

Supporting Information

Mechanistic Insights into Cu-Catalyzed Enantioselective Friedel-Crafts Reaction between Indoles and 2-Aryl-N-sulfonylaziridines

Ping Wang, Yang Zhao, Biplav Chapagain, Yonggang Yang, Wei Liu,* and Yong Wang*

College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou 215123, PR China

E-mail: yowang@suda.edu.cn; weiliu@suda.edu.cn

Contents:

Figure S1. Optimized geometries of the structures in the C–C bond formation. Key bond lengths are given in Å.....	S3
Figure S2. Optimized geometries of the structures in the oxidative addition, reductive elimination and catalyst release step. Key bond lengths are given in Å.....	S4
Figure S3. The energy decomposition analysis (EDA) for the four transitions states.	S5
Cartesian coordinates all structures.....	S6-S32
Total: 32 pages	

Complete Gaussian 09 reference

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.;

Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö .; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision D.01*; Gaussian, Inc.: Wallingford, CT, 2013.

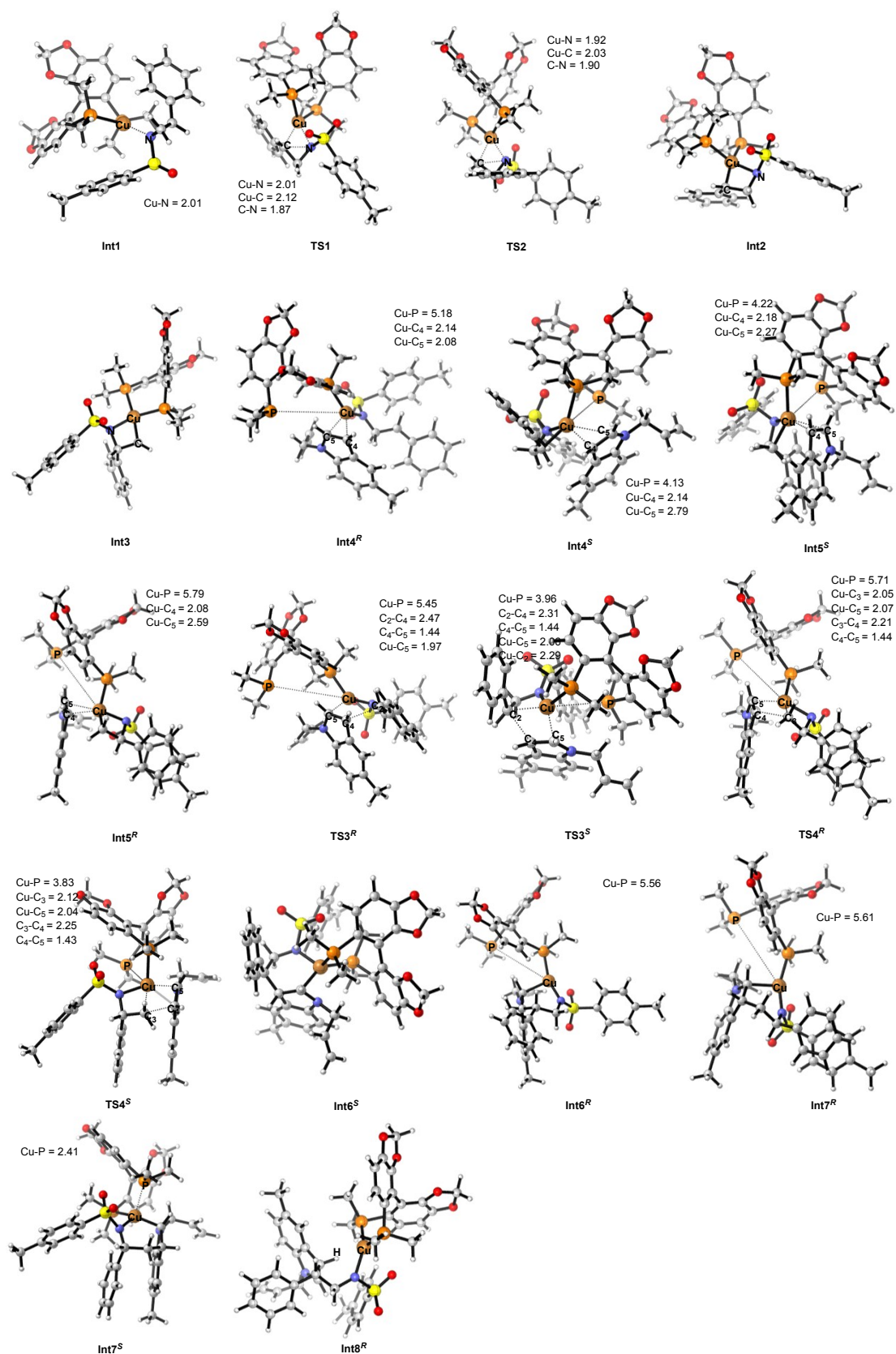


Figure S1. Optimized geometries of the structures in the C-C bond formation. Key bond lengths are given in Å.

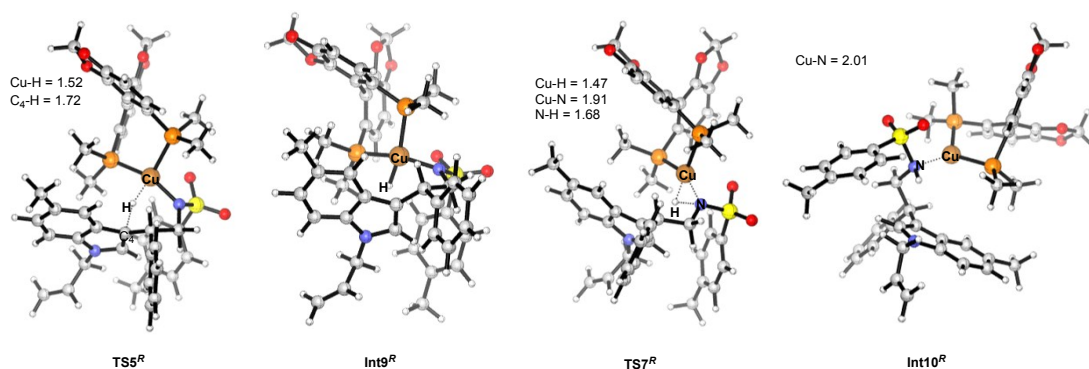
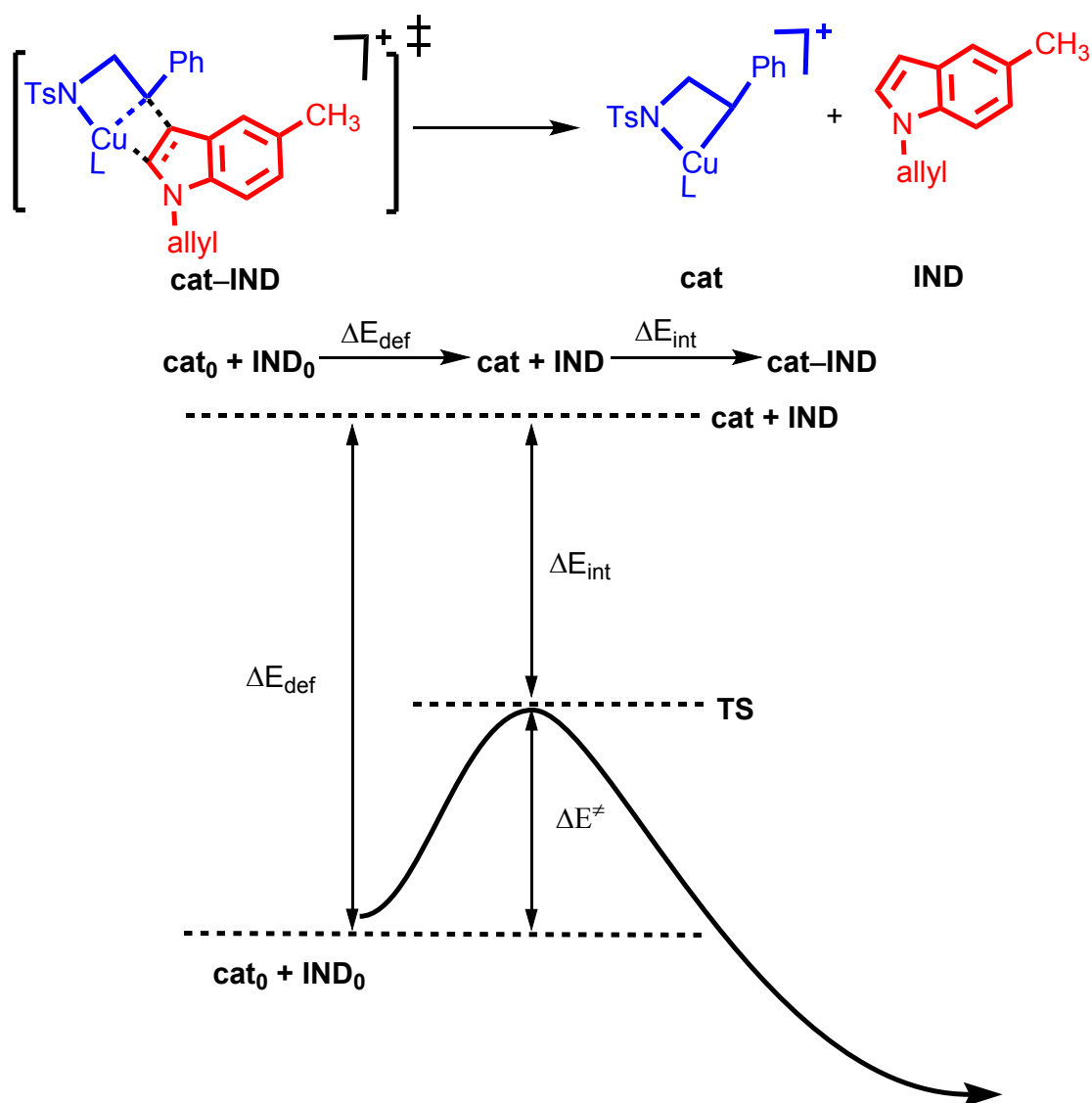


