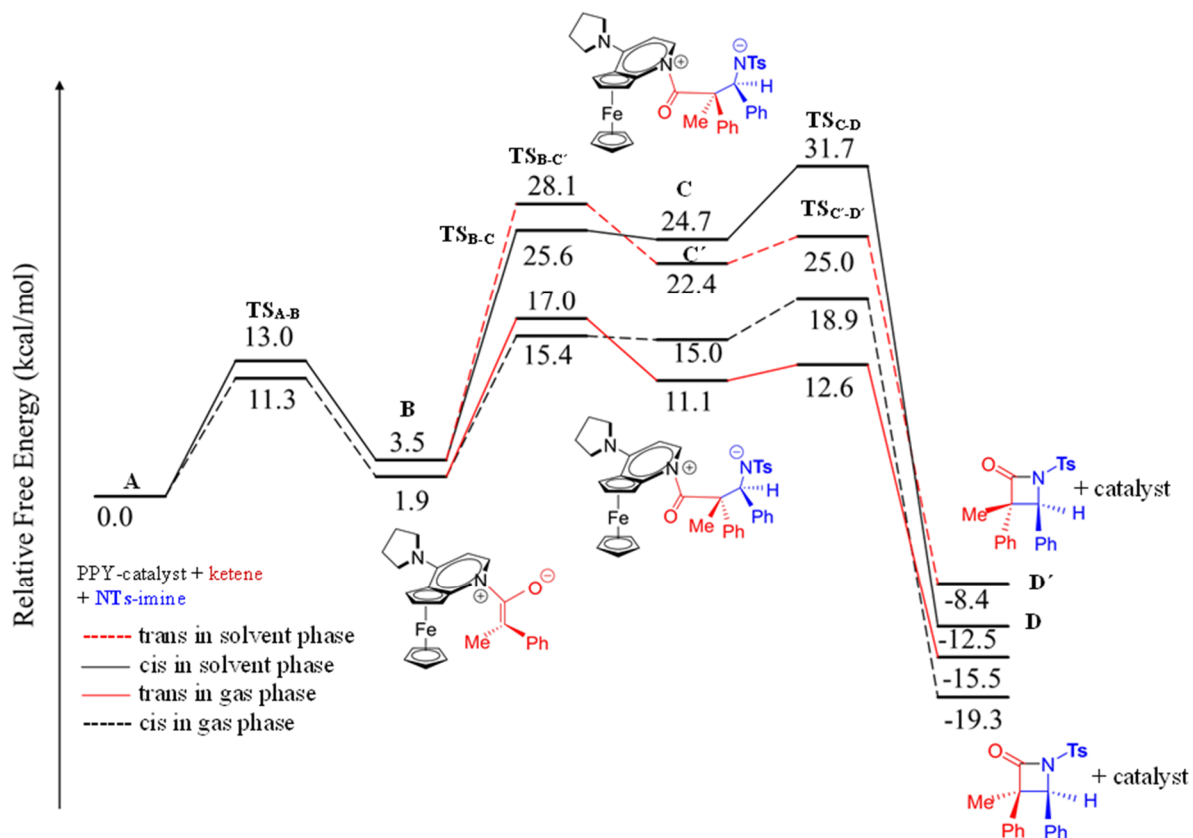


Fig. S3 Gibbs free energy profile for the ketene-first mechanism in gas and solvent (toluene) phase, comparing cis and trans selectivity of N-Ts imine.

Table S1. Optimized energies of reactants, intermediates, and products for the competing mechanisms of cycloaddition-catalyzed Staudinger reaction between ketene and N-Ts imine.

Name of molecules	Opt and Freq without dispersion for N-Ts, ketene-first (Hartree)	Opt and Freq with dispersion for N-Ts, ketene-first (Hartree)	Opt and Freq with dispersion for N-Ts, ketene-first in solvent phase (Hartree)
Reactants	-2655.011729	-2655.193217	-2635.312746
Intermediate-B	-2655.004973	-2655.190269	-2635.307168
Intermediate-C	-2654.964499	-2655.169312	-2635.273384
Intermediate-C`	-2654.970511	-2655.175527	-2635.277049
TSA-B	-2654.987763	-2655.175208	-2635.292029
TSB-C	-2654.963732	-2655.176642	-2635.271949
TSB-C`	-2654.961048	-2655.166103	-2635.267965
TSC-D	-2654.957243	-2655.163025	-2635.262228
TSC`-D`	-2654.968506	-2655.173100	-2635.272906
Catal+product-D	-2655.029491	-2655.223910	-2635.332666
Catal+product-D`	-2655.022172	-2655.217848	-2635.326291

Table S2. Optimized energies of reactants, intermediates, and products for the ketene-first mechanism of nucleophile-catalyzed Staudinger reaction involving N-Tf imine.

Name of molecules	Opt and Freq without dispersion for N-Tf, imine-first (Hartree)	Opt and Freq with dispersion for N-Tf, imine-first (Hartree)
Reactants	-2721.761756	-2721.930808
Intermediate-F	-2721.742033	-2721.925885
Intermediate-G	-2721.721492	-2721.915780
Intermediate-G`	-2721.713921	-2721.913348
TSE-F	-2721.740128	-2721.925978
TSF-G	-2721.717004	-2721.912138
TSF-G`	-2721.709054	-2721.904684
TSG-H	-2721.706676	-2721.885248
TSG`-H`	-2721.687089	-2721.879332
Catal+product-H	-2721.773150	-2721.955397
Catal+product-H`	-2721.771727	-2721.956774

continued

Name of molecules	Opt and Freq without dispersion for N-Tf, ketene-first (Hartree)	Opt and Freq with dispersion for N-Tf, ketene-first (Hartree)
Reactants	-2721.761756	-2721.930808
Intermediate-J	-2721.750431	-2721.927334
Intermediate-K	-2721.724645	-2721.916946
Intermediate-K`	-2721.732160	-2721.922293
TSE-J	-2721.746368	-2721.917550
TSJ-K	-2721.719600	-2721.910708
TSJ-K`	-2721.720711	-2721.911900
TSK-L	-2721.715227	-2721.909790
TSK-L`	-2721.724689	-2721.915725
Catal+product-L	-2721.773150	-2721.956619
Catal+product-L`	-2721.771727	-2721.958543

Optimized molecular structure of reactants, intermediates, and products for the competing mechanisms of cycloaddition-catalyzed Staudinger reaction between ketene and NTs-imine.

A. PPY-catalyst + ketene + N-Ts imine

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C	-3.36219600	6.32284800	-0.23765900
H	-1.59525700	5.81578100	-1.31878600
C	-4.18033000	4.68289600	1.31054700
H	-3.03832500	2.86903900	1.46708600
C	-4.31266600	5.93696000	0.70804400
H	-3.43777500	7.29442800	-0.72193500
H	-4.90442600	4.36160500	2.05688500
H	-5.13444800	6.59777900	0.97196700
C	0.00458700	3.90677000	-1.31065900
H	-0.39904600	4.14430700	-2.30807100
H	0.41698300	4.84795500	-0.91769800
H	0.84157700	3.22283100	-1.45458900
S	-2.14136500	-3.68424100	0.15955800
O	-2.74995000	-5.01583300	0.17509600
O	-0.72457300	-3.53525100	-0.22708400
N	-3.03093600	-2.78609400	-0.98328300
C	-3.31067800	-1.55048700	-0.75505200
H	-3.03312400	-1.03766200	0.17123000
C	-4.00228000	-0.71007800	-1.73253500
C	-4.09777000	0.66739700	-1.46567400
C	-4.55423700	-1.23584100	-2.91513600
C	-4.73409400	1.51147500	-2.37588200
H	-3.65239100	1.06969200	-0.55842900
C	-5.19489600	-0.38997000	-3.81311600
H	-4.47600200	-2.30189500	-3.10468400
C	-5.28458500	0.98317500	-3.54537000
H	-4.79554600	2.57538800	-2.16655300
H	-5.62876700	-0.79459500	-4.72358300
H	-5.78627700	1.63882800	-4.25250700
C	-3.44974600	-3.00852600	3.93034500
C	-3.25099600	-3.57302900	2.67193900
C	-2.36318800	-2.95886500	1.78463300
C	-1.68576100	-1.78849500	2.14149200
C	-1.91667700	-1.22697000	3.39524400
C	-2.79241200	-1.82900000	4.31022200
H	-4.13374800	-3.48770400	4.62658300

H	-3.76358500	-4.48160000	2.37543500
H	-1.01044400	-1.29720900	1.45133400
H	-1.41944600	-0.29481600	3.64803300
C	-3.01080300	-1.22504500	5.67707200
H	-3.95779600	-1.55545400	6.11568300
H	-2.20901900	-1.51622500	6.36880700
H	-3.01803600	-0.13079300	5.63191500

B 56 76 F

H C O N S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

TS_{B-C'}

%nprocshared=16

%mem=1GB

freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	4.54981300	-2.63308600	-1.08499500
C	3.52088800	-2.86137900	-0.10791900
C	3.76143300	-1.98272700	0.99768700
C	5.43412900	-1.62175000	-0.57414300
C	4.94304400	-1.21555500	0.70860400
Fe	3.50615700	-0.87549600	-0.75980200
C	4.99639800	4.75226900	0.41516700
C	4.76112400	4.57022700	1.92138000
C	3.47786200	3.73428600	1.96985100
N	3.55044700	2.90314300	0.75283000
C	4.58737000	3.39428000	-0.17353600
C	2.63625000	1.94403700	0.48454800
C	1.52576700	1.75566600	1.33495900
C	0.48890900	0.89762000	1.00649600
N	0.50548200	0.07781600	-0.05521900
C	1.60774300	0.14614700	-0.90194600
C	2.68474900	1.09172600	-0.68121300
H	6.02817300	5.01474400	0.16513100
H	4.34336500	5.54024500	0.02292800
H	5.59107600	4.01388000	2.37293100
H	4.65605900	5.51576600	2.46002000
H	3.41584100	3.10112500	2.86096600
H	2.58130100	4.36897600	1.94150400
H	5.43744800	2.69945400	-0.19873700

H	4.18429600	3.48415700	-1.18495000
H	1.37517800	2.39254200	2.19515400
H	-0.42855800	0.91780500	1.58243900
C	3.09260800	-0.08688800	-2.63473300
H	3.56308200	-0.44190200	-3.54192000
C	3.61816200	0.91280200	-1.77104700
H	4.54310200	1.44224900	-1.93094800
C	1.88290200	-0.59639800	-2.08286500
H	1.24920400	-1.35875200	-2.50636500
C	4.71055500	-3.37358400	-2.38231300
H	5.29862300	-4.29100700	-2.24085700
H	3.74415000	-3.66789800	-2.80355100
H	5.22846600	-2.76878800	-3.13364400
C	6.68169700	-1.12085200	-1.24419300
H	7.55410300	-1.72049800	-0.94958200
H	6.60667000	-1.17285000	-2.33510600
H	6.89693200	-0.08118700	-0.97628100
C	5.59216900	-0.22945300	1.63790500
H	6.26105200	-0.73842600	2.34613000
H	6.19682600	0.50422000	1.09443600
H	4.85135200	0.31875300	2.22891500
C	2.98272400	-1.91857500	2.28020000
H	3.47978200	-2.50574300	3.06503300
H	2.88923900	-0.89196800	2.64968300
H	1.97308600	-2.31798000	2.16259700
C	2.42549300	-3.88381000	-0.21335500
H	2.13274500	-4.05746800	-1.25316400
H	2.74993100	-4.84831800	0.20137200
H	1.52785100	-3.57864500	0.33128200
C	-0.75987800	-0.60754400	-0.56992000
O	-0.94847800	-0.43996500	-1.76603400
C	-1.55556700	-1.35616100	0.37426100
C	-2.44632300	-2.37388200	-0.27549200
C	-2.60012400	-3.66184000	0.28174500
C	-3.20214600	-2.09874500	-1.43918400
C	-3.44572100	-4.61597400	-0.28596000
H	-2.05528800	-3.93760800	1.17646700
C	-4.05219800	-3.05075900	-1.99970700
H	-3.11754700	-1.13200400	-1.91515100
C	-4.18254100	-4.31987100	-1.43163400
H	-3.52659400	-5.59623900	0.17826000
H	-4.61798500	-2.79304100	-2.89210700
H	-4.84487000	-5.06027900	-1.87267600
C	-0.88901300	-1.84072100	1.65760200
H	-1.63773200	-2.19309900	2.37027400
H	-0.20379500	-2.68082100	1.46985100
H	-0.31833700	-1.06952100	2.17240800
S	-2.45588700	2.59113800	0.26886300
O	-2.68535200	3.83079800	1.02597400
O	-1.20887200	2.48665000	-0.52217200
N	-2.57358600	1.36047700	1.37267200
C	-3.05470700	0.15612500	1.03822800
H	-3.55314300	0.01072400	0.07838300
C	-3.65555500	-0.61743900	2.16202800

C	-4.63014600	-1.59570300	1.90919300
C	-3.32420400	-0.32667500	3.49723400
C	-5.24321100	-2.27785800	2.96196600
H	-4.91717600	-1.81558400	0.88652300
C	-3.92990300	-1.01478100	4.54532600
H	-2.60778100	0.46370000	3.69443900
C	-4.89110100	-1.99640900	4.28230700
H	-5.99968800	-3.02765700	2.74563000
H	-3.66257900	-0.77659400	5.57195100
H	-5.36896100	-2.52756600	5.10164500
C	-6.13943100	2.75284100	-1.44561900
C	-5.08817200	2.87830500	-0.54149300
C	-3.81688400	2.42140000	-0.90117600
C	-3.59270100	1.84971100	-2.15455800
C	-4.65924800	1.73248200	-3.04909000
C	-5.94291100	2.17918400	-2.71214000
H	-7.12899400	3.10945500	-1.16791700
H	-5.23927100	3.33821500	0.42981900
H	-2.59783200	1.50513700	-2.41710500
H	-4.48746300	1.28772800	-4.02669500
C	-7.08834400	2.07129300	-3.69180100
H	-8.00118400	1.71171100	-3.20287700
H	-7.32418600	3.04767900	-4.13557400
H	-6.85120500	1.38607700	-4.51194900

H C O N S O

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Intermediate C

%nprocshared=16

%mem=800MB

freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	5.27179900	1.78496000	-1.27536000
C	4.01296700	2.17868100	-1.84427100
C	3.38359200	1.00692700	-2.38084000
C	5.42245600	0.36749800	-1.46508900
C	4.25580400	-0.11129200	-2.14799500
Fe	3.72360100	0.77875000	-0.33712700
C	4.38220500	-4.63254700	1.96128100
C	3.74188800	-5.29358300	0.73249000

C	2.55819100	-4.37332100	0.41942400
N	3.02541600	-3.03498900	0.84826900
C	4.25076700	-3.13191400	1.66502100
C	2.32044500	-1.91802300	0.59347000
C	1.05311000	-2.00094300	-0.03021700
C	0.24430100	-0.90401100	-0.22002300
N	0.59326300	0.36227000	0.13865900
C	1.88678700	0.55661900	0.66857600
C	2.75159900	-0.58299100	0.94777600
H	5.42263600	-4.92819000	2.12153300
H	3.81686900	-4.88519500	2.86555900
H	4.44653100	-5.30092300	-0.10757000
H	3.42269700	-6.32323100	0.91301200
H	2.29775900	-4.36092800	-0.64265100
H	1.66108900	-4.65487000	0.98571900
H	5.11389000	-2.75942800	1.09776400
H	4.15012000	-2.53447000	2.57397400
H	0.61295900	-2.95404000	-0.29194800
H	-0.80742000	-1.05126600	-0.52662300
C	3.79710900	1.35145800	1.67210400
H	4.53590000	2.03156200	2.07466500
C	3.95472700	-0.05208100	1.54484800
H	4.82651600	-0.60609600	1.85162100
C	2.54473800	1.73961500	1.11730100
H	2.17364200	2.74462000	1.02300400
C	6.28674500	2.70060400	-0.65207200
H	6.99554500	3.06976700	-1.40607600
H	5.81654600	3.57559900	-0.19299100
H	6.87112100	2.19342900	0.12254200
C	6.62246800	-0.44912700	-1.07640400
H	7.37083200	-0.45886600	-1.88086400
H	7.11205700	-0.04993700	-0.18226800
H	6.35504700	-1.49116800	-0.87135600
C	4.00285700	-1.52210200	-2.59652800
H	4.35118000	-1.67391300	-3.62728700
H	4.52510700	-2.24883000	-1.96592200
H	2.93619700	-1.76590800	-2.57204900
C	2.07981200	0.97133500	-3.12553600
H	2.24433400	1.10739400	-4.20343500
H	1.56055800	0.01615600	-2.99655000
H	1.40538200	1.76595000	-2.79456200
C	3.45831000	3.57381700	-1.90517600
H	3.89666300	4.21571200	-1.13494600
H	3.67423900	4.03680500	-2.87781700
H	2.37393700	3.58259100	-1.76206500
C	-0.27188700	1.51583500	-0.09628500
O	0.29489300	2.58266600	-0.20234700
C	-1.81762400	1.41088700	-0.29308700
S	-3.37072300	-2.22419200	0.30173800
O	-2.64524500	-3.41596300	-0.19653800
O	-3.93445900	-2.26349600	1.66993800
N	-2.42667300	-0.96976200	-0.00256900
C	-5.77401900	-2.11343300	-3.00038900
C	-4.69256800	-2.32862300	-2.15063500

C	-4.80514500	-2.02530300	-0.78924400
C	-6.00127300	-1.51046100	-0.28906100
C	-7.07897200	-1.29456100	-1.15270600
C	-6.98531200	-1.59112400	-2.51691800
H	-5.68340700	-2.35933800	-4.05707900
H	-3.76394000	-2.74764000	-2.52551700
H	-6.08409400	-1.30452200	0.77315400
H	-8.01058500	-0.89579000	-0.75596900
C	-8.16034500	-1.38479000	-3.44539300
H	-7.85429200	-0.90343400	-4.38215500
H	-8.63012700	-2.34036200	-3.71501800
H	-8.93150400	-0.76015300	-2.98247400
C	-2.67053400	0.33389300	0.55528700
C	-2.40566000	2.80853000	0.01791600
C	-3.43925700	3.33620900	-0.76896300
C	-2.00199900	3.55272900	1.13863900
C	-4.03817100	4.56041200	-0.46047000
H	-3.79785000	2.79314900	-1.63572700
C	-2.59246700	4.77695000	1.44730100
H	-1.21778400	3.17678400	1.78497800
C	-3.61492900	5.29091800	0.64787500
H	-4.83686100	4.93790300	-1.09386000
H	-2.25298400	5.32668200	2.32139000
H	-4.07588600	6.24528600	0.88862700
H	-3.70061000	0.67370200	0.34773600
C	-2.47700000	0.46160300	2.07491000
C	-3.33956100	1.26893900	2.82826600
C	-1.46763000	-0.23398300	2.75318200
C	-3.18036600	1.40811000	4.20820900
H	-4.15096900	1.79089000	2.32818100
C	-1.29811900	-0.09288500	4.13085600
H	-0.84618200	-0.93398300	2.20533400
C	-2.14974800	0.73531300	4.86530400
H	-3.86840000	2.03587200	4.76926900
H	-0.51309200	-0.65078100	4.63648200
H	-2.02488900	0.83680400	5.94054800
C	-1.98183900	1.08701500	-1.80946400
H	-3.02585400	0.85553500	-2.03247900
H	-1.66124100	1.94318900	-2.41241800
H	-1.40849500	0.20861000	-2.10431200