Figure S2. Optimized geometries of the structures in the oxidative addition, reductive elimination and catalyst release step. Key bond lengths are given in Å.



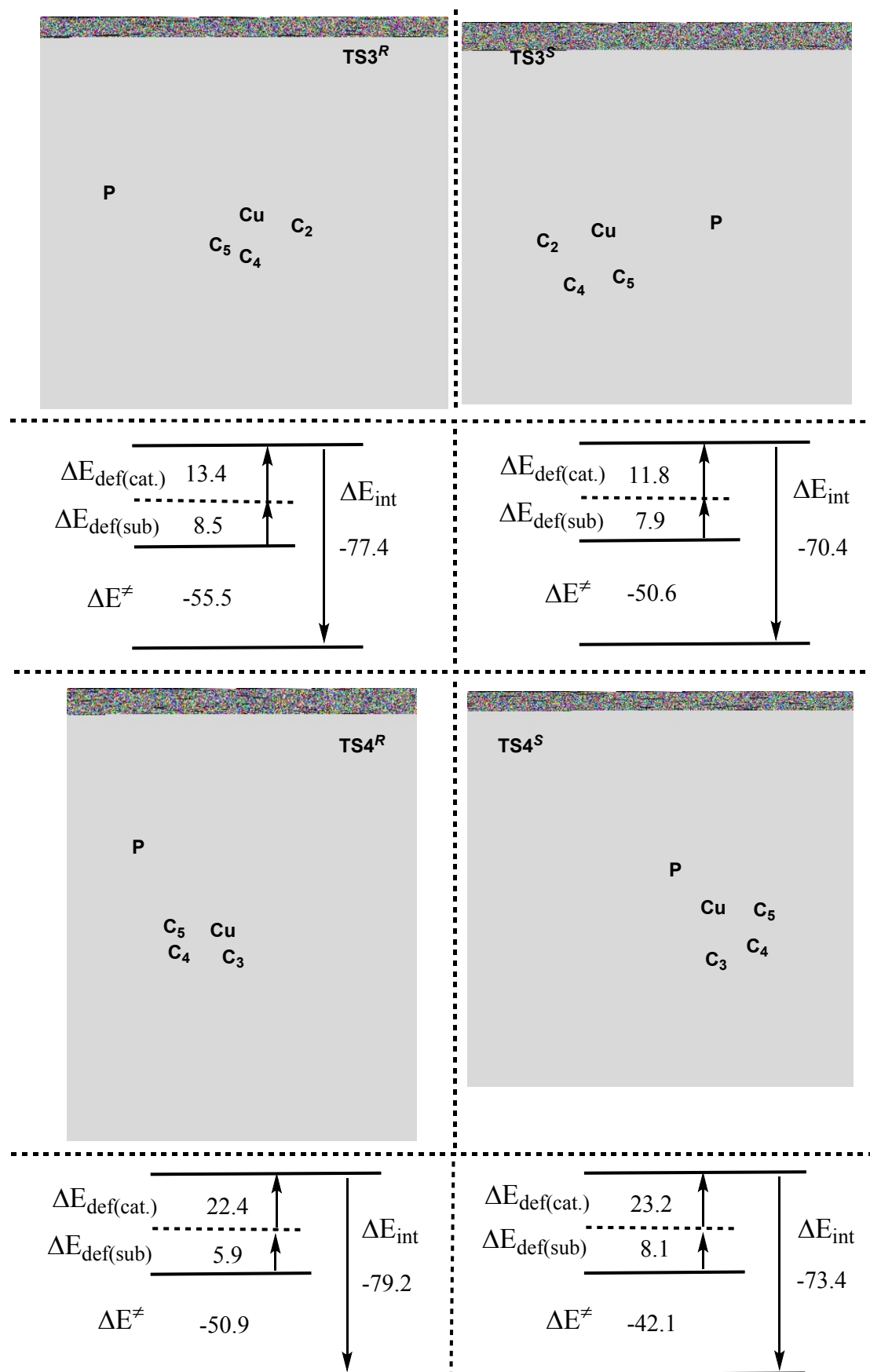


Figure S3. The energy decomposition analysis (EDA) for the four

transitions states.

Cartesian coordinates all structures.

Int1

$\Delta E = -4504.440633$ au

$\Delta G = -4504.516209$ au

C	-3.02622900	-3.17132400	-0.73507500	C	0.41678500	2.33839100	-2.52479500
C	-3.12936700	-1.78392800	-0.77379600	H	0.64549900	3.21116300	-1.90820900
C	-1.36657200	-1.57790700	0.80795500	H	1.34690900	2.01594900	-3.00221800
C	-1.28160600	-2.96868400	0.84390500	H	-0.31223600	2.60968200	-3.29442400
C	-2.10715700	-3.79853500	0.06969500	C	-0.48398400	-0.36713000	-2.70396300
H	-0.55725100	-3.44771500	1.49188900	H	-1.32968500	-0.11377500	-3.34963100
H	-2.03301800	-4.87896300	0.11415700	H	0.41509300	-0.48406100	-3.31760200
O	-3.92541700	-3.71912000	-1.58919100	H	-0.69123500	-1.31256600	-2.19770600
O	-4.09762600	-1.42650800	-1.65905800	C	3.63323100	2.11948300	0.26464700
C	-4.74371800	-2.64025100	-2.03719800	C	3.93076100	1.15519500	1.35108600
H	-5.72362300	-2.70080100	-1.54980500	H	4.45893400	2.29941900	-0.42070400
H	-4.83425700	-2.68085600	-3.12347400	H	3.40622100	1.21218100	2.29961600
C	-4.07853800	2.36141500	0.42041300	H	4.93812600	0.74889900	1.37688000
C	-3.72648500	1.01562400	0.45307600	N	3.08593800	0.73170100	0.22128900
C	-1.75830300	1.46971700	-0.80125600	C	2.61380800	3.20017600	0.34820100
C	-2.12436800	2.81463800	-0.82704900	C	1.47299200	3.05680100	1.14411500
C	-3.29160000	3.29262800	-0.21154600	C	2.76353900	4.34933800	-0.42442600
H	-1.49593500	3.53389600	-1.33870400	C	0.48585000	4.03339100	1.14707500
H	-3.56311400	4.34122600	-0.24173500	H	1.36245000	2.19162000	1.79692900
O	-5.23601800	2.54539800	1.10595700	C	1.78304200	5.33952000	-0.40811500
O	-4.65340900	0.32150600	1.16788600	H	3.64415700	4.46996600	-1.04905800
C	-5.71919900	1.23950900	1.40722300	C	0.63872900	5.17858800	0.36723900
H	-6.56170900	0.99976900	0.74778400	H	-0.40076000	3.90406200	1.75949700
H	-6.00785900	1.19203700	2.45809400	H	1.91263400	6.23361500	-1.00923100
C	-2.32176500	-0.94452200	-0.03645000	H	-0.12784100	5.94670100	0.37346700
C	-2.57438200	0.52295200	-0.12220200	S	3.80957100	-0.30132300	-0.97542600
Cu	1.09434500	0.44905400	0.27569800	C	3.24678600	-1.87536400	-0.40297300
P	-0.16643800	-0.56894100	1.74805100	C	3.91552400	-2.50303000	0.64568400
C	-1.16210500	0.52028100	2.83893300	C	2.13014200	-2.45113600	-1.00260500
H	-1.57674400	1.35084800	2.26337300	C	3.43042800	-3.71723100	1.11337900
H	-1.98161200	-0.02424600	3.31689200	H	4.80739800	-2.05947900	1.07579000
H	-0.50277900	0.92842000	3.61210400	C	1.66507000	-3.66808600	-0.52383400
C	0.59637500	-1.73203300	2.93734600	H	1.64582300	-1.95910800	-1.83816800
H	1.22258800	-1.14398500	3.61578200	C	2.30075400	-4.31470100	0.54041200
H	-0.14107600	-2.28287700	3.52956300	H	3.94355200	-4.21590100	1.93064400
H	1.24937900	-2.43445900	2.41242200	H	0.79329800	-4.12094500	-0.98582200
P	-0.14329500	0.95161500	-1.48000500	C	1.79751100	-5.64223600	1.04089200