Fe 0
LANL2DZ

H C O N S 0
6-31G*

Fe 0
LANL2DZ

Intermediate C'


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%nprocshared=16
%mem=1GB
# freq=noraman b3lyp/gen pseudo=read
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Title Card Required

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0 1
C      5.18210800   -1.98648000    0.47512300
C      3.96400100   -2.15840800    1.21866400
C      3.73371700   -0.96102800    1.97083600
C      5.70861000   -0.68347200    0.77781400
C      4.81008200   -0.04793500    1.69508400
Fe     3.82482500   -0.52592300   -0.07831900
C      4.36765000    5.33093400   -0.94156200
C      3.80808700    5.65708900    0.45030700
C      2.65644300    4.65739000    0.60240700
N      3.10513100    3.47886300   -0.16747700
C      4.27282100    3.80039000   -1.01013200
C      2.40100800    2.32922700   -0.19605300
C      1.14949600    2.23597600    0.45786800
C      0.30695000    1.15329100    0.29087500
N      0.65937300    0.04400000   -0.39580600
C      1.93364200    0.00623300   -0.96395700
C      2.82184800    1.15028200   -0.92040500
H      5.39078500    5.68587200   -1.09314600
H      3.73652500    5.77815600   -1.71789400
H      4.56852400    5.47760800    1.21961000
H      3.46792200    6.69136900    0.54776700
H      2.46698600    4.38153000    1.64449200
H      1.72200000    5.04857000    0.17823900
H      5.17683300    3.32730900   -0.60377500
H      4.11958900    3.43681500   -2.02861500
H      0.73111500    3.09058700    0.97041100
H     -0.74166600    1.17596100    0.59161900
C      3.81481600   -0.54144700   -2.15493500
H      4.52915800   -1.10035300   -2.74450500
C      4.00587500    0.77775100   -1.66129900
H      4.88521200    1.37779800   -1.83021700
C      2.56319900   -1.03920100   -1.69182000
H      2.13971400   -2.00950400   -1.90183100
C      5.82353700   -3.01739200   -0.40944700
H      6.44331400   -3.70813800    0.17864800
H      5.07688400   -3.61883600   -0.93788900
H      6.47290400   -2.55901500   -1.16193700
C      6.99622400   -0.11044700    0.25767900
H      7.84337700   -0.40422500    0.89252600
H      7.21438900   -0.45738400   -0.75748700
H      6.97192000    0.98405100    0.23512200
C      4.99888900    1.29570100    2.33983200
H      5.56464000    1.20260900    3.27737400
H      5.55419000    1.98486000    1.69484200
H      4.04100000    1.76499000    2.58603000
C      2.62500000   -0.71612400    2.95422700
H      2.99053600   -0.82871200    3.98427400
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H	2.20815500	0.29236300	2.86347900
H	1.80326900	-1.42348000	2.82265400
C	3.11930300	-3.40049600	1.23485200
H	3.18125500	-3.94267700	0.28649500
H	3.44743200	-4.08718700	2.02742200
H	2.06393800	-3.17558000	1.41190100
C	-0.38872900	-0.88913800	-0.96678500
O	-0.31988200	-1.04373700	-2.15538700
C	-1.36113800	-1.66121900	-0.04523300
C	-1.38290300	-3.12860400	-0.52541000
C	-1.00379700	-4.18529800	0.31630200
C	-1.79444900	-3.45627400	-1.83158200
C	-1.03408200	-5.51322600	-0.12046300
H	-0.68770600	-3.98973400	1.33434800
C	-1.82482400	-4.77953900	-2.26886800
H	-2.08259700	-2.67008100	-2.51788600
C	-1.44471300	-5.81828100	-1.41579200
H	-0.73882600	-6.30632500	0.56203300
H	-2.14975400	-4.99738700	-3.28302800
H	-1.47208500	-6.84981500	-1.75718700
C	-0.99164300	-1.54487700	1.43902000
H	-1.66228000	-2.16735300	2.03527500
H	0.03795300	-1.86182400	1.63253100
H	-1.11482300	-0.51958100	1.78604600
S	-3.00349600	1.60209700	-1.08360400
O	-2.11358500	2.77965900	-0.92310900
O	-3.22519700	1.06607100	-2.44961600
N	-2.48756500	0.49795600	-0.04060000
C	-2.77842200	-0.89627500	-0.29980700
H	-3.02121600	-1.07275600	-1.35485100
C	-3.89897200	-1.47616700	0.56467400
C	-4.59331000	-2.63251100	0.17789000
C	-4.26968600	-0.84806600	1.76166300
C	-5.61506600	-3.15540300	0.97255500
H	-4.33850200	-3.12444100	-0.75622100
C	-5.28905800	-1.36961800	2.55941900
H	-3.76499500	0.07296500	2.03376100
C	-5.96360200	-2.52886000	2.17079200
H	-6.14426100	-4.04891400	0.64982200
H	-5.56489900	-0.86246000	3.48114600
H	-6.76231200	-2.93282600	2.78821200
C	-5.98189100	3.54815800	0.92445800
C	-4.72823800	3.13685100	0.47583600
C	-4.63221800	2.17975000	-0.53738200
C	-5.79133200	1.64656200	-1.10241900
C	-7.04127400	2.06547800	-0.64483000
C	-7.15881600	3.01583200	0.37753400
H	-6.05051600	4.30238800	1.70639100
H	-3.82088300	3.56932000	0.88508600
H	-5.70567700	0.92690700	-1.90973700
H	-7.94125800	1.65142000	-1.09519700
C	-8.51504900	3.44416200	0.88956700
H	-8.50445100	4.48413100	1.23500100
H	-9.28364200	3.35373900	0.11413900

H -8.83652000 2.82443800 1.73814700

Fe 0
LANL2DZ

H C O N S 0
6-31G*

Fe 0
LANL2DZ

TS_{c-d}

nprocshared=16
%mem=800MB
opt=(ts,calcfc,noeigen) freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1
C -4.37824200 2.07552400 1.75916000
C -3.12250100 1.75318200 2.37859900
C -3.04478400 0.32805000 2.50362000
C -5.08873200 0.84849800 1.52347800
C -4.25951800 -0.22936000 1.97194600
Fe -3.29069000 0.86374100 0.48463500
C -5.70468000 -3.33657900 -2.92292000
C -5.31761700 -4.44748000 -1.93635900
C -3.90628000 -4.04151000 -1.49693900
N -3.92476400 -2.56896900 -1.55865500
C -5.10721000 -2.07367300 -2.28595800
C -2.86500600 -1.82097500 -1.16701900
C -1.66563100 -2.43141400 -0.74655000
C -0.50047400 -1.69791800 -0.53351300
N -0.44821800 -0.36455000 -0.57089800
C -1.63309200 0.31172100 -0.81887600
C -2.85567500 -0.37585600 -1.18956300
H -6.78372300 -3.24881200 -3.07782800
H -5.23788400 -3.51799000 -3.89793500
H -5.99646600 -4.44792300 -1.07513900
H -5.33817500 -5.44637200 -2.38042100
H -3.66316200 -4.37899900 -0.48405100
H -3.14179900 -4.44113000 -2.17838300
H -5.81774200 -1.60495900 -1.59138800
H -4.81578600 -1.33036900 -3.03190800
H -1.57145500 -3.50844400 -0.72169000
H 0.44614800 -2.21298700 -0.41026300
C -3.20214800 1.91321900 -1.30917900
H -3.67793700 2.87441800 -1.45195400
C -3.83158900 0.64894300 -1.48320400
H -4.85614800 0.50634200 -1.78790700
C -1.86854500 1.71482000 -0.85222300
H -1.14024100 2.48270700 -0.63556200

C	-4.88744400	3.46317800	1.49115300
H	-5.41522100	3.86523400	2.36737400
H	-4.07027300	4.15338100	1.25819500
H	-5.58959800	3.48427700	0.65138800
C	-6.47638300	0.72810900	0.96070600
H	-7.23081900	0.79243800	1.75702500
H	-6.69489800	1.52459400	0.24179700
H	-6.62590600	-0.22958600	0.45086500
C	-4.61257200	-1.68905500	1.98395400
H	-5.06503700	-1.97418800	2.94413600
H	-5.33047600	-1.94415100	1.19806200
H	-3.72607500	-2.31597900	1.84259400
C	-1.95637600	-0.47844300	3.15394100
H	-2.30442200	-0.89895700	4.10731600
H	-1.63806600	-1.31565000	2.52290500
H	-1.07170400	0.12538400	3.36597400
C	-2.12945200	2.76572700	2.87509200
H	-1.95314900	3.56041200	2.14298400
H	-2.49200400	3.24114900	3.79700600
H	-1.16271700	2.31067900	3.10181100
C	0.92035700	0.41585100	-1.02077000
O	0.84852400	0.72530500	-2.18989000
C	1.63254700	1.23873000	0.12005700
C	1.62562300	2.75621200	-0.09686000
C	1.48683500	3.64092700	0.98838200
C	1.78240500	3.32792800	-1.37442400
C	1.50432400	5.02664100	0.81282400
H	1.36821600	3.25920500	1.99564000
C	1.79367400	4.71153800	-1.55134800
H	1.87981400	2.68188900	-2.23466400
C	1.65650500	5.57147800	-0.46099200
H	1.40070800	5.67613800	1.67874900
H	1.91621800	5.11619000	-2.55279800
H	1.67096400	6.64929100	-0.60187700
C	1.07491400	0.84230600	1.49481600
H	1.69081500	1.25807700	2.29820500
H	0.04887500	1.19375000	1.62702200
H	1.09079400	-0.24387800	1.59537600
S	3.12058400	-2.12631300	-0.94406300
O	2.07867600	-3.17452000	-1.06713700
O	4.08244700	-1.99168000	-2.05213200
N	2.33198200	-0.75734900	-0.52452800
C	3.00427200	0.46098500	-0.05150600
H	3.45007500	0.31263500	0.94325900
C	4.06961400	1.11250000	-0.92037400
C	5.07575500	1.85716900	-0.28930700
C	4.08407800	1.01682500	-2.31855700
C	6.06495800	2.50662500	-1.02916700
H	5.08414100	1.92897000	0.79683500
C	5.07420900	1.66193900	-3.05988500
H	3.32716100	0.42602800	-2.81889300
C	6.06580900	2.41061300	-2.42148100
H	6.83517300	3.07946600	-0.51837800
H	5.07494500	1.57047500	-4.14312400

H	6.83799900	2.90708700	-3.00402800
C	4.10682700	-2.52462900	0.51761400
C	3.52568500	-3.22566800	1.57692800
C	5.44235000	-2.12426100	0.58460100
C	4.28679400	-3.51926900	2.70645900
H	2.49578900	-3.55843500	1.49765300
C	6.19081600	-2.42136300	1.72436200
H	5.88798800	-1.60434400	-0.25691800
C	5.62781600	-3.11762500	2.80213100
H	3.83715900	-4.07793100	3.52473600
H	7.23351200	-2.11503000	1.77172300
C	6.43799100	-3.41559100	4.04262400
H	7.50486900	-3.50610200	3.81247000
H	6.33313100	-2.61551600	4.78818900
H	6.11356800	-4.34696900	4.51931700

H C O N S O

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

TSC'D'

%nprocshared=16

%mem=1GB

freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	4.96920500	-1.91239700	0.83842600
C	3.72216400	-2.14000600	1.51555100
C	3.35455600	-0.92575900	2.18157900
C	5.37977500	-0.55972900	1.10049000
C	4.37830200	0.05015400	1.92192100
Fe	3.54787100	-0.59270200	0.12067500
C	4.70181700	5.01047600	-1.32791200
C	4.15604900	5.52317900	0.01270100
C	2.89381400	4.67813300	0.21565400
N	3.22154900	3.39350200	-0.42582000
C	4.42603100	3.50089800	-1.26789300
C	2.39074200	2.32455700	-0.36281300
C	1.13007900	2.42600800	0.26028700
C	0.18729300	1.40397700	0.17048800
N	0.42547300	0.21224700	-0.37591200
C	1.69930800	-0.01028800	-0.86944900
C	2.69901200	1.03909600	-0.94671300

H	5.76279600	5.22943300	-1.47753900
H	4.14482700	5.45838100	-2.15889500
H	4.87445800	5.32604800	0.81735700
H	3.93891800	6.59480300	0.01025400
H	2.65050500	4.52659400	1.27264500
H	2.01972900	5.13532900	-0.27010600
H	5.26546500	2.96148800	-0.80846300
H	4.24305400	3.07245600	-2.25639100
H	0.80540900	3.35995600	0.69806600
H	-0.83438300	1.55469000	0.49318800
C	3.53493000	-0.88219200	-1.93757400
H	4.19740800	-1.57423400	-2.44007100
C	3.84888300	0.46665200	-1.61000100
H	4.78280200	0.95567600	-1.83690300
C	2.23874900	-1.19650000	-1.44044600
H	1.72042200	-2.13852300	-1.53833700
C	5.75103900	-2.93600000	0.06486000
H	6.40543900	-3.51603300	0.73058800
H	5.09517700	-3.64756100	-0.44667000
H	6.38966100	-2.47044500	-0.69275200
C	6.66281100	0.07216000	0.64079800
H	7.48793300	-0.16911500	1.32522100
H	6.95496400	-0.27645700	-0.35540600
H	6.58607800	1.16387300	0.60066100
C	4.40827900	1.43840000	2.49469000
H	4.83456800	1.43546300	3.50770600
H	5.01501600	2.11855000	1.88826600
H	3.40162100	1.86330600	2.56521900
C	2.17718800	-0.70526200	3.08846500
H	2.50192400	-0.65286500	4.13694700
H	1.65373400	0.22995000	2.86138100
H	1.44799800	-1.51474200	3.01383200
C	2.99219200	-3.45174500	1.56736100
H	3.09892800	-4.01108900	0.63284100
H	3.38468500	-4.08456800	2.37571100
H	1.92215300	-3.31846400	1.74644400
C	-0.80305900	-0.68821400	-1.09046800
O	-0.59132600	-0.78743700	-2.27859400
C	-1.45230400	-1.81039300	-0.19220800
C	-1.35584200	-3.20294200	-0.81521100
C	-0.86932900	-4.30789900	-0.09902100
C	-1.77959100	-3.42128100	-2.14091800
C	-0.80811300	-5.58042100	-0.67470100
H	-0.54064700	-4.19183600	0.92773700
C	-1.71739300	-4.68913700	-2.71643400
H	-2.13554300	-2.58645800	-2.73265800
C	-1.23229800	-5.77760500	-1.98717400
H	-0.43264600	-6.41572100	-0.08854200
H	-2.04908200	-4.82490000	-3.74266100
H	-1.18844200	-6.76611500	-2.43733500
C	-0.94548100	-1.75898600	1.24911000
H	-1.50355500	-2.45288000	1.88451700
H	0.11589000	-2.01648100	1.29489600
H	-1.06813600	-0.75899000	1.66842800

S	-3.05495400	1.23211100	-1.60959800
O	-2.06383500	2.28262800	-1.90347500
O	-3.68981200	0.47339900	-2.70419900
N	-2.32774300	0.23739300	-0.49365000
C	-2.86671500	-1.12744200	-0.32036700
H	-3.33164000	-1.48241400	-1.24651000
C	-3.83678300	-1.34932200	0.82262100
C	-4.59462100	-2.53007800	0.85355100
C	-3.98770200	-0.43006400	1.86792500
C	-5.47205000	-2.79022200	1.90650600
H	-4.49490700	-3.24843100	0.04313000
C	-4.87052000	-0.68498400	2.91926600
H	-3.42423100	0.49672900	1.83639000
C	-5.61282200	-1.86693000	2.94557900
H	-6.05108500	-3.71037900	1.91159700
H	-4.98122400	0.04499900	3.71758300
H	-6.30104100	-2.06421500	3.76364100
C	-5.18490200	3.77544100	0.75631000
C	-4.14203500	3.16226900	0.06396400
C	-4.40425300	2.03556700	-0.71742400
C	-5.70229200	1.53422500	-0.82143700
C	-6.73586500	2.15800500	-0.12405200
C	-6.49508200	3.28067700	0.68002900
H	-4.98234900	4.65906200	1.35784900
H	-3.13468500	3.56424600	0.10172500
H	-5.89456700	0.67638600	-1.45672900
H	-7.74804200	1.76910900	-0.21001200
C	-7.61712500	3.93069200	1.45585000
H	-7.39281200	4.97766800	1.68582000
H	-8.56006600	3.90032000	0.89891100
H	-7.78928200	3.41556800	2.41066000

H C O N S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Product D + catalyst

%nprocshared=16

%mem=800MB

opt freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	4.71080200	-2.91420600	-1.26004600
C	3.50026800	-3.39973400	-0.65550900
C	3.39637500	-2.82324500	0.65248500
C	5.36214100	-2.04523500	-0.31677200
C	4.54742400	-1.98544500	0.86057200
Fe	3.46785300	-1.32924300	-0.79369800
C	5.63869900	4.00997800	0.61543900
C	5.48743700	3.73542500	2.11881200
C	4.11529100	3.05713700	2.20640300
N	4.00367000	2.32640900	0.93894500
C	5.00996200	2.76844600	-0.03657400
C	2.95804800	1.48279600	0.68203200
C	1.90071400	1.33671300	1.58791800
C	0.80178500	0.49008900	1.30635300
N	0.64807400	-0.24237200	0.21816300
C	1.67036200	-0.14105100	-0.68725100
C	2.84859200	0.70071800	-0.52990200
H	6.67608700	4.16087200	0.30266900
H	5.07111800	4.90624000	0.33774000
H	6.26914900	3.04627600	2.46027100
H	5.54456800	4.63913200	2.73226100
H	4.03652000	2.36922200	3.05574900
H	3.30667100	3.79862600	2.30445100
H	5.76330600	1.98577300	-0.20448500
H	4.54605200	3.00036500	-0.99989800
H	1.87945900	1.90157400	2.51162400
H	-0.01101900	0.45048800	2.02981200
C	2.98124700	-0.39009000	-2.57662400
H	3.34661000	-0.72546100	-3.53887100
C	3.66654400	0.50885800	-1.70654600
H	4.61511700	0.97301600	-1.92711700
C	1.78922600	-0.83288600	-1.93653000
H	1.07120000	-1.54433900	-2.32157100
C	5.24175500	-3.30999700	-2.60876400
H	5.85749600	-4.21810000	-2.54125100
H	4.43292900	-3.51768500	-3.31690900
H	5.86831900	-2.52525200	-3.04526000
C	6.68992200	-1.37075500	-0.51501800
H	7.51774400	-2.02110000	-0.19878700
H	6.86125300	-1.11446500	-1.56578400
H	6.76378300	-0.44599300	0.06665200
C	4.84639800	-1.22644700	2.12151900
H	5.31372900	-1.87744900	2.87362600
H	5.53107600	-0.39181800	1.93982900
H	3.93380700	-0.81273500	2.56331800
C	2.30727000	-3.07199000	1.65584200
H	2.62448800	-3.80620600	2.40978900
H	2.02580600	-2.15479000	2.18276300
H	1.40311900	-3.45969700	1.17744500
C	2.53441100	-4.36914400	-1.27583000
H	2.52325100	-4.28470200	-2.36739100
H	2.80105100	-5.40672200	-1.03036900
H	1.51244200	-4.20003100	-0.92281600
C	-3.78223900	-0.70816100	-1.09218700