H 0.72756900 -5.76308500 0.84746100
H 2.31617700 -6.46342100 0.53311800
H 1.97080300 -5.75951100 2.11428700
O 3.14042000 0.03830700 -2.21753600
O 5.25126500 -0.19913600 -0.83772300

TS1

$\Delta E = -4504.408835$ au

$\Delta G = -4504.485460$ au

C -2.45566100 -3.84678600 0.65734100
C -2.93350700 -2.66110800 0.10945500
C -1.33829700 -1.41178000 1.35044300
C -0.86444300 -2.60804900 1.88605800
C -1.40861700 -3.85525800 1.54561600
H -0.04078200 -2.59765400 2.58937500
H -1.02119500 -4.77742100 1.96157900
O -3.14258900 -4.89677700 0.14067600
O -3.92600800 -2.93890800 -0.77925700
C -4.19780800 -4.33150900 -0.63160700
H -5.14933900 -4.46385800 -0.10351400
H -4.22007500 -4.80256300 -1.61546300
C -4.87997600 1.22648200 -0.64839700
C -4.22675600 0.20205100 0.03069900
C -2.35586800 0.39227800 -1.42383200
C -3.02575700 1.41011700 -2.10148800
C -4.30616800 1.85072700 -1.72870800
H -2.56415000 1.88026000 -2.96330300
H -4.82136500 2.63356500 -2.27309600
O -6.08563000 1.45982300 -0.06827100
O -5.00742100 -0.23174400 1.05667300
C -6.26897200 0.40856100 0.87701600
H -6.99296400 -0.31490300 0.48374400
H -6.60089100 0.82936600 1.82705700
C -2.39853700 -1.42521300 0.40321200
C -2.96721000 -0.24385700 -0.30734500
Cu 0.50727900 1.01569500 -0.04184000
P -0.53611900 0.17044000 1.77250200
C -1.83557900 1.14865800 2.61555700
H -2.57176700 1.49173300 1.88542700
H -2.34042900 0.56007300 3.38670100
H -1.37280900 2.02812900 3.07271400
C 0.64539100 -0.21332400 3.11150800
H 1.07103200 0.73450600 3.45455200
H 0.17992600 -0.72238800 3.96061400
H 1.46075300 -0.82037700 2.70950400

P -0.60122500 0.04849400 -1.80248500
C -0.31680100 0.69774200 -3.49202900
H -0.37495100 1.78879100 -3.54044300
H 0.70208000 0.40471400 -3.76366600
H -1.01724300 0.27722300 -4.21987500
C -0.40174200 -1.75079700 -2.06890600
H -1.22540800 -2.16060400 -2.66013000
H 0.54460600 -1.89021500 -2.59889100
H -0.32260700 -2.27575700 -1.11719800
C 1.96288800 2.38202300 -0.74550800
C 3.28764800 2.06801700 -0.19357400
H 1.85420100 2.21510500 -1.81333300
H 3.65587500 2.62392700 0.66720900
H 4.06944000 1.93533800 -0.94271900
N 2.54890700 0.86388200 0.18367800
C 0.93477900 3.14764300 -0.04026600
C 1.13235000 3.70161600 1.24427100
C -0.33530000 3.27393800 -0.64106500
C 0.09865800 4.35772900 1.88586500
H 2.09604100 3.61079900 1.73322200
C -1.37507900 3.92662000 0.02091300
H -0.48596000 2.93620800 -1.66053400
C -1.15962000 4.46487900 1.28005200
H 0.26565100 4.79366000 2.86543700
H -2.34424200 4.00854900 -0.45913500
H -1.96497000 4.97741600 1.79635600
S 2.93528300 -0.52426700 -0.70921500
C 4.63991600 -0.77088800 -0.31386600
C 5.60255500 -0.61363300 -1.30496900
C 4.98833600 -1.12473600 0.98999700
C 6.93947300 -0.81504700 -0.97871100
H 5.30449800 -0.35467900 -2.31542500
C 6.32637000 -1.31602900 1.29447100
H 4.22190600 -1.25497700 1.74681800
C 7.32059300 -1.16728900 0.31771100
H 7.69729800 -0.70203400 -1.74830500
H 6.60895100 -1.59305400 2.30626300
C 8.76503700 -1.41090300 0.66519000
H 9.03651600 -0.90810300 1.59858600
H 8.94891500 -2.48194300 0.80551100
H 9.43506000 -1.05669300 -0.12207700
O 2.12421500 -1.57169200 -0.10539800
O 2.82078500 -0.25913400 -2.14434400

TS2

$\Delta E = -4504.388955$ au

$\Delta G = -4504.468250$ au

C -4.84377200 2.30419400 -0.40298500
C -4.51363900 0.97405400 -0.15930500
C -2.29818600 1.36068300 -0.93004200
C -2.64126800 2.69113500 -1.16648000
C -3.92479900 3.19436000 -0.90250300
H -1.90742700 3.37578400 -1.57640800
H -4.17928400 4.23081200 -1.08885600
O -6.13328600 2.52499900 -0.04456300
O -5.58590700 0.32911400 0.37159400
C -6.67513400 1.24690300 0.27897800
H -7.35640200 0.92611500 -0.51717900
H -7.18434800 1.30247900 1.24224100
C -3.35222900 -3.28712100 -0.81309600
C -3.55237200 -1.91812800 -0.95983900
C -2.22751500 -1.49289700 0.96659700
C -2.02266600 -2.86665300 1.09357300
C -2.57902400 -3.79530900 0.20220500
H -1.40866500 -3.25046900 1.89924300
H -2.40857600 -4.85944700 0.31140100
O -3.98247500 -3.94841700 -1.81562200
O -4.30303600 -1.68465000 -2.06994400
C -4.74494800 -2.96664900 -2.51318000
H -5.80715400 -3.09119700 -2.27325300
H -4.56451300 -3.06218700 -3.58485500
C -3.25607600 0.45948700 -0.38741000
C -2.99804700 -0.98130900 -0.11447600
Cu 0.37509800 0.39110500 0.89811000
P -0.57870100 0.79420000 -1.15862100
C -0.61410400 -0.60442700 -2.34354000
H -0.86736200 -1.52950100 -1.82172200
H -1.32967200 -0.43328700 -3.15259800
H 0.38934300 -0.71438200 -2.76644400
C 0.27061100 2.11933800 -2.09123300
H 1.28412700 1.76626400 -2.30359200
H -0.23184000 2.36337700 -3.03209100
H 0.37345200 3.02218600 -1.48265900
P -1.36954500 -0.35447600 2.10443000
C -0.89908600 -1.36171100 3.55485900
H -0.09398900 -2.05050100 3.28770900
H -0.51425200 -0.68394200 4.32320000
H -1.74566400 -1.91794000 3.96805500
C -2.61606900 0.81052700 2.77134300