S	-3.35505000	2.21626100	1.31311300
O	-4.63887300	2.69594400	1.81641100
O	-2.26985000	1.81231800	2.20882700
N	-3.66565600	0.83001400	0.35188900
C	-3.12955900	5.08043100	-1.53967800
C	-3.62932400	4.16428300	-0.61724800
C	-2.72751300	3.40589600	0.13390800
C	-1.34756200	3.55102300	-0.02308100
C	-0.87110000	4.47598700	-0.95067000
C	-1.74901900	5.25336000	-1.71951400
H	-3.82480100	5.67047700	-2.13160200
H	-4.69640900	4.02688400	-0.48716800
H	-0.66320200	2.95627600	0.57256900
H	0.20209800	4.59432700	-1.07894300
C	-1.22218600	6.27252800	-2.70190500
H	-1.88221500	6.37003800	-3.57027500
H	-1.14816600	7.26491700	-2.23726000
H	-0.22324200	6.00440500	-3.06099700
C	-2.93065600	-0.46493800	0.24379000
C	-4.74445400	-1.88091000	-1.14018700
C	-4.26217700	-3.19184100	-1.00308700
C	-6.11078100	-1.69009600	-1.38643400
C	-5.12476100	-4.28246800	-1.09883900
H	-3.20766200	-3.36071000	-0.80386300
C	-6.97445300	-2.78413800	-1.48398800
H	-6.49817200	-0.68428800	-1.51371000
C	-6.48630200	-4.08249100	-1.33993000
H	-4.73314500	-5.28956000	-0.98148100
H	-8.03126300	-2.61605600	-1.67452400
H	-7.15911100	-4.93274900	-1.41456500
H	-1.87263100	-0.31166300	0.01088800
C	-3.06634700	-1.38999000	1.42389400
C	-1.97078500	-2.18827700	1.77934400
C	-4.25261800	-1.49052100	2.16277800
C	-2.06532000	-3.08493100	2.84572900
H	-1.03945500	-2.08377400	1.22738400
C	-4.34321600	-2.38146800	3.23117100
H	-5.10172200	-0.86302200	1.90882500
C	-3.25224000	-3.18507900	3.57297800
H	-1.20676500	-3.69504200	3.11510200
H	-5.26715100	-2.44686000	3.79961100
H	-3.32552900	-3.87757900	4.40758700
C	-4.40640500	0.67721200	-0.81669000
O	-5.16990200	1.41832800	-1.39046700
C	-2.90484600	-0.65562500	-2.35673600
H	-2.33267000	-1.58341900	-2.46087900
H	-3.53655300	-0.53880500	-3.24305300
H	-2.19922300	0.18189100	-2.31850900

H C O N S O
6-31G*

Fe 0
LANL2DZ

Fe 0
LANL2DZ

Product D' + catalyst

%nprocshared=16
%mem=1GB
freq=noraman b3lyp/gen pseudo=read

Title Card Required

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0 1
C      4.83244100    2.10226200    1.38302800
C      3.62529900    2.58878300    0.77226000
C      3.52835000    2.01262100   -0.53607200
C      5.48864600    1.23457000    0.44185200
C      4.68151400    1.17610800   -0.74061700
Fe     3.59182000    0.51854600    0.90553800
C      5.28478000   -4.91777200   -0.91049300
C      5.08463400   -4.55009200   -2.38804000
C      3.78649600   -3.73513500   -2.36304400
N      3.81893700   -3.06279500   -1.05926700
C      4.82573000   -3.65401100   -0.16622500
C      2.84485300   -2.17665300   -0.68651600
C      1.74549100   -1.91378400   -1.51015000
C      0.70863900   -1.04389500   -1.09848000
N      0.66233100   -0.37909500    0.04183700
C      1.73882300   -0.58440900    0.86378000
C      2.86061000   -1.46553600    0.57297700
H      6.31515000   -5.19206900   -0.66529500
H      4.63929400   -5.76291300   -0.64329400
H      5.91460900   -3.92626300   -2.74141700
H      5.01486900   -5.42115300   -3.04587200
H      3.73075100   -2.99999400   -3.17411900
H      2.90255900   -4.38683800   -2.44573100
H      5.66596700   -2.96230400   -0.00904600
H      4.39325800   -3.88623200    0.81135000
H      1.63009400   -2.42245200   -2.45881300
H     -0.14645600   -0.92604000   -1.76250400
C      3.19154300   -0.50629500    2.66271300
H      3.63949600   -0.24614900    3.61330200
C      3.76960600   -1.37898000    1.69349300
H      4.70826100   -1.89684900    1.81777200
C      1.97859100    0.02441700    2.13934300
H      1.32029300    0.73626400    2.61893500
C      5.35542100    2.49660700    2.73530400
H      5.96914500    3.40660800    2.67370900
H      4.54230600    2.69983700    3.43998700
H      5.98167500    1.71240500    3.17310100
C      6.81292600    0.55513100    0.64669500
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H	7.64458000	1.19954400	0.32827800
H	6.98098500	0.30385200	1.69916400
H	6.88246100	-0.37361200	0.07093100
C	4.99128600	0.41915300	-2.00019600
H	5.47966200	1.06659200	-2.74210700
H	5.66145100	-0.42534700	-1.81079100
H	4.08098500	0.01929300	-2.45892100
C	2.43646800	2.25388300	-1.53766300
H	2.70953100	3.05628100	-2.23819100
H	2.22928500	1.35506100	-2.12702200
H	1.50082000	2.53826900	-1.04738800
C	2.65292700	3.55583900	1.38578100
H	2.63635700	3.47314000	2.47746200
H	2.91594600	4.59465300	1.14021200
H	1.63391900	3.38038700	1.02599000
C	-2.83126500	-1.83315100	-0.57065500
O	-2.34234600	-2.67388100	-1.26285000
C	-3.43895700	-1.75849700	0.84594200
C	-4.63469000	-2.68748400	1.03320800
C	-4.83125900	-3.41532900	2.21357000
C	-5.59019400	-2.81322000	0.00893900
C	-5.94869000	-4.23973600	2.37038800
H	-4.11360800	-3.34604100	3.02370500
C	-6.70268200	-3.63758300	0.16301000
H	-5.46834400	-2.26395800	-0.92173400
C	-6.88808100	-4.35538900	1.34718800
H	-6.07920000	-4.79273100	3.29701300
H	-7.42353200	-3.72040000	-0.64586100
H	-7.75513800	-4.99916600	1.46817400
C	-2.34717000	-1.89592300	1.91210300
H	-2.71238900	-1.57561500	2.89307100
H	-2.02435000	-2.93965300	1.97838100
H	-1.47422800	-1.28993500	1.65888600
S	-3.50853900	0.33663000	-2.27426900
O	-2.63435200	-0.27134900	-3.27622300
O	-4.97167300	0.28089800	-2.39988200
N	-3.08237800	-0.38997900	-0.78771200
C	-3.85608100	-0.26001300	0.48173900
H	-4.93007100	-0.22008400	0.27967000
C	-3.46503300	0.87198200	1.39654000
C	-4.43728100	1.40868800	2.25218200
C	-2.15981900	1.38405600	1.44116500
C	-4.11654400	2.43290000	3.14421700
H	-5.45387700	1.02241000	2.21676700
C	-1.84471200	2.41454300	2.32816500
H	-1.39047100	0.97544600	0.79057300
C	-2.81686300	2.94093500	3.18245100
H	-4.88260500	2.83789300	3.80035700
H	-0.83138100	2.80861600	2.34957900
H	-2.56464300	3.74374200	3.87059700
C	-1.36288600	3.76149400	-2.03724700
C	-1.70766000	2.42168400	-2.18779100
C	-3.04704200	2.04935300	-2.04667700
C	-4.03510300	2.99472600	-1.77258100

C	-3.66887500	4.33215700	-1.62519300
C	-2.33289400	4.73501600	-1.74862200
H	-0.32363800	4.05907100	-2.15296800
H	-0.95406400	1.67641000	-2.41787500
H	-5.07102900	2.68439200	-1.69172500
H	-4.43509000	5.07408300	-1.41515400
C	-1.93731300	6.17996900	-1.55891200
H	-1.14132500	6.47211500	-2.25245500
H	-2.78712800	6.85259800	-1.71205100
H	-1.56096400	6.35235600	-0.54183800

H C O N S O

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Optimized molecular structure of reactants, intermediates, and products for the ketene-first mechanism of nucleophile-catalyzed Staudinger reaction involving N-Tf imine.

E. PPY-catalyst + ketene + N-Ts imine

%nprocshared=16

%mem=800MB

opt=modredundant freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	-3.15575900	-4.14241500	1.00972200
C	-1.93775200	-4.52321800	0.34833300
C	-1.96111200	-3.97276900	-0.97538500
C	-3.93950100	-3.36694900	0.08630200
C	-3.20039000	-3.25992100	-1.13666000
Fe	-2.10295200	-2.45699500	0.44070600
C	-4.85288300	2.58389900	-1.03025100
C	-4.71142600	2.30461500	-2.53347500
C	-3.27949200	1.77037900	-2.64593300
N	-3.06964500	1.05952700	-1.37683800
C	-4.08879700	1.42207800	-0.37663900
C	-1.93929500	0.34116200	-1.13520000
C	-0.90183700	0.26952600	-2.07935700
C	0.28452800	-0.44805700	-1.81179300
N	0.56280100	-1.11911800	-0.70771300
C	-0.43794100	-1.09718900	0.23082600
C	-1.70298400	-0.38768900	0.09317400

H	-5.89305300	2.63361000	-0.69408700
H	-4.36285500	3.53042200	-0.78106300
H	-5.42659400	1.53593600	-2.85203100
H	-4.86963700	3.19131100	-3.15400300
H	-3.14665300	1.08888300	-3.49392600
H	-2.55653200	2.59252100	-2.74886100
H	-4.75412200	0.56910900	-0.18006600
H	-3.61389900	1.72123300	0.55973000
H	-0.97447600	0.80132300	-3.01971000
H	1.06621800	-0.43707500	-2.57249900
C	-1.64994600	-1.41145400	2.17530000
H	-1.94275100	-1.74597800	3.16225500
C	-2.45178400	-0.61665000	1.30629200
H	-3.42955500	-0.23379900	1.55241500
C	-0.44258300	-1.75506400	1.50373100
H	0.35599300	-2.37576400	1.88547000
C	-3.57196600	-4.54809700	2.39513800
H	-4.11515200	-5.50381300	2.38298700
H	-2.70857100	-4.67337400	3.05665700
H	-4.23283300	-3.80482100	2.85306500
C	-5.31452000	-2.81956600	0.34472900
H	-6.09067400	-3.54693000	0.06729200
H	-5.45966900	-2.57682900	1.40246500
H	-5.50343000	-1.90781100	-0.23172500
C	-3.64984600	-2.56601800	-2.39052800
H	-4.11080400	-3.27569500	-3.09192800
H	-4.38928300	-1.78770000	-2.17715900
H	-2.81070100	-2.08842500	-2.90680700
C	-0.90360500	-4.13872300	-2.02889100
H	-1.13123600	-4.98669900	-2.69047900
H	-0.81632600	-3.24455600	-2.65410200
H	0.08024300	-4.31785800	-1.58546600
C	-0.85491900	-5.38677600	0.93018400
H	-0.77614500	-5.25988700	2.01491600
H	-1.05221700	-6.45123400	0.73927100
H	0.12310300	-5.15305200	0.49802300
S	-1.03236700	4.08764600	0.46751400
O	-1.87165600	4.54886400	-0.64138300
O	-1.41916800	2.90311400	1.24329000
C	-0.92378000	5.50234100	1.68342700
F	-0.03853100	5.21195500	2.63810000
F	-2.13051500	5.66364000	2.23059000
F	-0.56229200	6.62387400	1.06435000
N	0.57506000	4.08641300	-0.02673000
C	1.17598300	2.93872600	-0.04490500
H	0.66705300	2.02220400	0.26981400
C	2.55909500	2.81360000	-0.47732000
C	3.14559000	1.53536900	-0.51377400
C	3.31408000	3.94367200	-0.85085000
C	4.47179100	1.39003900	-0.91822100
H	2.55720500	0.66176600	-0.24232300
C	4.63593200	3.79191100	-1.24705200
H	2.84641500	4.92235900	-0.82078300
C	5.21433700	2.51574400	-1.28050000

H	4.92345200	0.40479400	-0.95204000
H	5.22034500	4.66228900	-1.53180500
H	6.24893300	2.39761500	-1.59122400
C	4.32571900	-2.40634500	2.35414800
O	4.31243600	-2.21650500	3.51227500
C	4.32400800	-2.63306000	1.04847000
C	5.43756200	-2.15770800	0.20564700
C	5.40096800	-2.34765500	-1.18803500
C	6.56379000	-1.50692400	0.75202400
C	6.44853100	-1.90518200	-1.99930800
H	4.54761600	-2.83766200	-1.64480100
C	7.60247300	-1.06499700	-0.06035400
H	6.62581800	-1.34709200	1.82640200
C	7.55440800	-1.26071100	-1.44520400
H	6.39297400	-2.06686100	-3.07284500
H	8.45732100	-0.56783300	0.39091100
H	8.36901900	-0.92002200	-2.07804600
C	3.13418100	-3.39014700	0.47453700
H	2.51446400	-2.74287600	-0.15860000
H	3.47974200	-4.25049500	-0.11199500
H	2.49237200	-3.77712300	1.27217900

B 15 75 F
B 62 77 F

H C O N F S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

TS_{E-F}

%nprocshared=16

%mem=800MB

opt=(modredundant,ts,calcfc,noeigen) freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

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C	4.35712900	-2.39134900	-0.50499200
C	4.07372400	-1.94025800	0.82543200
C	5.67630000	-0.52204700	-0.08455400
C	4.89169800	-0.78508800	1.08485200
Fe	3.65347600	-0.43147000	-0.55087300

C	3.54281600	5.03596000	1.73580900
C	3.38903700	4.49701400	3.16503100
C	2.39057300	3.34652700	2.99278400
N	2.66938800	2.83489000	1.64042200
C	3.51864900	3.76474000	0.87482600
C	2.04679700	1.73627600	1.14384300
C	1.04248000	1.07953100	1.88445900
C	0.29965900	0.03640600	1.32942400
N	0.51351600	-0.48806600	0.13114700
C	1.54802300	0.03735300	-0.60951400
C	2.32691100	1.18302000	-0.16125500
H	4.45696200	5.61723000	1.58618900
H	2.69074200	5.67601400	1.47931900
H	4.34747500	4.11146500	3.53253600
H	3.03373200	5.24816300	3.87567100
H	2.52370700	2.55451800	3.73758400
H	1.35206900	3.70226800	3.06055200
H	4.52867600	3.35072200	0.75050300
H	3.09634100	3.94319500	-0.11694700
H	0.75612600	1.43483600	2.86510300
H	-0.54050400	-0.37815900	1.88006400
C	3.04357400	0.56092700	-2.27623000
H	3.59320900	0.53278800	-3.20767400
C	3.27010500	1.48026200	-1.21448500
H	4.00991200	2.26435000	-1.22767100
C	2.02764300	-0.35848300	-1.89292600
H	1.64363800	-1.16762900	-2.49517100
C	5.96260700	-1.65063800	-2.43319100
H	6.82709600	-2.32848200	-2.40163400
H	5.25523100	-2.05915200	-3.16205800
H	6.31783300	-0.68978200	-2.81901600
C	6.70858200	0.55904000	-0.23578000
H	7.70554400	0.19592700	0.05026400
H	6.77620600	0.91449300	-1.26920000
H	6.48521400	1.42375700	0.39818400
C	4.95775400	-0.03978100	2.38724000
H	5.71291100	-0.47967400	3.05344700
H	5.22344200	1.01241900	2.24243900
H	3.99951300	-0.07045800	2.91547600
C	3.13766900	-2.58046800	1.80967900
H	3.67504700	-3.27671000	2.46876400
H	2.65254200	-1.83405200	2.44670700
H	2.34258400	-3.14285400	1.31403700
C	3.77709000	-3.60229600	-1.17831500
H	3.65488200	-3.44923400	-2.25532900
H	4.42881600	-4.47669700	-1.04321100
H	2.79718100	-3.86009700	-0.76687900
S	-2.07397900	0.26273300	-2.16768100
O	-1.01310700	-0.03024700	-3.15117800
O	-3.47371900	0.29929900	-2.60945100
C	-1.75700700	2.02582300	-1.63751600
F	-2.62709400	2.40503700	-0.68919400
F	-1.88361700	2.84384600	-2.68744100
F	-0.51328400	2.16745700	-1.13968600

N	-1.95321600	-0.55630200	-0.77758600
C	-0.89974900	-1.39759100	-0.63973700
H	-0.34896200	-1.68682200	-1.53634400
C	-1.11323700	-2.53008000	0.32124900
C	-0.28423900	-3.65831000	0.26562600
C	-2.16579400	-2.50089600	1.24564400
C	-0.48773100	-4.73262200	1.13113300
H	0.51307100	-3.69835400	-0.47308300
C	-2.36334200	-3.57181400	2.11933500
H	-2.84199500	-1.65234700	1.24268900
C	-1.52442900	-4.68701500	2.06770600
H	0.15434500	-5.60739700	1.06983900
H	-3.18645600	-3.53962100	2.82803300
H	-1.68581600	-5.52402200	2.74189100
C	-7.94194100	2.28003600	0.45061100
O	-8.72506800	3.01217900	0.93382700
C	-7.05386500	1.47036900	-0.10452300
C	-6.90540000	0.07760500	0.36816100
C	-5.92306700	-0.75574000	-0.19585600
C	-7.73128900	-0.45546200	1.37899800
C	-5.78080500	-2.07573100	0.23906200
H	-5.26241600	-0.38491900	-0.97265200
C	-7.58131400	-1.76975400	1.80881400
H	-8.50249400	0.16600300	1.83040300
C	-6.60337200	-2.59246700	1.24020100
H	-5.01343500	-2.69692900	-0.21466300
H	-8.23436800	-2.15468900	2.58842900
H	-6.49042900	-3.62167100	1.57093900
C	-6.20878700	2.03495800	-1.23761000
H	-5.14459900	2.02366400	-0.98287800
H	-6.33394600	1.43896300	-2.14854000
H	-6.49176500	3.06673100	-1.46815300

H C O N F S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Intermediate F

%nprocshared=16

%mem=800MB

opt=(modredundant) freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

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C	-4.32013800	-1.95043000	-0.83182200
C	-3.79495800	-1.00362400	-1.77094900
C	-5.31690800	0.10837900	-0.40966000
C	-4.41406800	0.26883800	-1.50997800
Fe	-3.38664500	-0.38341200	0.18191900
C	-2.21913900	5.40912400	0.65024300
C	-1.88718500	5.52889700	-0.84392700
C	-1.08437600	4.25336200	-1.12294900
N	-1.65150400	3.26503900	-0.18592000
C	-2.50264700	3.91105800	0.83002800
C	-1.27230100	1.96703300	-0.19375700
C	-0.24752200	1.52615000	-1.06228200
C	0.27693500	0.24643600	-0.97078900
N	-0.19182000	-0.70131500	-0.15375300
C	-1.28198600	-0.38316100	0.63883600
C	-1.82857200	0.96376500	0.68245800
H	-3.06658700	6.02775200	0.95841800
H	-1.35236300	5.69916200	1.25514500
H	-2.80741700	5.53283300	-1.44014000
H	-1.32266100	6.43204000	-1.09080600
H	-1.18853100	3.90458900	-2.15552700
H	-0.01363300	4.39584800	-0.92094600
H	-3.56095000	3.68172200	0.64496100
H	-2.24185600	3.55548700	1.82936100
H	0.24937300	2.21094800	-1.73377600
H	1.14647900	-0.02655700	-1.55690100
C	-2.94568800	-0.36340000	2.21859500
H	-3.63652200	-0.68989400	2.98423900
C	-2.88326000	0.94568100	1.66989000
H	-3.51553600	1.76758100	1.96495100
C	-2.00108200	-1.19779200	1.55828500
H	-1.80932400	-2.23561400	1.78156400
C	-6.07827500	-1.88609600	1.10720600
H	-7.03107000	-2.26361500	0.71045100
H	-5.56322800	-2.73153400	1.57415100
H	-6.31745900	-1.16688800	1.89720200
C	-6.21040000	1.16907700	0.16734900
H	-7.18988700	1.17479200	-0.33066000
H	-6.39015500	1.01124100	1.23571300
H	-5.77987500	2.16895700	0.04794600
C	-4.19943900	1.52241900	-2.30854700
H	-4.86965500	1.55257400	-3.17885300
H	-4.39541600	2.42201600	-1.71613000
H	-3.17386600	1.58856600	-2.68507300
C	-2.82711700	-1.28577200	-2.88429600
H	-3.35998100	-1.52331900	-3.81569900
H	-2.18313900	-0.42416900	-3.08791000
H	-2.17153000	-2.12934600	-2.65559000
C	-4.01244200	-3.41971200	-0.77721600
H	-4.03332000	-3.80259900	0.24804200
H	-4.74853800	-3.99419200	-1.35660600

H	-3.02640600	-3.64305100	-1.19362700
S	1.88566500	-1.60889300	2.46969800
O	0.69805600	-2.28436800	3.04214200
O	3.21889600	-1.96771800	2.97579500
C	1.72495700	0.15759700	3.05859700
F	2.72200100	0.91647800	2.57365200
F	1.75380400	0.22336100	4.39534900
F	0.55857800	0.70621300	2.64432900
N	1.88650900	-1.48907100	0.88317300
C	0.74516900	-1.93200700	0.18952100
H	0.08238700	-2.57615100	0.77432400
C	1.10144400	-2.62746300	-1.11828500
C	0.16398700	-3.45584200	-1.74766700
C	2.37357000	-2.48925500	-1.68492900
C	0.47745700	-4.11515100	-2.93658500
H	-0.81063500	-3.60317400	-1.28795900
C	2.68578200	-3.14015500	-2.88074900
H	3.11539900	-1.89790100	-1.15839200
C	1.74006400	-3.95035600	-3.51183400
H	-0.25640900	-4.76535400	-3.40601400
H	3.67756100	-3.02561900	-3.31037500
H	1.98937200	-4.46462400	-4.43635600
C	3.94548200	2.09717000	-2.05319800
O	2.78202100	2.23070700	-2.18870400
C	5.25469700	1.96613900	-1.93203300
C	5.85174500	1.09066000	-0.89596500
C	7.24480900	0.91799300	-0.84556900
C	5.05943500	0.41226900	0.05112800
C	7.82317000	0.08904000	0.11843500
H	7.88560900	1.42740000	-1.55851600
C	5.63755600	-0.41822500	1.00746900
H	3.97766000	0.52607500	0.05429400
C	7.02667000	-0.58253600	1.04443500
H	8.90398400	-0.02881800	0.13809600
H	4.99842800	-0.93394300	1.71883500
H	7.47884200	-1.22937500	1.79116000
C	6.11097300	2.74406300	-2.91992700
H	6.79095600	3.42273600	-2.39067600
H	6.71780900	2.06360300	-3.52971300
H	5.50022000	3.34540300	-3.59995400

H C O N F S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

TSF-G'

```
%nprocshared=16
%mem=800MB
# freq=noraman b3lyp/gen pseudo=read
```

Title Card Required

```
0 1
C      3.47052100   -3.22881400   -0.84283200
C      2.33403400   -3.30368100    0.03314300
C      2.59916500   -2.47360100    1.16997600
C      4.44667500   -2.36466800   -0.23566200
C      3.90524000   -1.89421400    1.00379300
Fe     2.67541400   -1.33613100   -0.58319600
C      5.51158300    3.73324900    0.39533500
C      5.24415100    3.65115500    1.90481000
C      3.78845000    3.17618900    1.97299900
N      3.63091200    2.33941100    0.76752800
C      4.76168500    2.51560900   -0.16285100
C      2.50620100    1.63153600    0.52476900
C      1.38491600    1.74925000    1.37930600
C      0.15472500    1.19740000    1.05790100
N     -0.03682500    0.39652200   -0.00067600
C      1.05839300    0.09243700   -0.79311200
C      2.33529500    0.76129100   -0.61545200
H      6.57485100    3.71246700    0.14091700
H      5.08475800    4.65508900   -0.01614700
H      5.90449900    2.90968700    2.36978400
H      5.38981600    4.60292700    2.42245600
H      3.57466500    2.59201100    2.87386600
H      3.08625200    4.02083000    1.94184200
H      5.39927100    1.62124700   -0.16212200
H      4.39755700    2.68066700   -1.17951500
H      1.41346200    2.40533200    2.23788400
H     -0.73435800    1.46320500    1.62824600
C      2.43462900   -0.58227500   -2.50306900
H      2.80065800   -1.08880400   -3.38596100
C      3.18585300    0.31463800   -1.69618400
H      4.20785400    0.60115000   -1.88370500
C      1.14368000   -0.76408500   -1.92656500
H      0.36649200   -1.41721500   -2.29434800
C      3.64397100   -3.98414200   -2.12977800
H      4.10283000   -4.96593800   -1.94857700
H      2.68618800   -4.16108500   -2.62887400
H      4.29039600   -3.44826400   -2.83228900
C      5.80803000   -2.05473700   -0.78988000
H      6.53604200   -2.82375700   -0.49726400
H      5.80089900   -2.01368700   -1.88398600
H      6.18721200   -1.09447500   -0.42481600
C      4.59564600   -1.01587600    2.00809700
H      5.08687400   -1.62015300    2.78322800
H      5.36775300   -0.39269500    1.54562200
H      3.88704200   -0.35237000    2.51420200
C      1.72361400   -2.30344100    2.37768800
```

H	2.04545000	-2.97574700	3.18546800
H	1.76410800	-1.28138700	2.76915600
H	0.67908400	-2.53147100	2.15494900
C	1.10956700	-4.14459200	-0.18492400
H	0.90501700	-4.29053700	-1.25014300
H	1.23953900	-5.14022100	0.26174800
H	0.21931800	-3.69557300	0.26089100
S	-2.55691500	2.21731100	-1.32944500
O	-2.21441000	1.71542000	-2.67233100
O	-3.78853600	2.96974400	-1.09449000
C	-1.22976000	3.51286400	-1.02771100
F	-1.18636800	3.87929100	0.25789700
F	-1.47604900	4.58978200	-1.77798900
F	-0.01206000	3.03392800	-1.36879500
N	-2.40485900	1.06196700	-0.19258800
C	-1.46204800	0.02057800	-0.47488300
H	-1.33587400	-0.07747100	-1.55591400
C	-1.86712600	-1.33348100	0.08516600
C	-2.35764700	-2.29686200	-0.80262800
C	-1.79944000	-1.63873600	1.45008900
C	-2.76305000	-3.55128400	-0.34217000
H	-2.44841100	-2.05453800	-1.85872800
C	-2.20226900	-2.89285100	1.91202900
H	-1.44438200	-0.89728600	2.15870900
C	-2.68018700	-3.85407400	1.01675600
H	-3.15149300	-4.28334900	-1.04434000
H	-2.15052500	-3.11575100	2.97453300
H	-2.99656700	-4.82802000	1.38036900
C	-3.28534300	1.30333600	1.56758800
O	-2.55054800	2.02636400	2.20218400
C	-4.40409300	0.54842400	1.67280200
C	-5.12288200	-0.26545700	0.67364200
C	-5.64628700	-1.51766200	1.06014800
C	-5.41042300	0.17299700	-0.63398400
C	-6.38261200	-2.30739300	0.17779400
H	-5.46099800	-1.88561000	2.06487500
C	-6.13730700	-0.62245400	-1.51961800
H	-5.09519300	1.16158400	-0.93977900
C	-6.62684800	-1.86990700	-1.12512000
H	-6.76501600	-3.26982400	0.51172600
H	-6.34199800	-0.24865600	-2.52045000
H	-7.20387700	-2.48140400	-1.81474300
C	-4.94686600	0.53103600	3.10380200
H	-6.04099100	0.60831000	3.09901200
H	-4.68794200	-0.39408800	3.64179500
H	-4.54775900	1.36656400	3.68460500