H -3.54720200 0.29641700 3.02586100
H -2.20439000 1.27373500 3.67346900
H -2.82988500 1.59642200 2.04427200
C 2.95138400 1.41702600 1.33491200
C 1.67840500 1.38849100 2.09555100
H 3.83193800 1.12170200 1.91095000
H 0.99618000 2.23584000 1.96485500
H 1.71223000 0.92059600 3.07334300
N 2.27707300 0.30013300 0.66363300
C 3.20833700 2.54354600 0.37147100
C 2.86707800 3.85756600 0.68276900
C 3.79679600 2.25683100 -0.86173100
C 3.10152400 4.87858600 -0.23654200
H 2.42620800 4.09505000 1.64801400
C 4.03285100 3.27550000 -1.77690400
H 4.05643100 1.22897800 -1.10365100
C 3.68045900 4.58849500 -1.46760100
H 2.83538600 5.90097600 0.01271600
H 4.49311800 3.04793900 -2.73342300
H 3.86243000 5.38318500 -2.18411200
S 2.66538200 -1.25457400 1.24494500
C 4.06055800 -1.61793700 0.23234800
C 3.86351400 -1.86299000 -1.12713600
C 5.33428300 -1.58956400 0.79127400
C 4.97077200 -2.07910200 -1.93201000
H 2.85971400 -1.89145400 -1.53818200
C 6.43009500 -1.81147400 -0.03464500
H 5.46095200 -1.40980100 1.85343900
C 6.26771600 -2.05614200 -1.40050800
H 4.83100100 -2.27479600 -2.99131700
H 7.42819800 -1.79575900 0.39273000
C 7.45673600 -2.32241800 -2.28444100
H 7.59349200 -3.40071100 -2.42475400
H 7.32381900 -1.87678800 -3.27459400
H 8.37701900 -1.92472400 -1.84910700
O 3.07048300 -1.22708300 2.64429400
O 1.50080900 -2.04446300 0.84533600

Int2

$\Delta E = -4504.415799$ au

$\Delta G = -4504.491525$ au

C 2.33476600 -3.93557700 -0.38130100
C 2.91690800 -2.73790800 0.02375500
C 1.22622500 -1.51377200 -1.10944600
C 0.64227300 -2.71917700 -1.49407500

C 1.18566300 -3.96048200 -1.13366200
 H -0.27438000 -2.71653900 -2.07033100
 H 0.71814700 -4.89181600 -1.42893900
 O 3.04417800 -4.97619600 0.11949900
 O 3.99841500 -2.99856600 0.80565100
 C 4.20478400 -4.40837400 0.72029600
 H 5.07853500 -4.61199000 0.09059600
 H 4.33126400 -4.81810700 1.72344200
 C 5.02388600 1.16014900 0.18996600
 C 4.32335600 0.03303900 -0.23000500
 C 2.51076100 0.59633900 1.19623000
 C 3.21940600 1.72734400 1.60323500
 C 4.49389200 2.03625600 1.10623600
 H 2.79442300 2.39755700 2.34197600
 H 5.03678400 2.91458300 1.43410400
 O 6.21021900 1.22700100 -0.46052900
 O 5.04955600 -0.62786100 -1.16832600
 C 6.32956100 0.00239900 -1.18259400
 H 7.06091800 -0.64435900 -0.68511500
 H 6.61630700 0.21475400 -2.21321100
 C 2.39272000 -1.50516300 -0.29624800
 C 3.06090100 -0.28334800 0.22339500
 Cu -0.64024800 1.01845100 0.19553100
 P 0.41766700 0.04994100 -1.55516100
 C 1.70883000 1.12226400 -2.29597700
 H 2.24991200 1.67195300 -1.52261100
 H 2.41691000 0.53167500 -2.88409900
 H 1.21547800 1.84889600 -2.94701300
 C -0.71465500 -0.30510700 -2.93409400
 H -1.10660100 0.65044700 -3.29426300
 H -0.20364200 -0.81916600 -3.75322900
 H -1.55164900 -0.89932000 -2.56317700
 P 0.80720600 0.36944600 1.79520600
 C 0.72630300 1.18716700 3.42679800
 H 0.82013000 2.27246500 3.35710900
 H -0.25019000 0.95433100 3.86173400
 H 1.50835000 0.80735900 4.09060500
 C 0.52698800 -1.38448700 2.22815600
 H 1.39583600 -1.79618400 2.74961300
 H -0.35741200 -1.41853000 2.86968900
 H 0.30534900 -1.97973200 1.34186900
 C -1.65120600 2.40179200 1.13790500
 C -3.00309600 1.90983700 0.68460100
 H -1.46274700 2.47210500 2.20542900

H -3.57775000 2.65014400 0.11799400
 H -3.60603800 1.58067300 1.53505000
 N -2.55110200 0.80089600 -0.18793500
 C -0.84285900 3.25644100 0.27208500
 C -1.11256800 3.36540900 -1.11179000
 C 0.30264200 3.91120500 0.78114700
 C -0.28006800 4.11872300 -1.93543300
 H -1.98786900 2.87771900 -1.53025200
 C 1.12653700 4.65040000 -0.04568000
 H 0.51412900 3.85110700 1.84465400
 C 0.83816400 4.75407800 -1.41026300
 H -0.51314500 4.21165800 -2.99139800
 H 1.99300500 5.15655700 0.36684800
 H 1.48327900 5.34124200 -2.05579500
 S -2.91996800 -0.69458200 0.40268100
 C -4.66650400 -0.83881000 0.13483200
 C -5.49355700 -1.16717600 1.20198200
 C -5.18240700 -0.64919500 -1.14713100
 C -6.85928600 -1.30792600 0.97734100
 H -5.06712300 -1.31455200 2.18816300
 C -6.54579200 -0.79125200 -1.35066100
 H -4.52169000 -0.39146000 -1.96861300
 C -7.40466800 -1.12267800 -0.29398500
 H -7.51040200 -1.57057800 1.80620800
 H -6.95670600 -0.64728500 -2.34622100
 C -8.88568300 -1.25708600 -0.53238600
 H -9.34818200 -0.27122700 -0.65722400
 H -9.08906300 -1.83045200 -1.44207000
 H -9.38291100 -1.75524600 0.30388500
 O -2.20351600 -1.64729600 -0.44936000
 O -2.68801000 -0.77951800 1.85141300

Int3

$\Delta E = -4504.408329$ au

$\Delta G = -4504.485876$ au

C -4.38778100 2.60373700 -1.38906300
 C -4.41787200 1.43155900 -0.63723200
 C -2.22404600 0.87492200 -1.37552300
 C -2.20504100 2.05698800 -2.11571000
 C -3.28637100 2.95258900 -2.13206100
 H -1.33811200 2.30789400 -2.71517800
 H -3.25651200 3.86937000 -2.70855800
 O -5.54462000 3.28528300 -1.21022700
 O -5.58926800 1.35961200 0.04532600
 C -6.39991800 2.41614100 -0.47093000