H C O N F S O
6-31G*

Fe 0
LANL2DZ

Fe 0
LANL2DZ

TSF-G

%nprocshared=8
%mem=800MB
freq=noraman b3lyp/gen pseudo=read

Title Card Required

```
0 1
C      4.14610500   -2.88401000   -0.33703100
C      2.83784200   -3.12936800    0.20334600
C      2.67934800   -2.30626000    1.36531400
C      4.80290500   -1.91977300    0.50329200
C      3.89520900   -1.56021200    1.55096500
Fe     3.06729000   -1.11593500   -0.30941800
C      4.96870300    4.23254600    1.27422300
C      4.38136100    4.07910300    2.68440600
C      3.02108700    3.42260800    2.42367800
N      3.24633600    2.60458200    1.21600200
C      4.52453100    2.94611600    0.56403700
C      2.30462100    1.77005100    0.72543400
C      1.01809100    1.71151800    1.31110100
C     -0.02888500    1.02509900    0.71568900
N      0.12035800    0.25563800   -0.37133100
C      1.39405400    0.11467400   -0.89732000
C      2.50592300    0.92315000   -0.42783000
H      6.05568000    4.35106600    1.26733600
H      4.53164800    5.10440200    0.77417000
H      5.01002600    3.41590900    3.29021700
H      4.28312400    5.02844500    3.21739600
H      2.68808500    2.79340000    3.25532300
H      2.24077800    4.17199400    2.23145800
H      5.25433200    2.13827900    0.70962000
H      4.37914700    3.09106100   -0.50899000
H      0.77384800    2.32369900    2.16787100
H     -1.04507700    1.13113100    1.08518600
C      3.19852600   -0.35075900   -2.23834700
H      3.81869200   -0.79031900   -3.00802200
C      3.62956900    0.60815400   -1.28169500
H      4.62610600    1.01440400   -1.22461700
C      1.83914100   -0.69464300   -1.97973000
H      1.25079200   -1.42634200   -2.51217700
C      4.75364400   -3.57336100   -1.52558900
H      5.29220400   -4.48066200   -1.21895700
H      3.99272800   -3.87740400   -2.25109800
H      5.47052700   -2.93011900   -2.04609000
C      6.21308600   -1.42882300    0.33854400
H      6.92152200   -2.09153400    0.85439500
H      6.51093100   -1.39312300   -0.71443800
H      6.34728000   -0.42531400    0.75604700
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C	4.17595100	-0.62896900	2.69524600
H	4.52636500	-1.18553400	3.57537600
H	4.95052100	0.10317400	2.44501600
H	3.27784500	-0.07912700	2.99446000
C	1.49473500	-2.27993400	2.28756500
H	1.65360900	-2.95327500	3.14151100
H	1.31575900	-1.27793100	2.69139200
H	0.58104500	-2.60006600	1.78169300
C	1.84157000	-4.12015400	-0.32606900
H	1.91946400	-4.23021400	-1.41229600
H	2.01287600	-5.11184100	0.11551800
H	0.81305800	-3.83110800	-0.09795600
S	-2.39888500	1.82310600	-2.12083900
O	-1.73099800	1.49438200	-3.39384900
O	-3.77181600	2.32003300	-2.09790600
C	-1.40233600	3.28091100	-1.49225300
F	-1.69237300	3.54605400	-0.21034900
F	-1.65424400	4.36819300	-2.22488300
F	-0.07873900	3.01613400	-1.57315500
N	-2.22516600	0.64741000	-1.01326000
C	-1.10722200	-0.22842800	-1.18453100
H	-0.74103800	-0.18041200	-2.21411300
C	-1.44035900	-1.67681000	-0.86213500
C	-1.48769700	-2.59733200	-1.91617000
C	-1.76803000	-2.10782600	0.43086600
C	-1.84944000	-3.92730300	-1.68877800
H	-1.26445000	-2.26507300	-2.92783700
C	-2.12729100	-3.43715200	0.65914900
H	-1.77184100	-1.40273300	1.25589600
C	-2.16763100	-4.35066600	-0.39798900
H	-1.88925700	-4.62579700	-2.52024900
H	-2.39425300	-3.75441100	1.66343100
H	-2.45602500	-5.38243100	-0.21628000
C	-3.57062800	0.46170700	0.53914200
O	-2.96355100	0.88470800	1.49058900
C	-4.70729300	-0.11177400	0.08663200
C	-5.77945400	-0.30030100	1.09868800
C	-7.05639900	-0.74209700	0.68510300
C	-5.60614000	-0.07341900	2.48368400
C	-8.09085800	-0.94977200	1.59724300
H	-7.25100100	-0.91694200	-0.36675700
C	-6.64214400	-0.28331500	3.38956900
H	-4.64793000	0.27352500	2.85186300
C	-7.89606600	-0.72538700	2.95962200
H	-9.05858800	-1.28712300	1.23215000
H	-6.46481700	-0.09771600	4.44695900
H	-8.70219100	-0.88696800	3.67056900
C	-4.97556200	-0.54459900	-1.33170100
H	-5.37893300	-1.56547000	-1.34944400
H	-5.70212900	0.10985000	-1.83016000
H	-4.06480300	-0.53568900	-1.92438000

H C O N F S O
6-31G*

Fe 0
LANL2DZ

Fe 0
LANL2DZ

Intermediate G

%nprocshared=16
%mem=800MB
freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	4.14939400	-2.83658100	-0.39023700
C	2.85895800	-3.11563700	0.17555600
C	2.69814200	-2.29244400	1.33748500
C	4.79454000	-1.85167300	0.43455800
C	3.89648100	-1.51300700	1.49761400
Fe	3.02295300	-1.09953700	-0.34985400
C	4.91211700	4.29454600	1.10136900
C	4.39649600	4.13662400	2.53881300
C	3.03968600	3.44971500	2.34725600
N	3.22276200	2.63214200	1.13175500
C	4.46401700	2.99355900	0.42128700
C	2.27265400	1.78130600	0.68780600
C	1.01468700	1.70539300	1.32976100
C	-0.05193600	1.00550100	0.78858400
N	0.06186000	0.23950400	-0.31083800
C	1.31675200	0.10672200	-0.89057800
C	2.43572800	0.93104500	-0.46949100
H	5.99454000	4.43743800	1.04147700
H	4.43171100	5.15283000	0.61773700
H	5.06801100	3.49044000	3.11636200
H	4.30375400	5.08656900	3.07169500
H	2.76141800	2.81641100	3.19563400
H	2.23481300	4.18138300	2.19173700
H	5.21671300	2.20262300	0.54167700
H	4.26911300	3.12539500	-0.64559000
H	0.80228600	2.31535600	2.19683900
H	-1.07201700	1.08513600	1.19317300
C	3.07861500	-0.35334800	-2.29049000
H	3.67527400	-0.79453900	-3.07757800
C	3.53197900	0.61979600	-1.35941800
H	4.52621100	1.03532300	-1.33811700
C	1.73238700	-0.70814400	-1.98066800
H	1.13577100	-1.45144000	-2.48712500
C	4.75497900	-3.51584900	-1.58569300
H	5.31515200	-4.41177100	-1.28433700
H	3.99118900	-3.83662900	-2.30098600

H	5.45274900	-2.85982200	-2.11629000
C	6.18752000	-1.32287100	0.24232700
H	6.92571800	-1.97905100	0.72356200
H	6.45558100	-1.25561900	-0.81724700
H	6.30846600	-0.32639800	0.67991100
C	4.17443000	-0.56724700	2.63050600
H	4.59119700	-1.10335200	3.49418100
H	4.89608000	0.20593600	2.34791500
H	3.26132300	-0.06674000	2.96782500
C	1.52906400	-2.29635000	2.27938200
H	1.70875100	-2.98484800	3.11694900
H	1.34725800	-1.30462700	2.70613200
H	0.60922400	-2.61482600	1.78346600
C	1.88284200	-4.13779900	-0.33007800
H	1.94024000	-4.24793000	-1.41764600
H	2.09488900	-5.12258600	0.10923900
H	0.85123300	-3.88053100	-0.07981600
S	-2.46244100	1.80189600	-2.04992100
O	-1.68703600	1.45268400	-3.24705000
O	-3.84434300	2.24903800	-2.11950200
C	-1.54870900	3.27927500	-1.33780600
F	-1.90175800	3.49404200	-0.07036700
F	-1.83546300	4.35931100	-2.06652100
F	-0.21863300	3.07289300	-1.38812700
N	-2.31700500	0.57691500	-0.93519800
C	-1.16366900	-0.29877100	-1.05197100
H	-0.84761000	-0.27325600	-2.09469300
C	-1.48299900	-1.73909300	-0.68643700
C	-1.48742400	-2.69070000	-1.71355000
C	-1.82963100	-2.13346800	0.61429900
C	-1.81858000	-4.02228600	-1.45194400
H	-1.25494000	-2.38557100	-2.73175800
C	-2.15546000	-3.46541400	0.87441400
H	-1.88839300	-1.39457500	1.40757200
C	-2.14853100	-4.41234600	-0.15379900
H	-1.82536100	-4.74657700	-2.26180400
H	-2.44000000	-3.75737700	1.88135000
H	-2.41314000	-5.44539800	0.05515500
C	-3.32247500	0.44053600	0.25326400
O	-2.82802100	0.81923300	1.35258900
C	-4.53918700	-0.12845400	-0.05927300
C	-5.57481600	-0.29113300	0.98041100
C	-6.86201300	-0.76849600	0.62992900
C	-5.37072600	-0.00029700	2.35348300
C	-7.86784500	-0.95097300	1.57754300
H	-7.09116700	-0.99199600	-0.40582400
C	-6.37974600	-0.18601500	3.29523800
H	-4.40678000	0.37923500	2.66210300
C	-7.63849700	-0.66514100	2.92362700
H	-8.84065400	-1.31708000	1.25502300
H	-6.17671200	0.04999500	4.33847300
H	-8.42192000	-0.80762900	3.66412000
C	-4.88543900	-0.61708400	-1.44835800
H	-5.27927100	-1.64212300	-1.41343000

H	-5.64849200	0.00560100	-1.93523000
H	-4.01805400	-0.63391400	-2.10838000

H C O N F S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Intermediate G'

%nprocshared=16

%mem=800MB

freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	3.47128300	-3.22814100	-0.87655900
C	2.32610800	-3.33656200	-0.01598300
C	2.55895600	-2.51435800	1.13410900
C	4.42136600	-2.35129500	-0.24702800
C	3.85548300	-1.90820300	0.99160900
Fe	2.63281800	-1.35523300	-0.60422300
C	5.51193000	3.71396600	0.26224700
C	5.31263800	3.61566500	1.78127300
C	3.86240900	3.13647000	1.90926000
N	3.65352800	2.31100100	0.70354300
C	4.74340700	2.49780600	-0.27291700
C	2.51842900	1.60718500	0.50170800
C	1.43061100	1.72301600	1.39864900
C	0.18436500	1.18366000	1.12307800
N	-0.04801900	0.39252400	0.06036000
C	1.01843000	0.07996600	-0.77184900
C	2.30338600	0.74167200	-0.63512100
H	6.56272200	3.70133700	-0.03999400
H	5.06207100	4.63733900	-0.12023700
H	5.99455400	2.87087400	2.20828000
H	5.47966400	4.56228900	2.30189400
H	3.68915400	2.54276800	2.81248200
H	3.15817200	3.97998900	1.91742800
H	5.38403900	1.60630800	-0.30563400
H	4.33588800	2.66788400	-1.27224000
H	1.49612600	2.37298700	2.26017300
H	-0.70422900	1.45263500	1.71471300

C	2.33977400	-0.60903100	-2.51982200
H	2.67620300	-1.12077800	-3.41144000
C	3.11847100	0.28786600	-1.73989400
H	4.13581300	0.56910200	-1.95833800
C	1.06546200	-0.78147500	-1.90373200
H	0.27590400	-1.43361000	-2.24612600
C	3.67743200	-3.96584600	-2.16905800
H	4.14555100	-4.94379400	-1.99073600
H	2.73138100	-4.14913700	-2.68800300
H	4.33009300	-3.41379700	-2.85312100
C	5.78378100	-2.00927500	-0.77920000
H	6.52362500	-2.76467300	-0.48080400
H	5.79124900	-1.96154600	-1.87300700
H	6.13773900	-1.04379600	-0.40271400
C	4.51894700	-1.02968600	2.01369900
H	5.02777800	-1.63511400	2.77642000
H	5.27212900	-0.37461200	1.56432900
H	3.79118600	-0.39812500	2.53303000
C	1.66139800	-2.37420100	2.32917200
H	1.96138600	-3.07396400	3.12191100
H	1.70345300	-1.36511100	2.75239100
H	0.61830500	-2.58362300	2.08196700
C	1.12616800	-4.20577100	-0.25634900
H	0.93756400	-4.34633600	-1.32542600
H	1.27753900	-5.20223500	0.18158900
H	0.21942100	-3.78525800	0.18413700
S	-2.51450200	2.26683100	-1.25083300
O	-2.07424500	1.73795600	-2.54816600
O	-3.76490400	2.99504200	-1.08518800
C	-1.21506000	3.57095500	-0.85547700
F	-1.22802900	3.90871700	0.43166600
F	-1.47078500	4.64994100	-1.59866000
F	0.01424300	3.12063300	-1.17467900
N	-2.43541100	1.05206700	-0.12189400
C	-1.46793500	-0.00434800	-0.35451700
H	-1.38639000	-0.13055200	-1.43342900
C	-1.87991700	-1.32906200	0.26267600
C	-2.29751600	-2.35519400	-0.59069000
C	-1.89167800	-1.54061000	1.64840700
C	-2.70446700	-3.58841200	-0.07565200
H	-2.33343100	-2.18199100	-1.66353100
C	-2.29491800	-2.77379700	2.16168800
H	-1.61838600	-0.73789900	2.32639200
C	-2.69593700	-3.80140000	1.30219600
H	-3.03721400	-4.37146400	-0.75076900
H	-2.30919300	-2.92678100	3.23739500
H	-3.01488700	-4.75745400	1.70864600
C	-3.14862300	1.21948700	1.28122600
O	-2.43365000	1.79808900	2.14113100
C	-4.38063700	0.62516100	1.42695000
C	-5.12609600	-0.20788000	0.46508900
C	-5.76043900	-1.38269300	0.93574100
C	-5.30378300	0.09292300	-0.90293900
C	-6.48131300	-2.22300200	0.09003300

H	-5.66734300	-1.64957800	1.98418100
C	-6.01843000	-0.75293200	-1.75134000
H	-4.93187000	1.02985800	-1.29329600
C	-6.60848600	-1.92270600	-1.26816100
H	-6.94439400	-3.12045600	0.49587300
H	-6.13546600	-0.47626600	-2.79721500
H	-7.17313700	-2.57463700	-1.93035100
C	-4.92521000	0.70779200	2.84398800
H	-6.02035500	0.66402600	2.84971800
H	-4.56167700	-0.10796000	3.49182800
H	-4.60786200	1.64220000	3.31445200

H C O N F S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

TS_{G-H}

%nprocshared=16

%mem=800MB

opt=(ts,calcfc,noeigen) freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	-4.65581800	-2.88650800	-0.73528000
C	-3.47872900	-2.66865000	-1.53090300
C	-3.54274400	-1.33993600	-2.06519400
C	-5.45578100	-1.69264800	-0.78948200
C	-4.76639000	-0.73801700	-1.60600700
Fe	-3.57877700	-1.28967700	0.01548300
C	-6.12931400	3.33008400	2.77555300
C	-6.10589700	4.17440500	1.49287100
C	-4.72394200	3.86500100	0.90717200
N	-4.47641100	2.47529300	1.30818900
C	-5.40259000	2.03987500	2.36401500
C	-3.36581000	1.79522300	0.89042700
C	-2.38235900	2.41490700	0.11183700
C	-1.21085200	1.72643000	-0.27715000
N	-0.91990400	0.46890600	0.00589700
C	-1.87254900	-0.18432300	0.74327500
C	-3.11111000	0.41150800	1.22374000
H	-7.13846600	3.13513000	3.15024800
H	-5.56867300	3.83758700	3.56953000
H	-6.89044700	3.84127200	0.80274700
H	-6.25004200	5.24318200	1.67524200
H	-4.69308400	3.96118200	-0.18407500

H	-3.95433400	4.53544700	1.32125400
H	-6.11154800	1.29298700	1.97945200
H	-4.85857200	1.58939600	3.19945600
H	-2.47053000	3.45842400	-0.16322300
H	-0.45706300	2.27792800	-0.83607000
C	-3.01986800	-1.79272000	1.94694400
H	-3.28742500	-2.73109900	2.41564400
C	-3.82417700	-0.61541200	1.94837500
H	-4.78116200	-0.52640600	2.43842200
C	-1.85325100	-1.55371700	1.16590700
H	-1.06450800	-2.26169500	0.94914700
C	-5.01944200	-4.16242100	-0.03017200
H	-5.58469900	-4.83508000	-0.69085900
H	-4.13054700	-4.70723700	0.30479300
H	-5.64147400	-3.97451300	0.85122400
C	-6.80383300	-1.51082600	-0.15142100
H	-7.60651900	-1.87221200	-0.80972900
H	-6.88299700	-2.06327100	0.79074600
H	-7.01171100	-0.45749500	0.06387200
C	-5.24739000	0.63606400	-1.97605100
H	-5.73451400	0.63131400	-2.96123300
H	-5.97438800	1.02063600	-1.25356500
H	-4.41881300	1.35031600	-2.02157500
C	-2.54324600	-0.69462500	-2.98175000
H	-2.83203400	-0.82285200	-4.03458800
H	-2.45754400	0.37971300	-2.79130500
H	-1.54410500	-1.12234000	-2.85812100
C	-2.39297300	-3.67514000	-1.78494000
H	-2.23225400	-4.32538500	-0.91858200
H	-2.64156400	-4.32079600	-2.63903900
H	-1.44097600	-3.18489200	-2.01110600
S	3.23440100	2.79382800	-0.32281900
O	1.89627000	3.03525600	-0.85779700
O	3.75667600	3.47517700	0.85184300
C	4.42304300	3.15172600	-1.74790400
F	4.37077000	2.14788900	-2.62726400
F	5.65815800	3.31003200	-1.30576900
F	4.00751300	4.27565900	-2.33710300
N	3.36674600	1.10016500	-0.08542700
C	2.43971500	0.21449500	-0.57176300
H	1.38670600	0.45190600	-0.41625500
C	2.74536500	-0.94305500	-1.35617300
C	1.68168300	-1.84600600	-1.61301900
C	4.01285900	-1.19216600	-1.94893300
C	1.88531800	-2.96857800	-2.40569800
H	0.70734800	-1.63697200	-1.17978300
C	4.19663700	-2.31537900	-2.74062800
H	4.82652300	-0.49390400	-1.78942100
C	3.14213700	-3.21133500	-2.96942800
H	1.06416400	-3.65561600	-2.59132800
H	5.16645500	-2.49445700	-3.19640300
H	3.29861200	-4.08542500	-3.59537100
C	4.52255400	0.51484100	0.58735700
O	5.64912600	0.75183600	0.14007300

C	4.11685200	-0.36246700	1.65390700
C	5.05203100	-1.34131500	2.18695900
C	4.66919500	-2.16898100	3.27807500
C	6.33957000	-1.57551300	1.62822800
C	5.50564900	-3.16441100	3.76775200
H	3.69851300	-2.03851500	3.74116000
C	7.16804600	-2.57472600	2.12492800
H	6.67770900	-0.94485700	0.81861900
C	6.76317300	-3.37693900	3.19553100
H	5.17507800	-3.77846500	4.60154300
H	8.14630000	-2.72422900	1.67507800
H	7.41889900	-4.15254700	3.58218700
C	2.81466300	-0.16101700	2.40194500
H	2.19205500	-1.06430100	2.41456300
H	3.02449400	0.09263700	3.45065400
H	2.21480400	0.64859600	1.98880600

H C O N F S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

TS_G-H'

%nprocshared=16

%mem=800MB

opt=(ts,calcfc,noeigen) freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	3.15121900	-3.21322400	-0.05497200
C	2.19346400	-2.95912300	0.98578400
C	2.67778100	-1.86466900	1.77380300
C	4.23803800	-2.28505300	0.10292100
C	3.94379900	-1.44944600	1.22901500
Fe	2.45055400	-1.27476100	-0.21251100
C	5.28118600	3.84261600	-1.27666100
C	5.33754400	4.18860400	0.21828200
C	3.95008200	3.77105100	0.71878100
N	3.59428500	2.63009500	-0.13748700
C	4.48647600	2.52870700	-1.30468900
C	2.45428500	1.91301700	0.05545700
C	1.52790800	2.28092000	1.04765000
C	0.29611700	1.62082500	1.17008900
N	-0.07835100	0.58599400	0.44235400
C	0.82029100	0.11531300	-0.48217500

C	2.09863500	0.76071600	-0.74104300
H	6.26818400	3.73811200	-1.73625300
H	4.73565200	4.62023100	-1.82394600
H	6.11190000	3.59428800	0.71784800
H	5.54646500	5.24452100	0.41124500
H	3.95157300	3.47451400	1.77366500
H	3.21874200	4.58477900	0.60039100
H	5.15357600	1.66087600	-1.20823500
H	3.90724700	2.41390600	-2.22438100
H	1.70748000	3.13740500	1.68393600
H	-0.42860100	1.97959800	1.89678500
C	1.85262600	-1.03393000	-2.18722000
H	2.05200800	-1.76624300	-2.95853300
C	2.73800900	0.00965000	-1.79655100
H	3.70406700	0.19382600	-2.23862400
C	0.70190800	-1.01109700	-1.35066800
H	-0.13706200	-1.68982500	-1.41102200
C	3.06072300	-4.30555200	-1.08240100
H	3.49715600	-5.24081600	-0.70434400
H	2.02185800	-4.51724500	-1.35525800
H	3.59750900	-4.04435600	-2.00027800
C	5.47803900	-2.23281600	-0.74375000
H	6.24382100	-2.92654300	-0.36957200
H	5.26934800	-2.50771000	-1.78290300
H	5.92165800	-1.23169800	-0.74996100
C	4.82618500	-0.37656400	1.80119500
H	5.43789700	-0.76859500	2.62594200
H	5.51419800	0.02898500	1.05206700
H	4.23964200	0.45800500	2.19937000
C	2.02695900	-1.27929900	2.99413100
H	2.40989700	-1.75204400	3.90963800
H	2.21799900	-0.20449300	3.07492200
H	0.94202300	-1.41231900	2.98372900
C	0.93185800	-3.74028600	1.21903600
H	0.44082100	-4.01434700	0.28012100
H	1.13953600	-4.66923800	1.76848300
H	0.21116400	-3.16803700	1.81001400
S	-2.46943700	1.66928200	-1.67159900
O	-1.06246900	1.58517400	-2.05194800
O	-3.53698000	1.58510800	-2.66110400
C	-2.65063500	3.37718700	-0.91754700
F	-3.90051900	3.60930400	-0.53753600
F	-2.28573200	4.28075500	-1.83167100
F	-1.84206400	3.49498300	0.15087800
N	-2.85188900	0.59947800	-0.45634000
C	-2.08732200	-0.09789000	0.52147500
H	-1.69440200	-1.06006400	0.22634200
C	-2.37435100	0.11668600	1.93725700
C	-1.98418900	-0.87315700	2.86429500
C	-3.01482200	1.27867200	2.41444100
C	-2.22655100	-0.70985800	4.22257900
H	-1.50870900	-1.78022400	2.50053400
C	-3.25685000	1.43234300	3.77962600
H	-3.34505100	2.03622200	1.71626200

C	-2.86248500	0.44820900	4.68756500
H	-1.92679200	-1.48561100	4.92209700
H	-3.76092700	2.32761200	4.13299000
H	-3.05167000	0.57685000	5.74973700
C	-4.28321700	0.18126300	-0.20386800
O	-5.09275600	1.03328800	0.14083500
C	-4.37606100	-1.23708400	-0.11849600
C	-3.62235200	-2.19218200	-0.93630300
C	-3.39560400	-3.50829600	-0.46616000
C	-3.13406400	-1.87939100	-2.22702800
C	-2.68532300	-4.43977500	-1.22046300
H	-3.77271900	-3.79838600	0.50987200
C	-2.42127900	-2.81377000	-2.97689300
H	-3.35790100	-0.91094200	-2.65916600
C	-2.18300700	-4.09891900	-2.48020300
H	-2.52884000	-5.44053900	-0.82418200
H	-2.07222500	-2.54007800	-3.96968000
H	-1.64167200	-4.83001200	-3.07493000
C	-5.50165900	-1.76131500	0.74124200
H	-5.11562200	-2.34583500	1.59049900
H	-6.08186700	-0.92874600	1.14243300
H	-6.17676800	-2.42191600	0.18103500

H C O N F S O

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Product H + catalyst

%nprocshared=16

%mem=800MB

opt freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	4.90182200	-2.83606400	-0.68275500
C	3.95554300	-3.23812500	0.32183100
C	3.95589300	-2.24376000	1.35372200
C	5.49599200	-1.59560300	-0.26331100
C	4.90931200	-1.22854200	0.99113600
Fe	3.43786900	-1.39084300	-0.47183500
C	4.00071100	4.55263600	-0.93480000
C	4.07856500	4.74725100	0.58649800
C	3.03766500	3.75284800	1.11268300
N	3.07938600	2.65228900	0.14197800
C	3.78251800	3.03903100	-1.08972200

C	2.32724900	1.52326900	0.30988600
C	1.47445800	1.37496000	1.40996300
C	0.62575700	0.25177700	1.53190100
N	0.54968000	-0.76213600	0.68874400
C	1.41006600	-0.68127300	-0.37489600
C	2.32342700	0.42440100	-0.63125700
H	4.89363000	4.89819500	-1.46401800
H	3.13935100	5.09710700	-1.33960700
H	5.07576500	4.47771700	0.95484200
H	3.86924900	5.77306700	0.90291800
H	3.27263700	3.38957500	2.11956800
H	2.03137200	4.19838300	1.14518300
H	4.74086300	2.50706200	-1.17576700
H	3.18398900	2.79955200	-1.97313500
H	1.38614900	2.15700900	2.15285200
H	-0.06152000	0.22488400	2.37610200
C	2.55438800	-1.14065500	-2.33176300
H	2.90609700	-1.64086600	-3.22503300
C	3.04733000	0.10437000	-1.84042700
H	3.81067400	0.69511200	-2.32276500
C	1.59124900	-1.65001100	-1.41503400
H	1.06454600	-2.59236300	-1.48408300
C	5.26216600	-3.61331200	-1.91732800
H	6.09053000	-4.30860400	-1.72032500
H	4.41842300	-4.20880600	-2.28120500
H	5.57782300	-2.95490600	-2.73351900
C	6.58565900	-0.85525400	-0.98564800
H	7.57822300	-1.22370700	-0.69004600
H	6.50547300	-0.97388600	-2.07126000
H	6.56071800	0.21754300	-0.76762800
C	5.26052800	-0.02813600	1.82340200
H	6.03675200	-0.27311000	2.56206100
H	5.64125800	0.79419300	1.20912100
H	4.39076700	0.34668000	2.37273300
C	3.13906900	-2.26755300	2.61332800
H	3.70450900	-2.71501000	3.44295900
H	2.84408900	-1.25896400	2.91922800
H	2.21990200	-2.84622900	2.48570900
C	3.13541600	-4.49680100	0.30872900
H	2.89474200	-4.81165300	-0.71190900
H	3.67393600	-5.32578800	0.78922100
H	2.19012400	-4.36427300	0.84390400
C	-3.67646600	-0.40056900	-1.28588400
S	-2.81020700	2.64152100	0.77674800
O	-3.84195800	3.66552100	0.78488300
O	-2.11093100	2.19632000	1.97490700
N	-3.37808100	1.26758900	-0.01112900
C	-2.95924500	-0.16832100	0.12525600
C	-4.86701400	-1.33947800	-1.35342200
C	-4.70978400	-2.69113400	-1.01043300
C	-6.11597800	-0.90179800	-1.81380300
C	-5.77759400	-3.58062800	-1.11539400
H	-3.75107800	-3.04771000	-0.64457500
C	-7.18524100	-1.79502600	-1.91965300

H	-6.25195400	0.13546500	-2.10281500
C	-7.02103000	-3.13505700	-1.57059300
H	-5.63863900	-4.62209400	-0.83782000
H	-8.14693700	-1.43782400	-2.27830600
H	-7.85366300	-3.82857300	-1.65237200
H	-1.87609000	-0.27494600	0.03392200
C	-3.43651000	-0.86696500	1.36890400
C	-2.57435900	-1.78039600	1.99135000
C	-4.71091900	-0.64822100	1.90945400
C	-2.98864900	-2.47492300	3.13007200
H	-1.57359500	-1.92600800	1.58906200
C	-5.11816600	-1.33698900	3.05060600
H	-5.38327900	0.06528000	1.44205800
C	-4.26008300	-2.25554900	3.66158100
H	-2.31110600	-3.17786600	3.60776600
H	-6.10682700	-1.15629200	3.46379300
H	-4.58007700	-2.79058000	4.55188200
C	-3.99377700	1.10768200	-1.27330500
O	-4.48143800	1.90404200	-2.02958300
C	-2.65791700	-0.70438600	-2.40306900
H	-2.28982800	-1.73092200	-2.30964500
H	-3.13640300	-0.59502400	-3.38113600
H	-1.79979800	-0.02499300	-2.35511400
C	-1.48742500	3.23402000	-0.42331100
F	-0.77532300	2.18855200	-0.86340200
F	-0.67808200	4.08231600	0.21572300
F	-2.05016500	3.84626600	-1.45996900

H C O N F S O

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Product H' + catalyst

%nprocshared=16

%mem=800MB

opt freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	4.23384300	-2.77213600	-0.15311800
C	3.22804000	-2.87073500	0.86869300
C	3.37896400	-1.75033100	1.74904600
C	5.01559200	-1.59329800	0.10537500
C	4.48643400	-0.96110000	1.27756800
Fe	3.01925500	-1.09727100	-0.19056700
C	4.47657600	4.60272800	-1.17958000

C	4.54488400	4.90681800	0.32398400
C	3.33201300	4.15187700	0.88013900
N	3.20945200	2.98534500	-0.00115300
C	4.01244200	3.13860500	-1.22276800
C	2.28147300	2.00647900	0.22622500
C	1.35669500	2.10659700	1.27119000
C	0.36156200	1.12132500	1.46677100
N	0.20011400	0.02560300	0.74893000
C	1.10394600	-0.12357600	-0.27094600
C	2.16542700	0.81987900	-0.59266900
H	5.42869200	4.75067400	-1.69771800
H	3.72932400	5.24576600	-1.65958900
H	5.46947300	4.50210500	0.75310900
H	4.50844900	5.97599600	0.55189200
H	3.46986700	3.83547500	1.92059900
H	2.42187100	4.77071400	0.83960300
H	4.87211000	2.45279700	-1.21654600
H	3.41467000	2.92190000	-2.11270500
H	1.34305700	2.97472800	1.91837100
H	-0.36045900	1.27878900	2.26703100
C	2.24484600	-0.93633800	-2.10911500
H	2.55608600	-1.57070900	-2.92915800
C	2.88478600	0.27854500	-1.72282600
H	3.73892600	0.70865200	-2.22231600
C	1.18894400	-1.21427900	-1.19578300
H	0.53459400	-2.07523600	-1.20006300
C	4.47591900	-3.76496400	-1.25472400
H	5.17944900	-4.54728700	-0.93607800
H	3.55133300	-4.26495200	-1.56150900
H	4.90187600	-3.28748100	-2.14336400
C	6.21034600	-1.14101700	-0.68536200
H	7.13596100	-1.59329900	-0.30187200
H	6.12515300	-1.42048700	-1.74066300
H	6.33766400	-0.05421100	-0.64171600
C	5.02495300	0.27410900	1.94190800
H	5.75067700	0.01706500	2.72646500
H	5.53426800	0.92906500	1.22763700
H	4.22668700	0.85783100	2.41132500
C	2.54771300	-1.46867800	2.96716300
H	2.94950800	-1.98409700	3.85104300
H	2.51636800	-0.39868600	3.19400700
H	1.51338000	-1.79657400	2.82733100
C	2.21724500	-3.97257100	1.01314700
H	1.96240600	-4.41525800	0.04486900
H	2.59915000	-4.78033500	1.65360200
H	1.28899400	-3.60640000	1.46290400
C	-4.11267300	-1.32521600	-0.31450600
S	-3.50592100	2.41738100	-0.46406700
O	-4.68525700	3.12646200	-0.93490300
O	-2.75563600	2.80806600	0.72179100
N	-3.87260800	0.78008300	-0.31003700
C	-3.25855600	-0.28440200	0.54705400
H	-2.18750700	-0.37997100	0.34738800
C	-3.49704100	-0.16819000	2.02988500

C	-2.56960300	-0.76270000	2.89744800
C	-4.61312300	0.48251500	2.57209300
C	-2.76919400	-0.73101200	4.27876300
H	-1.67486900	-1.22054400	2.48288000
C	-4.80744000	0.52085900	3.95286400
H	-5.32373300	0.97588700	1.91509200
C	-3.89080100	-0.09214100	4.81020800
H	-2.04050100	-1.19401500	4.93895900
H	-5.67412100	1.03536000	4.35903500
H	-4.04375400	-0.06036900	5.88560600
C	-4.56100200	-0.11567800	-1.15989600
O	-5.21686400	0.06256800	-2.15043500
C	-2.28955900	2.39702200	-1.89012200
F	-1.27709500	1.57887500	-1.59926900
F	-1.82749300	3.63404900	-2.07412000
F	-2.89800800	1.97438700	-2.99660700
C	-3.28712000	-2.36196500	-1.06307400
C	-3.46192400	-2.58839600	-2.43477700
C	-2.37569100	-3.16050700	-0.35622200
C	-2.73231000	-3.58624700	-3.08565000
H	-4.16909500	-1.98364600	-2.99318500
C	-1.65140200	-4.15991500	-1.00647400
H	-2.23263900	-3.00165800	0.70939900
C	-1.82603700	-4.37475900	-2.37622000
H	-2.87673900	-3.74565600	-4.15088800
H	-0.95241900	-4.77133000	-0.44164300
H	-1.26277500	-5.15345500	-2.88355600
C	-5.29717600	-1.99027300	0.40492000
H	-4.93524500	-2.72416900	1.13196500
H	-5.91912000	-1.26283400	0.93360600
H	-5.91815100	-2.51057400	-0.33088400

H C O N F S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Optimized molecular structure of reactants, intermediates, and products for the imine-first mechanism of nucleophile-catalyzed Staudinger reaction involving N-Tf imine.

TS_{E-J}

%nprocshared=16

%mem=800MB

opt=(modredundant,ts,calcfc,noeigen) freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	2.08444800	-2.49728800	1.71042900
C	1.42519400	-1.43971800	2.42607600
C	2.36838000	-0.37661000	2.61385000
C	3.44261700	-2.09024400	1.46883200
C	3.61624900	-0.78071300	2.02302900
Fe	2.10954500	-0.76268000	0.58493200
C	6.53337500	0.51398500	-3.13544400
C	7.19290500	1.45344700	-2.11540800
C	5.99920900	2.21841500	-1.53189200
N	4.89743600	1.24731600	-1.58685800
C	5.23114500	0.09375800	-2.43816200
C	3.67793000	1.50646300	-1.03945500
C	3.39257500	2.76031400	-0.47070700
C	2.11120000	3.06334100	0.01761800
N	1.09143800	2.22129800	0.06330600
C	1.32923100	0.96435900	-0.43411300
C	2.59408800	0.55094000	-1.02389600
H	7.15545500	-0.34566200	-3.40066400
H	6.30395800	1.06007500	-4.05807800
H	7.68785700	0.87277400	-1.32782500
H	7.93663500	2.12137900	-2.55889200
H	6.16978900	2.54743100	-0.50085200
H	5.76108900	3.10962300	-2.13252100
H	5.38083900	-0.80789600	-1.82847500
H	4.42645600	-0.10723400	-3.15026500
H	4.13515900	3.54754800	-0.46694500
H	1.90735300	4.07228600	0.36970800
C	1.08310600	-1.20668500	-1.17346800
H	0.64594000	-2.17256600	-1.38521000
C	2.42386000	-0.81850300	-1.45447400
H	3.15730300	-1.45040600	-1.92981600
C	0.42562900	-0.13887800	-0.49988700
H	-0.58768700	-0.13756400	-0.12670200
C	1.49204200	-3.83011400	1.35057400
H	1.69381800	-4.57195800	2.13645300
H	0.40824700	-3.77715800	1.22231300
H	1.91113400	-4.22186300	0.41816500
C	4.49904800	-2.92256100	0.79919900
H	5.03026000	-3.55154600	1.52740300
H	4.06726900	-3.58995400	0.04648100
H	5.24938300	-2.30054900	0.29966000
C	4.88589800	0.02174200	2.04153100
H	5.43875000	-0.13556200	2.97836000
H	5.55278900	-0.25482000	1.21845000
H	4.68259800	1.09446400	1.95645600
C	2.12828900	0.91189100	3.34662000
H	2.50278400	0.85606900	4.37854600
H	2.63170500	1.75400300	2.85981400
H	1.06288700	1.15365600	3.39770100
C	0.01049400	-1.46717700	2.93221500
H	-0.63094100	-2.09690300	2.30924900

H	-0.03145000	-1.86897400	3.95438700
H	-0.43120300	-0.46591700	2.95659800
C	-0.82564700	3.00550600	-0.29690200
O	-1.10979600	2.48750300	-1.33543900
C	-1.11908300	3.87731600	0.69520600
C	-2.24426600	4.80565500	0.43542400
C	-2.71126200	5.65186500	1.46523200
C	-2.88169600	4.92322700	-0.82261100
C	-3.75788000	6.55010500	1.25473900
H	-2.25206100	5.61125300	2.44672000
C	-3.92584500	5.82232600	-1.02640100
H	-2.54303000	4.31320300	-1.65331500
C	-4.37892000	6.64408900	0.00983200
H	-4.08650100	7.18167300	2.07706400
H	-4.38322900	5.88678200	-2.01130600
H	-5.19284100	7.34509700	-0.15373700
C	-0.43074600	3.91143500	2.03593500
H	0.01783200	4.89260200	2.24899600
H	-1.14280300	3.70824900	2.84813300
H	0.34914700	3.15382600	2.09014000
S	-2.70388300	-4.01556800	-1.29828900
O	-3.22542300	-5.01191800	-2.22740600
O	-1.39072800	-3.39552100	-1.51923500
C	-2.60172100	-4.83064800	0.38122000
F	-2.30893200	-3.91279000	1.31398400
F	-1.62429500	-5.73829700	0.34314500
F	-3.75073100	-5.42261700	0.69152300
N	-3.92168900	-2.90368600	-0.94654200
C	-3.61870400	-1.65536100	-1.11265500
H	-2.61781400	-1.35705100	-1.44373700
C	-4.56952800	-0.58698500	-0.85670200
C	-4.13085100	0.74655100	-0.95962200
C	-5.90325600	-0.86198700	-0.49203800
C	-5.01207100	1.79205300	-0.68872700
H	-3.10345700	0.96964500	-1.24000700
C	-6.77725700	0.18464400	-0.23246100
H	-6.22758700	-1.89516300	-0.42182900
C	-6.33129400	1.51046800	-0.32780800
H	-4.66644100	2.81933500	-0.75281100
H	-7.80627500	-0.02432200	0.04592000
H	-7.01755200	2.32667200	-0.11825300

H C O N F S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Intermediate J

%nprocshared=16

%mem=800MB

opt=(modredundant) freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	-2.29511400	2.70816900	1.38767100
C	-1.99614700	1.57111300	2.21459400
C	-3.14248400	0.71256600	2.21047100
C	-3.63435600	2.55386500	0.88434500
C	-4.15395300	1.31502500	1.38453400
Fe	-2.43648600	0.98269700	0.26067100
C	-6.49545600	-1.48775800	-3.19316000
C	-6.89776600	-2.50248400	-2.11357100
C	-5.54696500	-2.97767800	-1.56633300
N	-4.67387600	-1.80009300	-1.70799200
C	-5.28087800	-0.77706800	-2.57783400
C	-3.43767900	-1.74477800	-1.15504900
C	-2.88533400	-2.88469300	-0.52658700
C	-1.59915100	-2.87970800	0.00054100
N	-0.80902400	-1.80435900	0.03787300
C	-1.28074700	-0.64650500	-0.56209700
C	-2.58352400	-0.58244400	-1.20316400
H	-7.29483500	-0.78701600	-3.44946000
H	-6.19854000	-2.00921600	-4.11057100
H	-7.47092800	-2.00862700	-1.32013200
H	-7.50041200	-3.32916700	-2.49958600
H	-5.60062700	-3.28970800	-0.51809800
H	-5.15153600	-3.82204600	-2.14996600
H	-5.58540300	0.09513100	-1.98525300
H	-4.56777500	-0.44630400	-3.33693600
H	-3.42613700	-3.82098300	-0.50765700
H	-1.16501200	-3.78727500	0.40150400
C	-1.46274500	1.42299500	-1.52390700
H	-1.22095900	2.43060700	-1.83288500
C	-2.68693500	0.74319700	-1.77476700
H	-3.51751100	1.15224100	-2.32672200
C	-0.61699200	0.59650200	-0.73465000
H	0.36355800	0.84597200	-0.37066100
C	-1.38100100	3.87307000	1.13388500
H	-1.41794100	4.58741000	1.96804800