H -7.16131500 1.99892000 -1.13956100
 H -6.84883400 2.96484700 0.35747500
 C -4.47081600 -2.80861300 0.73822700
 C -4.36231400 -1.63540900 -0.00548000
 C -2.63803800 -0.86360200 1.43278300
 C -2.74643500 -2.04849900 2.16257800
 C -3.66604500 -3.05145100 1.82564700
 H -2.11501100 -2.22134200 3.02582800
 H -3.74011500 -3.97005800 2.39462800
 O -5.42187800 -3.60136000 0.19876400
 O -5.23472100 -1.67036000 -1.04195700
 C -5.99951200 -2.86580700 -0.87960300
 H -7.03363600 -2.60807300 -0.63106400
 H -5.94316900 -3.45848700 -1.79467500
 C -3.35932300 0.55242100 -0.58226500
 C -3.44871400 -0.64705200 0.28512400
 Cu 0.41718100 0.08265200 0.61462300
 P -0.74627300 -0.20197300 -1.34641200
 C -1.27072300 -1.89748000 -1.77006700
 H -1.74286400 -2.37891400 -0.91189200
 H -1.96732900 -1.88782200 -2.61288900
 H -0.36579900 -2.45394900 -2.02567900
 C 0.27572700 0.34830900 -2.74938200
 H 1.08988100 -0.37360300 -2.84023500
 H -0.30495500 0.37694000 -3.67581100
 H 0.70972400 1.33089500 -2.54917200
 P -1.36102000 0.33765800 1.90648500
 C -1.05023600 0.04410500 3.67943600
 H -0.54610500 -0.91021400 3.84516500
 H -0.40160700 0.83744500 4.05847400
 H -1.99142900 0.05962400 4.23594600
 C -2.02982500 2.03756400 1.87837700
 H -3.02634900 2.06248300 2.32839300
 H -1.35414300 2.66820200 2.46423900
 H -2.08149300 2.43117900 0.86249600
 C 2.83377000 0.51575100 1.15948100
 C 1.61961400 0.49475900 2.06833200
 H 3.63689800 -0.12406500 1.54591200
 H 1.35698000 1.44478200 2.53749600
 H 1.61013500 -0.34733300 2.76072500
 N 2.17142900 -0.06211800 -0.03592000
 C 3.39516600 1.89227900 0.88683000
 C 4.04504000 2.56610100 1.92412500
 C 3.27495800 2.50988900 -0.35564900

C 4.56301900 3.83942400 1.72291600
 H 4.15573300 2.08483000 2.89378800
 C 3.79466400 3.78735300 -0.55832000
 H 2.78790200 1.97453200 -1.16395700
 C 4.43709100 4.45473500 0.47834300
 H 5.07160800 4.35034000 2.53469800
 H 3.70075600 4.25890100 -1.53204100
 H 4.84628200 5.44737400 0.31862400
 S 2.55600800 -1.65593500 -0.30220200
 C 4.30725600 -1.58108800 -0.55823400
 C 4.81982500 -0.73738800 -1.54178500
 C 5.14247500 -2.36472200 0.23073400
 C 6.19283200 -0.68201400 -1.72878100
 H 4.15474000 -0.12715600 -2.14369300
 C 6.51520200 -2.29921700 0.02375700
 H 4.71750800 -3.00981000 0.99219100
 C 7.05924500 -1.46167100 -0.95354600
 H 6.60160100 -0.02066800 -2.48723800
 H 7.17475700 -2.90808800 0.63551700
 C 8.54668400 -1.41746600 -1.18459400
 H 9.09909600 -1.59988900 -0.25860900
 H 8.84451000 -2.18867900 -1.90431100
 H 8.86103700 -0.45091300 -1.58796400
 O 2.29252600 -2.46734700 0.88885200
 O 1.88012600 -2.03517500 -1.54305200

Int4^R

$\Delta E = -5023.840990$ au

$\Delta G = -5023.936398$ au

Cu -0.39699000 -0.24032000 -0.31060400
 C -4.39781900 0.32998600 -0.61385600
 H -4.04014400 1.17842100 -1.19714600
 N -2.13245500 0.34233900 0.32163800
 S -2.21355100 1.44321700 1.52183700
 C -3.40807100 2.61880300 0.89787700
 C -4.73115400 2.54906000 1.32601800
 C -3.03885400 3.49460000 -0.12548500
 C -5.69266200 3.35675900 0.71937300
 H -4.99210800 1.87762400 2.13803400
 C -4.00611300 4.28971200 -0.71991500
 H -2.00265000 3.54143900 -0.44620100
 C -5.34897300 4.23123400 -0.31056900
 H -6.72380400 3.30433100 1.05846400
 H -3.72124900 4.97870000 -1.51071400
 C -6.38064500 5.12757300 -0.94462100

H	-6.19061500	5.26800700	-2.01308600	C	4.82220500	-0.17255800	-2.21917900
H	-6.36227800	6.11882400	-0.47785200	C	2.69060900	0.36521200	-1.32482600
H	-7.39061500	4.72595600	-0.82197800	C	2.13864300	0.04416000	-2.56853200
O	-0.92346900	2.12123100	1.61292700	C	2.90265800	-0.38450700	-3.66115000
O	-2.80430600	0.87336300	2.73362300	H	1.06242800	0.13022100	-2.70096100
C	-1.43032800	-3.16484700	0.57211500	H	2.45388100	-0.62804800	-4.61676500
C	-1.63945500	-2.88759000	-0.79711700	O	5.22508300	-0.90115300	-4.30711800
C	-2.84505400	-3.26745700	-1.40175700	O	6.16819000	-0.39404500	-2.27351900
C	-3.83408000	-3.88936500	-0.64317200	C	6.45898800	-0.63071500	-3.64770600
C	-3.61524400	-4.09364400	0.73458100	H	6.91651800	0.26602400	-4.08369100
C	-2.42785800	-3.73852900	1.35899800	H	7.11569800	-1.49692300	-3.73535500
C	0.42401100	-2.14539300	-0.18828900	C	4.79865800	0.56052000	0.14109900
C	-0.48066500	-2.15887700	-1.25464400	C	4.08885000	0.24460100	-1.12745800
H	-3.00562000	-3.08079900	-2.46128100	P	4.28095300	-2.06663400	0.95840300
H	-4.39636400	-4.56634100	1.32461100	C	5.64258000	-2.92022900	0.03827400
H	-2.28734200	-3.90023900	2.42176900	H	5.78349400	-2.44878400	-0.93730500
H	1.50104400	-2.01361600	-0.20709800	H	6.58927600	-2.86835200	0.58563700
H	-0.19315100	-2.01200700	-2.28824900	H	5.37467700	-3.96982400	-0.11801400
N	-0.15456700	-2.75549300	0.90706700	C	4.50388900	-2.83115000	2.62780400
C	-5.11239300	-4.36672300	-1.28934200	H	4.12769900	-3.85809900	2.57913900
H	-5.43702400	-3.69298300	-2.08926500	H	5.54837300	-2.86914800	2.95484900
H	-5.92514400	-4.44548800	-0.55980800	H	3.91515000	-2.29334500	3.37807500
H	-4.97852500	-5.36000000	-1.73255000	P	1.44266100	0.99623200	-0.13166200
C	0.38022300	-2.69169300	2.26229700	C	1.39365800	2.77659700	-0.55720300
H	0.23474500	-3.66485200	2.74320800	H	1.02440200	2.89934900	-1.57928100
H	1.45875100	-2.53035900	2.15781800	H	0.71456900	3.28007400	0.13559400
C	-0.26865900	-1.59265300	3.05971100	H	2.39319100	3.21773300	-0.48881800
C	-0.96584800	-1.78571500	4.17349400	C	2.07907100	1.01239000	1.58207700
H	-0.16326100	-0.58632600	2.65738300	H	2.96135400	1.64050600	1.71396000
H	-1.43662800	-0.95368800	4.68631700	H	1.25918400	1.40938400	2.18727800
H	-1.09156800	-2.77599000	4.60798800	H	2.30914500	-0.00132400	1.91786400
C	5.94531300	2.20697300	1.50962100	C	-5.72894700	-0.07125900	-0.82157900
C	5.29902100	1.82728300	0.33966300	C	-6.54628400	0.73218600	-1.65605200
C	5.00271500	-0.38264900	1.18262300	C	-6.27304600	-1.23364500	-0.21654500
C	5.65575300	0.01511200	2.34865500	C	-7.86822300	0.39279500	-1.86947900
C	6.13495800	1.32022800	2.54225700	H	-6.12337700	1.62588500	-2.10570600
H	5.80612500	-0.69732600	3.15190300	C	-7.58882500	-1.57444700	-0.45350500
H	6.63088200	1.61477400	3.45967800	H	-5.64705000	-1.86335600	0.40821100
O	6.27478500	3.52660600	1.44019500	C	-8.38253400	-0.76070900	-1.27165900
O	5.19021800	2.90801800	-0.49090500	H	-8.50025100	1.00893200	-2.49912100
C	6.01885800	3.91009600	0.09392400	H	-8.01123400	-2.46706700	-0.00570400
H	6.96679900	3.96642800	-0.45632300	H	-9.41925500	-1.03256900	-1.44571400
H	5.49423500	4.86620800	0.08180900	C	-3.38494100	-0.35651100	0.19214200
C	4.25656200	-0.48356100	-3.44998000	H	-3.79578600	-0.73134700	1.14336300