H	-0.34086800	3.55881100	1.01268700
H	-1.66317200	4.41664300	0.22719100
C	-4.35854700	3.53574300	0.00795500
H	-4.84184700	4.31933500	0.60749200
H	-3.67604200	4.03215500	-0.68914300
H	-5.14021800	3.05002400	-0.58502500
C	-5.53141900	0.75879400	1.16220300
H	-6.19721900	0.99405000	2.00451100
H	-5.99443700	1.17088000	0.25949900
H	-5.50948100	-0.33155700	1.05832300

C	-3.31408900	-0.55388400	2.99974800
H	-3.96174200	-0.38151900	3.87082700
H	-3.77352300	-1.35256100	2.40617500
H	-2.35754700	-0.92549200	3.37332100
C	-0.71746700	1.34914400	2.97360800
H	0.12084100	1.87971600	2.51387900
H	-0.80928500	1.71351800	4.00643000
H	-0.44357100	0.29075500	3.01839300
C	0.69045200	-1.89645000	0.44821100
O	1.43656700	-1.42131200	-0.43673900
C	0.93651200	-2.48933900	1.67785400
C	2.32289300	-2.75992600	2.10465900
C	2.57359500	-3.59346500	3.22214700
C	3.46337700	-2.22088800	1.45952300
C	3.86735800	-3.87562100	3.65849200
H	1.74510400	-4.04488900	3.75766200
C	4.75303100	-2.50272800	1.90203900
H	3.31463400	-1.56785300	0.61198700
C	4.97340600	-3.33406300	3.00340600
H	4.00729300	-4.52711600	4.51877700
H	5.59835800	-2.06116000	1.37796500
H	5.98267500	-3.55192600	3.34348400
C	-0.15177700	-2.87274500	2.66099900
H	-0.30451300	-3.96116100	2.75296300
H	0.10282300	-2.51898700	3.66953100
H	-1.11788800	-2.43487600	2.40868400
S	2.99727700	3.05942000	-0.89222300
O	3.54157700	4.39284500	-1.11286700
O	1.59849600	2.75196900	-1.22732000
C	3.12986700	2.69048200	0.94148500
F	2.76886200	1.42303400	1.16855200
F	2.28995300	3.50472300	1.59585800
F	4.36854000	2.88961900	1.38158400
N	4.09562900	1.94226400	-1.51541300
C	3.62648200	0.76004500	-1.77755900
H	2.58768200	0.48112900	-1.57742400
C	4.47162200	-0.27937000	-2.34660200
C	3.95239900	-1.58443900	-2.44391500
C	5.77731800	-0.00213000	-2.79854400
C	4.73874600	-2.59931800	-2.98771500
H	2.95846500	-1.79175200	-2.05401300
C	6.54760400	-1.01873900	-3.34723300
H	6.15957400	1.01012400	-2.71508900
C	6.02848000	-2.31760000	-3.44220900
H	4.34667900	-3.61014900	-3.05136600
H	7.55249500	-0.80795500	-3.70212000
H	6.63687600	-3.11046500	-3.86977000

H C O N F S 0
6-31G*

Fe 0
LANL2DZ

Fe 0
LANL2DZ

TSJ-k

%nprocshared=16

%mem=1GB

freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	-3.85433500	-2.88160300	-1.03830500
C	-2.70710400	-2.39716800	-1.75519600
C	-2.93917900	-1.02136300	-2.07813400
C	-4.80108100	-1.80495300	-0.93119400
C	-4.23185400	-0.65334500	-1.56661200
Fe	-3.01761000	-1.29792800	-0.00251400
C	-4.78147000	3.92878800	2.16124900
C	-4.25043200	4.69006300	0.93854000
C	-2.90164700	4.01368000	0.66930800
N	-3.11089600	2.61768500	1.10610500
C	-4.35376900	2.47966700	1.88911200
C	-2.18075500	1.65879400	0.91396200
C	-0.91943500	1.98636200	0.36344000
C	0.09932900	1.05806500	0.25282900
N	-0.03224800	-0.24080100	0.57569400
C	-1.26454000	-0.66120800	1.07620800
C	-2.35856500	0.27299300	1.28437200
H	-5.86312400	4.01931100	2.29321600
H	-4.29875200	4.29507400	3.07456700
H	-4.91940800	4.55067200	0.08132100
H	-4.14314700	5.76419200	1.11068000
H	-2.61240200	4.04397700	-0.38559200
H	-2.09447100	4.47471000	1.25493500
H	-5.11300100	1.94311200	1.30561200
H	-4.16463900	1.92153200	2.80883700
H	-0.67300400	3.00135900	0.08433300
H	1.09457400	1.38794700	-0.04258800
C	-3.00473300	-1.83225000	2.00663300
H	-3.59517000	-2.64452700	2.40903800
C	-3.44933200	-0.49218500	1.84570400
H	-4.42715000	-0.12995700	2.11767600
C	-1.68100800	-1.95450300	1.49690600
H	-1.07652600	-2.84644100	1.48073600
C	-4.05505800	-4.28532900	-0.54343300
H	-4.49622700	-4.91829800	-1.32564000
H	-3.10933100	-4.74833600	-0.24462200
H	-4.72781700	-4.31805100	0.31946300
C	-6.16240100	-1.89105000	-0.30244600
H	-6.91068000	-2.23191800	-1.03104200
H	-6.17941100	-2.59638600	0.53449800

H	-6.49663300	-0.91996000	0.07665300
C	-4.89118500	0.68441600	-1.74693300
H	-5.37386800	0.75657600	-2.73144600
H	-5.66686900	0.85881600	-0.99395200
H	-4.16839700	1.50422500	-1.67979900
C	-2.03649100	-0.12896100	-2.88011500
H	-2.36200300	-0.09168500	-3.92886000
H	-2.03347500	0.89863800	-2.50269500
H	-1.00400800	-0.48489500	-2.87223700
C	-1.50572900	-3.21200300	-2.14173600
H	-1.31014700	-4.01141000	-1.42070500
H	-1.65544700	-3.68516700	-3.12193200
H	-0.60110200	-2.60135900	-2.20902400
C	1.16642000	-1.17710500	0.68911400
O	1.14597700	-1.85907500	1.69730000
C	2.20179300	-1.10114800	-0.33627600
C	3.14206200	-2.28919000	-0.42566400
C	4.15869700	-2.24810800	-1.40655000
C	3.07120200	-3.44812700	0.37084100
C	5.04980900	-3.30490200	-1.58277000
H	4.26910000	-1.37085000	-2.03593500
C	3.96077600	-4.50925900	0.18497900
H	2.32435700	-3.51739000	1.14810400
C	4.95606700	-4.44929800	-0.78907700
H	5.82132800	-3.22729600	-2.34465700
H	3.87043800	-5.38920500	0.81777900
H	5.64946200	-5.27520500	-0.92476900
C	1.78195500	-0.63506900	-1.73541900
H	2.57776100	-0.07746600	-2.23059800
H	1.55440700	-1.50822800	-2.36053100
H	0.90451300	0.00738100	-1.73670900
S	3.78739700	2.37264300	-1.24251400
O	4.63255500	3.49036700	-0.80366700
O	4.32232700	1.47089100	-2.28636300
C	2.32217600	3.23773600	-2.01937900
F	1.47150600	2.36560900	-2.59532600
F	2.74560600	4.08832400	-2.95686800
F	1.62371200	3.93135100	-1.09709400
N	3.03548300	1.64008100	-0.01824900
C	3.45628900	0.39106900	0.37124400
H	4.28986800	-0.04627600	-0.17774100
C	3.53595500	0.16687700	1.84554700
C	4.32043000	-0.87652100	2.36210900
C	2.87241900	1.01737700	2.74464800
C	4.42452600	-1.07348400	3.73889800
H	4.86055800	-1.52905200	1.68397600
C	2.97235900	0.81527300	4.11976000
H	2.31381700	1.86024600	2.35112200
C	3.74645500	-0.23306100	4.62328600
H	5.04325700	-1.88182800	4.11986800
H	2.45845000	1.48836200	4.80180100
H	3.83148900	-0.38469700	5.69633800

H C O N F S O

6-31G*

Fe 0
LANL2DZ

Fe 0
LANL2DZ

TS_{J-k}'

%nprocshared=16
%mem=1GB
freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1			
C	4.40300000	-2.79413800	-0.07027900
C	3.21834300	-2.85942800	0.74038000
C	3.25377000	-1.76317100	1.66215900
C	5.17781000	-1.66351600	0.36239700
C	4.46469400	-1.02280900	1.42743700
Fe	3.31069700	-1.05203200	-0.30522300
C	4.63191800	4.74286200	-0.19290300
C	4.15249200	4.90091700	1.25708500
C	2.87826700	4.04999300	1.29336800
N	3.14414200	2.97000900	0.32219800
C	4.32550200	3.27214000	-0.50769800
C	2.28428200	1.94651500	0.13366600
C	1.04973700	1.91077200	0.81969900
C	0.06838400	0.98251100	0.51973100
N	0.24363900	-0.03468000	-0.34297900
C	1.48028300	-0.13392100	-0.97966900
C	2.51693300	0.86322200	-0.79490200
H	5.69075200	4.98004100	-0.32876600
H	4.05215000	5.39440500	-0.85655200
H	4.89728200	4.49548300	1.95218000
H	3.95974500	5.93969000	1.53793500
H	2.67544900	3.63030400	2.28400400
H	1.99743400	4.62731900	0.98114600
H	5.16506200	2.62225300	-0.22633900
H	4.10062100	3.11086000	-1.56419200
H	0.76589000	2.71338000	1.48528800
H	-0.93700800	1.11029100	0.90844200
C	3.22906100	-0.69941600	-2.35090200
H	3.83950500	-1.23117300	-3.06843200
C	3.61523800	0.47601600	-1.65074800
H	4.56229400	0.97770400	-1.76305900
C	1.93771700	-1.10585100	-1.91068400
H	1.37564700	-1.95616400	-2.26260500
C	4.78896800	-3.77828700	-1.13749300

H	5.31810600	-4.63907500	-0.70583100
H	3.91198500	-4.16595500	-1.66554800
H	5.45293900	-3.32984800	-1.88322800
C	6.52040500	-1.25813200	-0.17606400
H	7.33047300	-1.76552700	0.36574900
H	6.62812000	-1.51506300	-1.23484600
H	6.68939400	-0.18070500	-0.07764200
C	4.93902000	0.15726700	2.22738700
H	5.52279400	-0.17004900	3.09906100
H	5.58332300	0.81726200	1.63717600
H	4.10347500	0.75555100	2.60441200
C	2.25197600	-1.47137200	2.74223300
H	2.57172500	-1.90866000	3.69834100
H	2.12554400	-0.39550200	2.90008500
H	1.26895000	-1.88499900	2.50560100
C	2.16752500	-3.92993900	0.66466200
H	2.04551400	-4.30772000	-0.35516100
H	2.43522500	-4.78493400	1.30086800
H	1.19153800	-3.56747600	0.99878500
C	-0.92853300	-0.80874800	-0.94043800
O	-0.89953700	-0.85972600	-2.15313600
C	-1.92051400	-1.38530700	-0.03570300
C	-2.68668000	-2.51052700	-0.68096800
C	-2.89561400	-3.72836200	-0.00523100
C	-3.26547100	-2.38135900	-1.96381100
C	-3.63748400	-4.76506500	-0.57569900
H	-2.47740200	-3.88361500	0.98266000
C	-4.00987700	-3.41551500	-2.52815400
H	-3.13031300	-1.46523200	-2.52456200
C	-4.20234500	-4.61666800	-1.84101200
H	-3.77254100	-5.69056400	-0.02089000
H	-4.44388800	-3.27675800	-3.51527600
H	-4.78376000	-5.42054100	-2.28495100
C	-1.47429700	-1.66085900	1.39611000
H	-2.32554200	-1.97365000	2.00394600
H	-0.72577900	-2.46475100	1.44482200
H	-1.04923200	-0.78630200	1.88888200
S	-2.76351600	2.30502400	-1.08642000
O	-1.48497200	3.03623600	-1.08809700
O	-3.23445200	1.66542700	-2.32726800
C	-4.03237300	3.62442200	-0.72446400
F	-5.25047400	3.08009400	-0.60535400
F	-4.05565000	4.51302700	-1.72722000
F	-3.73774200	4.27178600	0.41136600
N	-2.89242200	1.39175300	0.24617200
C	-3.41717000	0.13966200	0.10804300
H	-3.82079400	-0.13664900	-0.86513200
C	-4.20689100	-0.35490000	1.26870000
C	-5.14999400	-1.38286800	1.09960400
C	-4.06996900	0.23015300	2.53945500
C	-5.92110600	-1.82375200	2.17581600
H	-5.28797300	-1.82745200	0.11978200
C	-4.83640500	-0.21572000	3.61384800
H	-3.37597000	1.05514300	2.66038100

C	-5.76323500	-1.24751400	3.43759500
H	-6.65124500	-2.61434300	2.02392900
H	-4.72053000	0.25062600	4.58913300
H	-6.36605800	-1.59020700	4.27474300

H C O N F S O

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Intermediate K

%nprocshared=16

%mem=1GB

opt freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	-4.04744600	-2.78889200	-0.80537800
C	-2.88795400	-2.41743200	-1.56856200
C	-3.05782700	-1.06077600	-1.99636800
C	-4.94159600	-1.66396900	-0.77605700
C	-4.32686100	-0.59465600	-1.50436500
Fe	-3.12029900	-1.17152700	0.09454400
C	-4.97359700	4.07867600	2.13053100
C	-4.54810100	4.79840900	0.84309600
C	-3.19619000	4.15431400	0.51658900
N	-3.32484000	2.77406100	1.03415000
C	-4.51656400	2.63289700	1.89381800
C	-2.37553600	1.84044200	0.83460800
C	-1.15693100	2.18287300	0.19607600
C	-0.09476400	1.30742100	0.10755800
N	-0.15697500	0.02106300	0.52582200
C	-1.36060500	-0.42725800	1.08066000
C	-2.48271700	0.47079300	1.28603200
H	-6.04684400	4.14196500	2.32947600
H	-4.44484900	4.50004100	2.99307700
H	-5.26555000	4.59899000	0.03856500
H	-4.46653500	5.88200900	0.96048100
H	-2.97794500	4.13908200	-0.55542200
H	-2.36973900	4.66890200	1.02446000
H	-5.29002100	2.05049600	1.37634500
H	-4.25712900	2.11905300	2.82201600
H	-0.97060000	3.19523300	-0.13499300
H	0.90976300	1.63936800	-0.18672900
C	-3.02004400	-1.62351400	2.12039800
H	-3.56363800	-2.44062400	2.57525000
C	-3.52028400	-0.30855200	1.92311900

H	-4.50191800	0.02760900	2.21483400
C	-1.71049600	-1.71597200	1.56695700
H	-1.08052100	-2.59141600	1.56066600
C	-4.30899200	-4.14184400	-0.20733800
H	-4.79458100	-4.80478800	-0.93654100
H	-3.38210000	-4.63063800	0.10888300
H	-4.96739600	-4.08064000	0.66499100
C	-6.30096800	-1.63917900	-0.13712400
H	-7.06629600	-2.01114600	-0.83192500
H	-6.34238000	-2.26834600	0.75792800
H	-6.59464100	-0.62612000	0.15596000
C	-4.92848000	0.75215600	-1.78854600
H	-5.44206200	0.75441800	-2.75981000
H	-5.66733100	1.03602100	-1.03204200
H	-4.16611700	1.53708900	-1.82428500
C	-2.13110500	-0.27420000	-2.87821900
H	-2.44901800	-0.33872700	-3.92789200
H	-2.11059900	0.78627100	-2.60807900
H	-1.10490900	-0.64327200	-2.82465500
C	-1.73476500	-3.32256500	-1.89512100
H	-1.52006900	-4.01666400	-1.07666100
H	-1.95246800	-3.92507300	-2.78750500
H	-0.81867000	-2.76172100	-2.09743300
C	1.09331100	-0.77664300	0.78062600
O	1.14524000	-1.30025900	1.86293200
C	2.18030300	-0.88880500	-0.29598400
C	2.75101600	-2.33447300	-0.36353100
C	3.76678000	-2.58337100	-1.30719600
C	2.29472000	-3.42958700	0.38392500
C	4.30411300	-3.85595200	-1.48970800
H	4.15991300	-1.77146400	-1.91023500
C	2.82708100	-4.70919500	0.19727600
H	1.54084800	-3.29693100	1.14719800
C	3.83367400	-4.93355600	-0.73793400
H	5.09302600	-4.00070300	-2.22311900
H	2.45038700	-5.53073000	0.80154900
H	4.24924600	-5.92791600	-0.87694200
C	1.64197400	-0.56516500	-1.71011000
H	2.45137800	-0.63231500	-2.43712100
H	0.87803400	-1.29541000	-1.99752300
H	1.23445500	0.43822400	-1.79969000
S	3.63489100	2.67840500	-0.57702700
O	3.09388500	3.96571500	-0.11318300
O	5.09158600	2.45067800	-0.60773200
C	3.19961000	2.72524500	-2.39884700
F	3.62270000	1.60251200	-3.02524100
F	3.74038100	3.77459500	-3.02895500
F	1.85357700	2.79110800	-2.56964200
N	2.77243100	1.48953900	0.00639100
C	3.35066400	0.16538100	0.09575400
H	4.12658200	-0.00552200	-0.66148900
C	3.98264400	-0.11865200	1.46260900
C	5.01164200	-1.06090300	1.59883200
C	3.57688700	0.59083700	2.60043200

C	5.60217700	-1.30461100	2.83948800
H	5.36682800	-1.60097500	0.72649300
C	4.16234200	0.34674400	3.84284900
H	2.82252300	1.36291000	2.49095000
C	5.17486200	-0.60589100	3.96960900
H	6.40541100	-2.03321600	2.91871300
H	3.83508800	0.91277300	4.71179700
H	5.63818200	-0.78998600	4.93587400

H C O N F S O

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Intermediate K'

%nprocshared=16

%mem=1GB

opt freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	4.34430400	-2.72015300	0.28604800
C	3.14301100	-2.66487400	1.07301600
C	3.19135400	-1.47419900	1.86811100
C	5.14235600	-1.56854200	0.60926700
C	4.42575300	-0.79491300	1.57901300
Fe	3.30352900	-0.99037800	-0.16738500
C	4.89719100	4.70765400	-0.70075700
C	4.42832700	5.03799200	0.72317000
C	3.11422300	4.25975900	0.84369700
N	3.32644300	3.07039100	-0.00838500
C	4.52038400	3.22809700	-0.86198900
C	2.42674400	2.07061600	-0.08272300
C	1.19207500	2.16281500	0.60560400
C	0.16394500	1.26457600	0.40061100
N	0.29054100	0.15523700	-0.36265900
C	1.52657800	-0.07661300	-0.97118600
C	2.60876300	0.88434100	-0.88920900
H	5.96593000	4.87771800	-0.85693300
H	4.34846100	5.31333100	-1.43079900
H	5.15347800	4.67076000	1.45898100
H	4.28721800	6.10835600	0.89410100
H	2.89125600	3.95663400	1.87138300
H	2.26224400	4.84148200	0.46738300

H	5.32700100	2.57163300	-0.50992600
H	4.28594900	2.96649700	-1.89619000
H	0.94907900	3.04247600	1.18459500
H	-0.85152100	1.46072100	0.74069600
C	3.25659000	-0.88213700	-2.24273300
H	3.84700500	-1.52399400	-2.88260700
C	3.69307500	0.34831300	-1.68065700
H	4.66498600	0.78766900	-1.83667000
C	1.94225600	-1.17142900	-1.77604600
H	1.34483300	-2.03341800	-2.03107300
C	4.72648700	-3.82538200	-0.65677600
H	5.24261500	-4.63583300	-0.12402400
H	3.84847600	-4.26196700	-1.14322900
H	5.40032300	-3.47221200	-1.44378400
C	6.50502000	-1.26057600	0.05698900
H	7.28910500	-1.74731900	0.65292800
H	6.61476700	-1.61298200	-0.97355100
H	6.71365700	-0.18575900	0.06261300
C	4.89500300	0.46747100	2.24320700
H	5.36911900	0.25118900	3.21049500
H	5.63206300	0.99858300	1.63271000
H	4.06253900	1.15224200	2.43419800
C	2.18954600	-1.04101900	2.89951700
H	2.51133900	-1.34861100	3.90414000
H	2.06149900	0.04611000	2.91616400
H	1.20672300	-1.48345900	2.72323900
C	2.06753700	-3.71267500	1.09924200
H	1.95074400	-4.19981500	0.12658600
H	2.30538900	-4.49633100	1.83183300
H	1.09522500	-3.29455800	1.37313700
C	-0.91827500	-0.54285600	-0.94386600
O	-0.90202400	-0.65632800	-2.13893100
C	-2.00622900	-1.16358300	-0.02862800
C	-2.29365600	-2.58319100	-0.57108100
C	-2.07652800	-3.72908000	0.20845100
C	-2.79416200	-2.76949700	-1.87384400
C	-2.35057600	-5.00857800	-0.28410900
H	-1.70125900	-3.64151200	1.22131500
C	-3.06768100	-4.04447100	-2.36667100
H	-2.96326200	-1.91340200	-2.51483200
C	-2.84815100	-5.17379200	-1.57447000
H	-2.17699400	-5.87337000	0.35137400
H	-3.45702900	-4.15250600	-3.37564600
H	-3.06570500	-6.16695500	-1.95851700
C	-1.58468700	-1.19271200	1.44802200
H	-2.33743100	-1.72240200	2.03523500
H	-0.62140800	-1.69230400	1.58739900
H	-1.51793900	-0.18336700	1.85292300
S	-3.01787800	2.33675800	-0.94337700
O	-1.93318300	3.33520500	-0.84486900
O	-3.50559400	1.93509800	-2.27846300
C	-4.47412700	3.25177400	-0.21523100
F	-5.56767500	2.47019700	-0.21147600
F	-4.75079600	4.36148100	-0.91655400

F	-4.21996600	3.61497700	1.05758200
N	-2.70693300	1.14894600	0.05639700
C	-3.25373200	-0.17267600	-0.20154000
H	-3.59021400	-0.26991900	-1.24043600
C	-4.41674900	-0.54691000	0.72081500
C	-5.28402800	-1.60142100	0.39759600
C	-4.65089000	0.16822200	1.90316100
C	-6.34176500	-1.94392500	1.24137700
H	-5.13969200	-2.15336100	-0.52610400
C	-5.70737900	-0.17349700	2.74900500
H	-4.01497800	1.01761700	2.12819900
C	-6.55439100	-1.23493200	2.42527100
H	-7.00594100	-2.75994000	0.96698400
H	-5.87532500	0.39984600	3.65765800
H	-7.38114600	-1.49756400	3.08069400

H C O N F S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

TS_{K-L}

%nprocshared=16

%mem=1GB

opt=(ts,calcfc,noeigen) freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	3.82661900	-3.02464400	0.22880600
C	2.77801700	-2.77193100	1.17862100
C	3.07120700	-1.53484600	1.83825300
C	4.77543100	-1.94759800	0.31445700
C	4.30346000	-1.02407900	1.30183400
Fe	2.90419800	-1.22915900	-0.22821100
C	5.32121700	3.94622100	-1.74136700
C	5.20014900	4.47699800	-0.30584800
C	3.81314400	3.98825800	0.12654200
N	3.63899200	2.72160200	-0.60726900
C	4.65507200	2.56501200	-1.66357900
C	2.56710900	1.91940100	-0.41106500
C	1.52261500	2.31241000	0.45249300
C	0.33042300	1.60152800	0.52431600
N	0.10647700	0.43896800	-0.09293700
C	1.15428900	-0.08844500	-0.83643500
C	2.38178200	0.65079400	-1.07600000
H	6.35372000	3.88543500	-2.09665000
H	4.76442800	4.59040300	-2.43157600
H	5.97229100	4.03062500	0.33196300

H	5.29328400	5.56414100	-0.23673400
H	3.74130400	3.81772600	1.20587400
H	3.02705000	4.70240000	-0.15648700
H	5.38109000	1.78928400	-1.38474300
H	4.18577600	2.27436400	-2.60644900
H	1.55913600	3.26023800	0.97104600
H	-0.50523900	2.01454000	1.06582800
C	2.45502000	-1.34291200	-2.25279800
H	2.79716800	-2.15084100	-2.88595200
C	3.18822800	-0.15998200	-1.95990600
H	4.16705900	0.07264900	-2.34733200
C	1.23004300	-1.32940100	-1.52808000
H	0.46075800	-2.08497100	-1.54786300
C	3.94851700	-4.24137800	-0.64410200
H	4.47168700	-5.05177900	-0.11761300
H	2.96801600	-4.62635300	-0.94151400
H	4.51305500	-4.03025600	-1.55802000
C	6.06124100	-1.84215800	-0.45494300
H	6.87859800	-2.35182500	0.07383300
H	5.98165500	-2.29917200	-1.44658300
H	6.36612600	-0.79961900	-0.59402300
C	5.00380300	0.21756600	1.77580500
H	5.65450700	-0.00175600	2.63403900
H	5.63415000	0.65567900	0.99504400
H	4.29003900	0.98343300	2.09646900
C	2.30093300	-0.90253700	2.96254600
H	2.86708100	-0.96359300	3.90203800
H	2.09119400	0.15621400	2.77438300
H	1.34510300	-1.40466200	3.12766500
C	1.61968000	-3.68485500	1.46298300
H	1.32142600	-4.25083900	0.57576200
H	1.87899700	-4.41219400	2.24511400
H	0.73650400	-3.13754400	1.80149900
C	-1.40367400	-0.10223400	-0.48034000
O	-1.44618800	-0.38543500	-1.66220800
C	-2.17797500	-0.88866500	0.66293900
C	-2.41476700	-2.37104300	0.36167500
C	-2.30617200	-3.34379600	1.37213200
C	-2.76559200	-2.82205000	-0.92587600
C	-2.53255000	-4.69827700	1.11632500
H	-2.04541800	-3.05855600	2.38459000
C	-2.98686100	-4.17506900	-1.18349000
H	-2.85116200	-2.10947800	-1.73236600
C	-2.87309500	-5.12344300	-0.16625800
H	-2.44239500	-5.41696700	1.92717500
H	-3.25679200	-4.48472800	-2.18997400
H	-3.05126600	-6.17633100	-0.36964900
C	-1.53898800	-0.67129300	2.04322500
H	-2.18471200	-1.07040600	2.83117300
H	-0.56206600	-1.15451200	2.12049000
H	-1.41526500	0.39398600	2.24320900
S	-2.94293900	2.69738500	-0.32777000
O	-1.76316400	3.33354000	-0.92759200
O	-4.27016500	2.87053000	-0.92298500

C	-3.12597500	3.52643700	1.34441000
F	-4.09551700	2.92951600	2.05723100
F	-3.42540400	4.82031000	1.20753700
F	-1.97864400	3.43557800	2.05627200
N	-2.53379600	1.19125600	0.07483600
C	-3.40965100	0.11790300	0.58130000
H	-3.76292200	0.33575600	1.59659200
C	-4.61569900	-0.28678000	-0.24550400
C	-5.70087500	-0.87511700	0.41690200
C	-4.68772600	-0.11777900	-1.63419800
C	-6.82832500	-1.30060900	-0.28643800
H	-5.66443200	-0.99925400	1.49758400
C	-5.81570000	-0.53817000	-2.33865400
H	-3.85974200	0.34182300	-2.16068300
C	-6.88858700	-1.13238500	-1.67040400
H	-7.65980400	-1.75373500	0.24748400
H	-5.85834800	-0.39269400	-3.41502100
H	-7.76795800	-1.45348100	-2.22299200

H C O N F S O

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

TS_k'-L'

%nprocshared=16

%mem=1GB

opt=(ts,calcfc,noeigen) freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	4.07001600	-2.78055000	0.53905900
C	2.84589600	-2.73378400	1.28966900
C	2.83657700	-1.51543500	2.04316300
C	4.82876900	-1.59936300	0.84784700
C	4.06182800	-0.81408600	1.76699900
Fe	3.00192900	-1.09401800	-0.00547000
C	5.18162800	4.31218200	-1.11658100
C	4.81164200	4.82680500	0.28172000
C	3.43290300	4.20193700	0.52510600
N	3.48594100	2.92585900	-0.21078900
C	4.64924300	2.87237400	-1.11449900
C	2.46363900	2.03817700	-0.18662300
C	1.26893700	2.32970100	0.50548100
C	0.13406400	1.53597100	0.36683500
N	0.10420000	0.38073200	-0.30090500

C	1.29407300	-0.05067500	-0.86452300
C	2.48776700	0.77483600	-0.88704700
H	6.25425200	4.35429400	-1.32556500
H	4.66500500	4.89908600	-1.88473000
H	5.52877700	4.46031900	1.02583500
H	4.78574700	5.91778600	0.34849300
H	3.22898600	4.02457500	1.58642800
H	2.62747900	4.83518800	0.12685500
H	5.40269100	2.17150300	-0.72949100
H	4.34608300	2.53958100	-2.10969000
H	1.15516100	3.26128600	1.04254400
H	-0.81920600	1.86639400	0.75689500
C	2.88636500	-1.17216500	-2.07943100
H	3.38083400	-1.93409600	-2.66712800
C	3.48040600	0.04505500	-1.64278200
H	4.49251700	0.34981500	-1.85523400
C	1.56247200	-1.25947100	-1.56462800
H	0.85669100	-2.05928800	-1.73159200
C	4.51270000	-3.91229400	-0.34425900
H	5.06933500	-4.66579000	0.23042800
H	3.65987400	-4.41993400	-0.80598100
H	5.16946700	-3.56745100	-1.14948700
C	6.20736800	-1.28255600	0.34159300
H	6.97464300	-1.71181100	1.00073200
H	6.37734700	-1.68982900	-0.66026100
H	6.38835200	-0.20338400	0.29614100
C	4.47778000	0.47977800	2.40616700
H	4.93504500	0.30379700	3.38983800
H	5.21151700	1.01788200	1.79793600
H	3.62048300	1.14365600	2.55806600
C	1.80169800	-1.06864500	3.03645700
H	2.14195500	-1.26210200	4.06336500
H	1.59705000	0.00453300	2.95768000
H	0.85314300	-1.59298100	2.90283700
C	1.81722700	-3.82755300	1.32791700
H	1.63946100	-4.25680400	0.33692000
H	2.14535800	-4.64403700	1.98618400
H	0.85694200	-3.47015800	1.70726800
C	-1.28225000	-0.19076600	-1.01944700
O	-1.13903300	-0.22911100	-2.22394200
C	-2.11630600	-1.24432600	-0.18960600
C	-2.30297900	-2.57495000	-0.91734600
C	-2.02919400	-3.80532800	-0.29894700
C	-2.78504400	-2.60563400	-2.24041700
C	-2.22867200	-5.01725600	-0.96628000
H	-1.66507200	-3.83590400	0.72175200
C	-2.98313200	-3.81332300	-2.90759300
H	-2.97983700	-1.67576000	-2.76046400
C	-2.70782400	-5.02771900	-2.27461100
H	-2.01346300	-5.95174600	-0.45386400
H	-3.35380300	-3.80259200	-3.92930400
H	-2.86714200	-5.96853400	-2.79518300
C	-1.58052700	-1.40535400	1.23308200
H	-2.25078700	-2.02356400	1.83705800

H	-0.59074800	-1.86810600	1.21963700
H	-1.49331700	-0.43689000	1.72833700
S	-3.06542200	2.18176200	-1.25329000
O	-1.87967000	2.90226200	-1.72863100
O	-4.17315200	1.84555600	-2.15580900
C	-3.81465300	3.37090800	-0.01273500
F	-4.96971300	2.90614600	0.47425900
F	-4.03733100	4.55042200	-0.60162000
F	-2.96536100	3.56579200	1.01803500
N	-2.55807700	0.93567100	-0.32119800
C	-3.37535700	-0.29441000	-0.21444100
H	-3.93109200	-0.47046600	-1.14058800
C	-4.33391600	-0.40285200	0.95162300
C	-5.34093800	-1.37860900	0.90364700
C	-4.23254300	0.40012200	2.09410700
C	-6.21741900	-1.55516000	1.97417400
H	-5.43707400	-2.00174200	0.01769800
C	-5.11314400	0.22934200	3.16398700
H	-3.47484000	1.17532000	2.13129900
C	-6.10552100	-0.75079400	3.11069200
H	-6.99283100	-2.31480700	1.91695200
H	-5.02576600	0.86853700	4.03909700
H	-6.79208500	-0.88103100	3.94321200

H C O N F S O

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Product L + catalyst

%nprocshared=16

%mem=800MB

opt freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	4.90182200	-2.83606400	-0.68275500
C	3.95554300	-3.23812500	0.32183100
C	3.95589300	-2.24376000	1.35372200
C	5.49599200	-1.59560300	-0.26331100
C	4.90931200	-1.22854200	0.99113600
Fe	3.43786900	-1.39084300	-0.47183500
C	4.00071100	4.55263600	-0.93480000
C	4.07856500	4.74725100	0.58649800
C	3.03766500	3.75284800	1.11268300
N	3.07938600	2.65228900	0.14197800

C	3.78251800	3.03903100	-1.08972200
C	2.32724900	1.52326900	0.30988600
C	1.47445800	1.37496000	1.40996300
C	0.62575700	0.25177700	1.53190100
N	0.54968000	-0.76213600	0.68874400
C	1.41006600	-0.68127300	-0.37489600
C	2.32342700	0.42440100	-0.63125700
H	4.89363000	4.89819500	-1.46401800
H	3.13935100	5.09710700	-1.33960700
H	5.07576500	4.47771700	0.95484200
H	3.86924900	5.77306700	0.90291800
H	3.27263700	3.38957500	2.11956800
H	2.03137200	4.19838300	1.14518300
H	4.74086300	2.50706200	-1.17576700
H	3.18398900	2.79955200	-1.97313500
H	1.38614900	2.15700900	2.15285200
H	-0.06152000	0.22488400	2.37610200
C	2.55438800	-1.14065500	-2.33176300
H	2.90609700	-1.64086600	-3.22503300
C	3.04733000	0.10437000	-1.84042700
H	3.81067400	0.69511200	-2.32276500
C	1.59124900	-1.65001100	-1.41503400
H	1.06454600	-2.59236300	-1.48408300
C	5.26216600	-3.61331200	-1.91732800
H	6.09053000	-4.30860400	-1.72032500
H	4.41842300	-4.20880600	-2.28120500
H	5.57782300	-2.95490600	-2.73351900
C	6.58565900	-0.85525400	-0.98564800
H	7.57822300	-1.22370700	-0.69004600
H	6.50547300	-0.97388600	-2.07126000
H	6.56071800	0.21754300	-0.76762800
C	5.26052800	-0.02813600	1.82340200
H	6.03675200	-0.27311000	2.56206100
H	5.64125800	0.79419300	1.20912100
H	4.39076700	0.34668000	2.37273300
C	3.13906900	-2.26755300	2.61332800
H	3.70450900	-2.71501000	3.44295900
H	2.84408900	-1.25896400	2.91922800
H	2.21990200	-2.84622900	2.48570900
C	3.13541600	-4.49680100	0.30872900
H	2.89474200	-4.81165300	-0.71190900
H	3.67393600	-5.32578800	0.78922100
H	2.19012400	-4.36427300	0.84390400
C	-3.67646600	-0.40056900	-1.28588400
S	-2.81020700	2.64152100	0.77674800
O	-3.84195800	3.66552100	0.78488300
O	-2.11093100	2.19632000	1.97490700
N	-3.37808100	1.26758900	-0.01112900
C	-2.95924500	-0.16832100	0.12525600
C	-4.86701400	-1.33947800	-1.35342200
C	-4.70978400	-2.69113400	-1.01043300
C	-6.11597800	-0.90179800	-1.81380300
C	-5.77759400	-3.58062800	-1.11539400
H	-3.75107800	-3.04771000	-0.64457500

C	-7.18524100	-1.79502600	-1.91965300
H	-6.25195400	0.13546500	-2.10281500
C	-7.02103000	-3.13505700	-1.57059300
H	-5.63863900	-4.62209400	-0.83782000
H	-8.14693700	-1.43782400	-2.27830600
H	-7.85366300	-3.82857300	-1.65237200
H	-1.87609000	-0.27494600	0.03392200
C	-3.43651000	-0.86696500	1.36890400
C	-2.57435900	-1.78039600	1.99135000
C	-4.71091900	-0.64822100	1.90945400
C	-2.98864900	-2.47492300	3.13007200
H	-1.57359500	-1.92600800	1.58906200
C	-5.11816600	-1.33698900	3.05060600
H	-5.38327900	0.06528000	1.44205800
C	-4.26008300	-2.25554900	3.66158100
H	-2.31110600	-3.17786600	3.60776600
H	-6.10682700	-1.15629200	3.46379300
H	-4.58007700	-2.79058000	4.55188200
C	-3.99377700	1.10768200	-1.27330500
O	-4.48143800	1.90404200	-2.02958300
C	-2.65791700	-0.70438600	-2.40306900
H	-2.28982800	-1.73092200	-2.30964500
H	-3.13640300	-0.59502400	-3.38113600
H	-1.79979800	-0.02499300	-2.35511400
C	-1.48742500	3.23402000	-0.42331100
F	-0.77532300	2.18855200	-0.86340200
F	-0.67808200	4.08231600	0.21572300
F	-2.05016500	3.84626600	-1.45996900

H C O N F S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ

Product L' + catalyst

%nprocshared=16

%mem=800MB

opt freq=noraman b3lyp/gen pseudo=read

Title Card Required

0 1

C	4.23384300	-2.77213600	-0.15311800
C	3.22804000	-2.87073500	0.86869300
C	3.37896400	-1.75033100	1.74904600
C	5.01559200	-1.59329800	0.10537500

C	4.48643400	-0.96110000	1.27756800
Fe	3.01925500	-1.09727100	-0.19056700
C	4.47657600	4.60272800	-1.17958000
C	4.54488400	4.90681800	0.32398400
C	3.33201300	4.15187700	0.88013900
N	3.20945200	2.98534500	-0.00115300
C	4.01244200	3.13860500	-1.22276800
C	2.28147300	2.00647900	0.22622500
C	1.35669500	2.10659700	1.27119000
C	0.36156200	1.12132500	1.46677100
N	0.20011400	0.02560300	0.74893000
C	1.10394600	-0.12357600	-0.27094600
C	2.16542700	0.81987900	-0.59266900
H	5.42869200	4.75067400	-1.69771800
H	3.72932400	5.24576600	-1.65958900
H	5.46947300	4.50210500	0.75310900
H	4.50844900	5.97599600	0.55189200
H	3.46986700	3.83547500	1.92059900
H	2.42187100	4.77071400	0.83960300
H	4.87211000	2.45279700	-1.21654600
H	3.41467000	2.92190000	-2.11270500
H	1.34305700	2.97472800	1.91837100
H	-0.36045900	1.27878900	2.26703100
C	2.24484600	-0.93633800	-2.10911500
H	2.55608600	-1.57070900	-2.92915800
C	2.88478600	0.27854500	-1.72282600
H	3.73892600	0.70865200	-2.22231600
C	1.18894400	-1.21427900	-1.19578300
H	0.53459400	-2.07523600	-1.20006300
C	4.47591900	-3.76496400	-1.25472400
H	5.17944900	-4.54728700	-0.93607800
H	3.55133300	-4.26495200	-1.56150900
H	4.90187600	-3.28748100	-2.14336400
C	6.21034600	-1.14101700	-0.68536200
H	7.13596100	-1.59329900	-0.30187200
H	6.12515300	-1.42048700	-1.74066300
H	6.33766400	-0.05421100	-0.64171600
C	5.02495300	0.27410900	1.94190800
H	5.75067700	0.01706500	2.72646500
H	5.53426800	0.92906500	1.22763700
H	4.22668700	0.85783100	2.41132500
C	2.54771300	-1.46867800	2.96716300
H	2.94950800	-1.98409700	3.85104300
H	2.51636800	-0.39868600	3.19400700
H	1.51338000	-1.79657400	2.82733100
C	2.21724500	-3.97257100	1.01314700
H	1.96240600	-4.41525800	0.04486900
H	2.59915000	-4.78033500	1.65360200
H	1.28899400	-3.60640000	1.46290400
C	-4.11267300	-1.32521600	-0.31450600
S	-3.50592100	2.41738100	-0.46406700
O	-4.68525700	3.12646200	-0.93490300
O	-2.75563600	2.80806600	0.72179100
N	-3.87260800	0.78008300	-0.31003700

C	-3.25855600	-0.28440200	0.54705400
H	-2.18750700	-0.37997100	0.34738800
C	-3.49704100	-0.16819000	2.02988500
C	-2.56960300	-0.76270000	2.89744800
C	-4.61312300	0.48251500	2.57209300
C	-2.76919400	-0.73101200	4.27876300
H	-1.67486900	-1.22054400	2.48288000
C	-4.80744000	0.52085900	3.95286400
H	-5.32373300	0.97588700	1.91509200
C	-3.89080100	-0.09214100	4.81020800
H	-2.04050100	-1.19401500	4.93895900
H	-5.67412100	1.03536000	4.35903500
H	-4.04375400	-0.06036900	5.88560600
C	-4.56100200	-0.11567800	-1.15989600
O	-5.21686400	0.06256800	-2.15043500
C	-2.28955900	2.39702200	-1.89012200
F	-1.27709500	1.57887500	-1.59926900
F	-1.82749300	3.63404900	-2.07412000
F	-2.89800800	1.97438700	-2.99660700
C	-3.28712000	-2.36196500	-1.06307400
C	-3.46192400	-2.58839600	-2.43477700
C	-2.37569100	-3.16050700	-0.35622200
C	-2.73231000	-3.58624700	-3.08565000
H	-4.16909500	-1.98364600	-2.99318500
C	-1.65140200	-4.15991500	-1.00647400
H	-2.23263900	-3.00165800	0.70939900
C	-1.82603700	-4.37475900	-2.37622000
H	-2.87673900	-3.74565600	-4.15088800
H	-0.95241900	-4.77133000	-0.44164300
H	-1.26277500	-5.15345500	-2.88355600
C	-5.29717600	-1.99027300	0.40492000
H	-4.93524500	-2.72416900	1.13196500
H	-5.91912000	-1.26283400	0.93360600
H	-5.91815100	-2.51057400	-0.33088400

H C O N F S 0

6-31G*

Fe 0

LANL2DZ

Fe 0

LANL2DZ