H -3.20940500 -1.28561000 -0.39438100

Int4^S

ΔE = -5023.839398 au

ΔG = -5023.928588 au

Cu 1.13039100 1.37926600 -1.10880900

N 1.97280000 1.21910700 0.57876700

S 1.48609300 1.08509100 2.13672100

C 2.35728000 -0.38052100 2.66439000

C 2.72046700 -1.35516400 1.74052700

C 2.58600300 -0.56562000 4.02550200

C 3.31269900 -2.52931700 2.19308700

H 2.53835100 -1.19375000 0.68364200

C 3.17080000 -1.74840300 4.45957800

H 2.31225900 0.20934500 4.73403200

C 3.54247900 -2.74784200 3.55367400

H 3.60012600 -3.28905200 1.47019500

H 3.34619500 -1.89797100 5.52140900

C 4.20066600 -4.01366700 4.03761800

H 5.25744900 -3.83649500 4.26824200

H 3.72542800 -4.38522300 4.95040700

H 4.15350800 -4.80368300 3.28289100

O 1.99872700 2.20659700 2.92739400

O 0.05861900 0.81185500 2.16983300

C 2.04824500 -1.62548900 -2.47282300

C 2.76647000 -0.42173400 -2.39948300

C 4.04866100 -0.42594700 -1.83978900

C 4.57261700 -1.60173600 -1.32218500

C 3.81240300 -2.78792500 -1.39829200

C 2.55458200 -2.82441100 -1.97130400

C 0.79675200 -0.07139400 -3.46299500

C 1.90530400 0.62337100 -2.95377700

H 4.64354100 0.48258500 -1.81625200

H 4.23910500 -3.70755600 -1.00740300

H 2.00427500 -3.75296100 -2.05123700

H -0.01969400 0.31494900 -4.05513000

H 2.25770400 1.51713900 -3.45466700

N 0.84608400 -1.36753000 -3.14606200

C 5.92098300 -1.62376700 -0.65150600

H 6.54063900 -2.44524600 -1.02446000

H 6.46514200 -0.68891900 -0.81092000

H 5.80210600 -1.76272600 0.42961300

C -0.22322700 -2.33046000 -3.40767900

H -0.71800900 -2.57738900 -2.46305900

H -0.95735900 -1.80864900 -4.03094500

C 0.25562200 -3.56911700 -4.11047400

C -0.14652800 -4.79023200 -3.77349000

H 0.92466000 -3.41673300 -4.95531600

H 0.16899200 -5.66557200 -4.33149400

H -0.82187000 -4.95858400 -2.93731200

C 2.74469800 2.56923800 -0.95174400

H 3.38088000 2.41018000 -1.81824200

C -3.22309400 1.51642200 2.91941800

C -3.32315500 0.38193400 2.12374100

C -2.14126600 1.45705100 0.38007300

C -2.05370500 2.59282900 1.18560000

C -2.60378300 2.65581700 2.46909100

H -1.50914500 3.46245500 0.83280500

H -2.52842300 3.54595200 3.08141100

O -3.85362500 1.30039500 4.10257400

O -4.03172800 -0.57511300 2.78644500

C -4.17549600 -0.08693900 4.11676400

H -5.20856400 -0.21701500 4.44185300

H -3.47729700 -0.61684700 4.77688100

C -4.80604100 -2.10599800 -1.25744300

C -4.36989100 -1.01614500 -0.51410000

C -2.28254400 -2.07624800 -0.08523600

C -2.74517200 -3.17061300 -0.82184300

C -4.00879200 -3.20931800 -1.43328800

H -2.12113700 -4.05217200 -0.91847800

H -4.34124900 -4.06883000 -2.00377900

O -6.04469000 -1.84784500 -1.76264900

O -5.32019900 -0.03591600 -0.55419500

C -6.47725400 -0.66692500 -1.09572100

H -7.16153300 -0.93586400 -0.28104900

H -6.95260300 0.00284600 -1.81259600

C -2.80717000 0.29446600 0.84788000

C -3.12215200 -0.93969600 0.06772300

P -1.23288000 1.52904700 -1.19333100

C -2.22071500 0.56362900 -2.40919900

H -3.28448000 0.75253600 -2.24098800

H -1.97423700 0.91288000 -3.41621200

H -2.04146100 -0.50876100 -2.33386600

C -1.60337600 3.21066800 -1.84241000

H -1.20039600 3.28688700 -2.85738700

H -2.68333300 3.38297100 -1.86765800

H -1.13028700 3.99022400 -1.24440100

P -0.55405500 -2.00522600 0.56082200

C 0.02178400 -3.74830000 0.30336000

H 0.13739000 -3.99263700 -0.75679000
H 1.01087900 -3.82514000 0.76678400
H -0.63675700 -4.48911100 0.76977800
C -0.82669900 -2.10882300 2.38843800
H -1.55490500 -2.88499000 2.64204400
H 0.13399400 -2.33863800 2.86150200
H -1.15477100 -1.14198700 2.76922100
C 3.19053800 1.97964800 0.35204600
H 4.06786800 1.33082900 0.24792600
H 3.40005400 2.73279900 1.12064600
C 1.92829000 3.77747800 -1.00589200
C 1.78837000 4.44091600 -2.24067700
C 1.33488200 4.34659300 0.14130100
C 1.10813400 5.64679300 -2.32781200
H 2.25024600 4.01696000 -3.12918400
C 0.66722200 5.55774000 0.04824900
H 1.41161600 3.84678900 1.10293600
C 0.55049200 6.20974300 -1.18166100
H 1.02237800 6.15365300 -3.28317900
H 0.23538400 5.99934200 0.94050300
H 0.02522300 7.15737300 -1.24470000

Int5^R

$\Delta E = -5023.845856$ au

$\Delta G = -5023.937606$ au

Cu -0.84972100 0.27105500 0.92431800
C -3.29463200 -0.31374400 1.10626200
C -2.35347200 0.24832000 2.13622800
H -3.78150800 0.52877600 0.59735800
H -2.60430100 1.20515000 2.57791700
H -2.01350500 -0.49881700 2.86213300
N -2.20017500 -0.90024700 0.28733600
C -4.33895300 -1.30730000 1.54006000
C -5.68297000 -0.94083400 1.58852700
C -3.97440200 -2.61443100 1.86727700
C -6.65366800 -1.86829500 1.95443900
H -5.97479500 0.07041900 1.31575500
C -4.94222800 -3.54328300 2.23069300
H -2.93028300 -2.90675400 1.79616700
C -6.28500400 -3.17234700 2.27267400
H -7.69880600 -1.57492100 1.98367700
H -4.65257000 -4.56096600 2.47471300
H -7.04121700 -3.89884400 2.55366200
S -2.34843200 -0.59981800 -1.34895700
C -4.01648500 -1.08172500 -1.67532300

C -4.98032200 -0.10723900 -1.90117600
C -4.35312100 -2.43008600 -1.56319500
C -6.31215700 -0.49531100 -2.00129600
H -4.68843100 0.93412700 -1.98905000
C -5.68550600 -2.79423900 -1.65643600
H -3.58411700 -3.17310700 -1.38204100
C -6.68403300 -1.83382300 -1.86177500
H -7.07491900 0.25755100 -2.17800300
H -5.96179800 -3.83916100 -1.54992300
C -8.12960000 -2.25099200 -1.90393600
H -8.28979600 -3.04383000 -2.64175400
H -8.78584300 -1.41425700 -2.15661600
H -8.43874200 -2.64388700 -0.92865000
O -1.42166400 -1.49568000 -2.03599700
O -2.20146600 0.84303700 -1.60429800
C -0.95653500 3.59334200 0.00758200
C -1.27929000 3.09374800 1.27399300
C -2.43498100 3.56039900 1.90525100
C -3.26585500 4.46086100 1.24545800
C -2.93188300 4.88904500 -0.05428800
C -1.77423000 4.47468300 -0.69059300
C 0.74814100 2.28610600 0.61486100
C -0.23322000 2.12285000 1.63272800
H -2.67700100 3.25522900 2.91968300
H -3.59645800 5.57996500 -0.56506700
H -1.52463200 4.81520900 -1.68906200
H 1.75351500 1.88030300 0.56632800
H 0.07398600 1.92896200 2.65600300
N 0.29943100 3.07953900 -0.35140500
C -4.51004900 4.99528700 1.90824900
H -4.42945000 6.07464900 2.07631500
H -4.68718300 4.51816600 2.87588400
H -5.39256000 4.82802300 1.28188300
C 0.98871700 3.36676800 -1.60610300
H 1.13298800 4.44988000 -1.67969400
H 1.97894300 2.90941100 -1.51443700
C 0.23762500 2.83559400 -2.79756700
C 0.17367800 3.48216100 -3.95684300
H -0.25908900 1.87704900 -2.66156800
H -0.34415900 3.05568600 -4.80948600
H 0.64110900 4.45398500 -4.10260100
C 4.99148300 -2.50619200 -2.21181100
C 4.50517600 -2.23496400 -0.93820600
C 4.74255700 0.10722600 -1.31484600

C 5.23243700 -0.18439300 -2.58689300
 C 5.35922300 -1.49672800 -3.06861100
 H 5.52931800 0.62108200 -3.24887500
 H 5.73262100 -1.70454200 -4.06438300
 O 4.98645100 -3.84959000 -2.42470300
 O 4.16910100 -3.40669600 -0.32103700
 C 4.68810700 -4.43664900 -1.16364200
 H 5.60618300 -4.84032600 -0.71964000
 H 3.93215300 -5.21205600 -1.29269500
 C 4.18307400 -0.53453000 3.29684900
 C 4.62118600 -0.70099400 1.98633200
 C 2.38770100 -0.63447600 1.18964400
 C 1.96560400 -0.47146300 2.51207200
 C 2.84790800 -0.41706600 3.59817200
 H 0.90159700 -0.40092800 2.72473600
 H 2.49988200 -0.29169200 4.61639200
 O 5.24727600 -0.49562200 4.13407600
 O 5.98160700 -0.76832700 1.97236400
 C 6.38109200 -0.83923600 3.33999700
 H 6.69480300 -1.86266300 3.57515300
 H 7.18174200 -0.12146400 3.52180600
 C 4.34226800 -0.95407000 -0.45962600
 C 3.77311500 -0.74697800 0.89999500
 P 4.48611800 1.83070500 -0.71065400
 C 6.07503500 2.15130200 0.18095600
 H 6.17253900 1.45808500 1.01978200
 H 6.93717600 2.01679200 -0.48002500
 H 6.07584000 3.17394200 0.57058000
 C 4.75970000 2.84253200 -2.23422500
 H 4.64680800 3.89752600 -1.96442800
 H 5.75534800 2.71235900 -2.67064700
 H 4.00637300 2.60688700 -2.99348200
 P 1.01737300 -0.81655600 -0.01515700
 C 0.74031600 -2.62196200 -0.03273300
 H 0.36403800 -2.93806600 0.94388600
 H -0.00821000 -2.85282200 -0.79275300
 H 1.68268700 -3.13884700 -0.23733400
 C 1.52708400 -0.40485800 -1.71701900
 H 2.26270300 -1.11095800 -2.10555000
 H 0.62089600 -0.46255200 -2.32517800
 H 1.94356400 0.60238100 -1.76927200

Int5^S

$\Delta E = -5023.853471$ au

$\Delta G = -5023.943654$ au

Cu 0.74176400 0.45712400 1.37184700
 N 1.07231400 -1.32568200 0.91455100
 S 0.40076400 -2.52082500 1.89245300
 C 0.80340800 -3.97550200 0.96855300
 C 0.04405700 -4.28620100 -0.15957200
 C 1.87866500 -4.76501000 1.35939100
 C 0.38879700 -5.39889700 -0.90968400
 H -0.79817300 -3.65676200 -0.43061100
 C 2.20802100 -5.87739000 0.59200600
 H 2.43215100 -4.52319200 2.26079600
 C 1.47619100 -6.20718700 -0.54997800
 H -0.19741400 -5.65504200 -1.78841500
 H 3.04376800 -6.50244500 0.89238300
 C 1.82652300 -7.41711300 -1.37523000
 H 1.02741100 -8.16472700 -1.32482600
 H 1.95811100 -7.15040600 -2.42899900
 H 2.74893700 -7.88779300 -1.02630200
 O 1.09065700 -2.56196600 3.17984600
 O -1.04056700 -2.31755500 1.86430400
 C 3.01019500 2.73871600 -0.08129400
 C 2.51127600 3.01286400 1.20313900
 C 3.37634900 3.50688000 2.18703300
 C 4.71162700 3.71922300 1.87771700
 C 5.17884700 3.42170700 0.57557900
 C 4.35273800 2.92920500 -0.41643600
 C 0.85093500 2.17775700 -0.09906700
 C 1.12465500 2.60078200 1.21167600
 H 3.00468600 3.71837200 3.18601800
 H 6.22813200 3.59244800 0.35096500
 H 4.72585700 2.71142800 -1.41089600
 H -0.10128900 1.93899200 -0.55752300
 H 0.37766800 2.98813900 1.88874500
 N 1.97200700 2.22092200 -0.84828100
 C 5.67610900 4.25887700 2.90297300
 H 6.10509900 5.21141300 2.57404000
 H 5.18640700 4.42561100 3.86592900
 H 6.50797100 3.56452700 3.06324900
 C 2.54526700 -1.36164200 0.86656500
 H 2.97997500 -2.18926000 1.43782400
 C 2.10709400 1.68202400 -2.19812200
 H 2.93057000 0.96313300 -2.20376800
 H 1.18606300 1.12766500 -2.39494600
 C 2.32153600 2.75499100 -3.22612800
 C 3.29775900 2.70619800 -4.12656200

H 1.61170700 3.58034300 -3.21366300
 H 3.41480300 3.47460100 -4.88382500
 H 4.01141000 1.88476300 -4.14219800
 C 2.61497300 -0.05648500 1.58431800
 H 3.19953700 0.74418000 1.14239400
 H 2.67466900 -0.14726600 2.67021600
 C 3.09792500 -1.34844100 -0.54046900
 C 4.38052600 -0.84053700 -0.75859900
 C 2.37119500 -1.85454400 -1.61635400
 C 4.93189600 -0.83971500 -2.03673300
 H 4.95701300 -0.44317700 0.07371600
 C 2.92484500 -1.85842500 -2.89462800
 H 1.37059400 -2.23881000 -1.44704000
 C 4.20327800 -1.35003400 -3.10988800
 H 5.93162400 -0.44574000 -2.19281100
 H 2.35563700 -2.26375200 -3.72597600
 H 4.63434800 -1.35852800 -4.10628300
 C -5.50253900 -0.77615500 0.65704000
 C -4.69975800 0.05315600 -0.11579500
 C -2.99246200 -0.00267200 1.53136900
 C -3.80371400 -0.84167900 2.29382200
 C -5.07295700 -1.25720500 1.86954200
 H -3.44746900 -1.21660500 3.24476100
 H -5.68522700 -1.91754400 2.47162300
 O -6.68183500 -0.99353700 0.01990200
 O -5.35404400 0.38161400 -1.26417200
 C -6.54825600 -0.39816700 -1.26765100
 H -7.40425600 0.25121900 -1.45937900
 H -6.46636700 -1.18554500 -2.02673600
 C -2.27550000 3.47400700 -1.70555800
 C -2.84280700 2.64643000 -0.74019300
 C -1.91629700 0.71456200 -1.79258000
 C -1.38144300 1.56067600 -2.76692000
 C -1.53749900 2.95737300 -2.74093300
 H -0.83309200 1.14207500 -3.60280800
 H -1.12182800 3.59162600 -3.51549500
 O -2.59206000 4.76975700 -1.43965700
 O -3.54965700 3.40912900 0.14268100
 C -3.60347300 4.71073000 -0.44000400
 H -4.58683700 4.85985900 -0.90205300
 H -3.40203600 5.45952200 0.32620400
 C -3.43026200 0.44332000 0.25662700
 C -2.66989400 1.27763500 -0.71911000
 P -1.44537300 0.63256900 2.26072400

C -1.90160000 2.36780800 2.67913000
 H -2.89342400 2.38419900 3.13942400
 H -1.18166100 2.77152800 3.39887800
 H -1.93279900 3.00895600 1.79672500
 C -1.34399600 -0.04955800 3.96042000
 H -0.46306700 0.38695600 4.44243100
 H -2.22725900 0.22314100 4.54578500
 H -1.22017100 -1.13209500 3.94447500
 P -1.57647500 -1.10660600 -1.79480600
 C -0.70947400 -1.32179700 -3.41804300
 H 0.27646500 -0.84811100 -3.40724900
 H -0.54604800 -2.39661800 -3.55276600
 H -1.28128300 -0.95355300 -4.27673500
 C -3.21209900 -1.84074900 -2.28588500
 H -3.77593000 -1.20005000 -2.96980400
 H -3.01181800 -2.79796400 -2.77902100
 H -3.81297800 -2.04765700 -1.39808800

TS3^R

$\Delta E = -5023.828456$ au

$\Delta G = -5023.923706$ au

Cu -0.77412900 -0.23864100 -0.30729300
 C -2.75839700 -1.23986100 -1.58158500
 H -1.88578300 -1.01628600 -2.19501700
 N -2.31160600 0.84736600 -0.59751300
 S -2.59979200 1.97792800 0.52442600
 C -3.79731300 3.06753400 -0.21246700
 C -4.99746900 3.30903400 0.44382600
 C -3.51943600 3.66898800 -1.43962200
 C -5.92761400 4.16694900 -0.13565500
 H -5.19098500 2.82908500 1.39700200
 C -4.45725400 4.52040700 -2.00402200
 H -2.57850700 3.46824000 -1.94224700
 C -5.67297700 4.78569900 -1.36019800
 H -6.86673500 4.35858900 0.37596700
 H -4.24594800 4.99275800 -2.95975400
 C -6.66709000 5.73888200 -1.97113400
 H -6.76797200 5.57373200 -3.04837400
 H -6.34402700 6.77630100 -1.82757400
 H -7.65529800 5.63305500 -1.51556900
 O -1.33150500 2.69881300 0.68678400
 O -3.21981000 1.41324400 1.72596900
 C -1.96282200 -1.68147100 2.31102600
 C -2.46082800 -2.39911500 1.21338200
 C -3.73973400 -2.95492400 1.28669000

C -4.52462900 -2.72907000 2.41488700
 C -4.01260000 -1.94555600 3.46458000
 C -2.73044900 -1.41897400 3.43886200
 C -0.27596500 -1.78200000 0.80829500
 C -1.43920600 -2.36058200 0.17663800
 H -4.10600000 -3.59793400 0.49456200
 H -4.63857900 -1.75882100 4.33255700
 H -2.35191400 -0.81364200 4.25401200
 H 0.75945200 -2.03967100 0.60500500
 H -1.31120700 -3.11507800 -0.58775800
 N -0.63005000 -1.35312500 2.05747200
 C -5.90097900 -3.33427100 2.52917600
 H -6.21511700 -3.79345400 1.58703300
 H -6.64376700 -2.57773700 2.80252400
 H -5.92707300 -4.11016300 3.30210400
 C 0.28926900 -0.76941000 3.02552700
 H 0.32603200 -1.41964600 3.90758400
 H 1.28028200 -0.80219300 2.55682500
 C -0.08449600 0.63687000 3.41293500
 C 0.03810100 1.10069200 4.65295000
 H -0.45138200 1.28253600 2.61656300
 H -0.20232400 2.13135900 4.89151500
 H 0.38237200 0.47205700 5.47204700
 C 5.52566700 2.85839200 -0.13051400
 C 4.96008100 1.77945700 -0.79906400
 C 4.69916500 0.60436700 1.26070300
 C 5.27360400 1.69410100 1.91306500
 C 5.69239400 2.84905000 1.23410900
 H 5.40374800 1.66978600 2.98929300
 H 6.12583000 3.69319000 1.75742300
 O 5.80606900 3.84901300 -1.02078900
 O 4.85204600 2.07367300 -2.12965600
 C 5.60084100 3.27614300 -2.30686500
 H 6.57041200 3.03800600 -2.76150600
 H 5.02930400 3.96799900 -2.92665300
 C 4.14655800 -2.54232700 -2.14167500
 C 4.66267300 -1.46395700 -1.42945500
 C 2.49049500 -0.54845400 -1.16776200
 C 1.98674500 -1.64220000 -1.87655300
 C 2.79961100 -2.66376000 -2.38504700
 H 0.91394500 -1.70851300 -2.04892700
 H 2.39279100 -3.50703000 -2.93002200
 O 5.14900900 -3.38955800 -2.47972600
 O 6.00999400 -1.61565700 -1.29625400

C 6.35889300 -2.72050800 -2.12643000
 H 6.85054500 -2.35400300 -3.03489900
 H 7.00177200 -3.40317000 -1.56972300
 C 4.52148400 0.64938700 -0.14727100
 C 3.88237400 -0.45122700 -0.91562400
 P 4.05316900 -0.88276700 2.14442200
 C 5.56810300 -1.94594900 2.18301000
 H 5.85895700 -2.19507800 1.15878900
 H 6.40735100 -1.43603300 2.66701900
 H 5.35354000 -2.87518500 2.71981600
 C 3.98529400 -0.31919000 3.90426200
 H 3.64804900 -1.16509700 4.51245500
 H 4.94807200 0.01637900 4.30345000
 H 3.25034800 0.48562700 4.01536900
 P 1.22695400 0.68466500 -0.69497000
 C 1.15265200 1.83346900 -2.11581300
 H 0.84138800 1.30285400 -3.01915700
 H 0.41398300 2.60617500 -1.88291900
 H 2.13343400 2.28729600 -2.28936600
 C 1.74351400 1.78584600 0.66318500
 H 2.59563500 2.41098400 0.39181400
 H 0.87120000 2.41528100 0.86358400
 H 1.98514900 1.22415800 1.56620900
 C -3.50884600 -2.39011700 -1.99936400
 C -2.89870900 -3.35760300 -2.82347700
 C -4.86201300 -2.55385800 -1.64355200
 C -3.61167700 -4.45605900 -3.26906800
 H -1.85708800 -3.23130300 -3.10975300
 C -5.57922000 -3.64565200 -2.11002600
 H -5.35046000 -1.82237700 -1.00898700
 C -4.95455700 -4.59964100 -2.91185900
 H -3.13392600 -5.19736900 -3.90056200
 H -6.62537100 -3.75885100 -1.84619300
 H -5.51661700 -5.45771500 -3.26651900
 C -3.38316700 -0.06035800 -0.92227000
 H -4.12146800 0.35747800 -1.63451700
 H -3.94673500 -0.38224300 -0.03039800

TS3^s

$\Delta E = -5023.827909$ au

$\Delta G = -5023.913799$ au

Cu 0.80846100 1.53153200 -0.75842800
 N 1.65073600 1.07261300 0.90891100
 S 1.24839700 0.53273500 2.38364300
 C 2.15934100 -0.99382900 2.55806000

C 2.71553800 -1.62432600 1.45137000
 C 2.24276000 -1.57467500 3.82209800
 C 3.35002900 -2.85269800 1.61505600
 H 2.64266100 -1.16289100 0.47221300
 C 2.86957000 -2.80433400 3.96652800
 H 1.81943100 -1.06680600 4.68280500
 C 3.43145300 -3.46445400 2.86674900
 H 3.78642200 -3.34198300 0.74763000
 H 2.92950500 -3.26145000 4.95058700
 C 4.12374700 -4.79077900 3.04556100
 H 5.09513200 -4.65937900 3.53570100
 H 3.53126800 -5.46418900 3.67274800
 H 4.29819000 -5.28534300 2.08584800
 O 1.75439900 1.45008700 3.41107100
 O -0.17242400 0.20969900 2.39820800
 C 2.51435600 -0.69872900 -2.41123400
 C 3.27194200 0.43507400 -2.08051600
 C 4.57943100 0.28957700 -1.61747400
 C 5.11950200 -0.98352500 -1.46654500
 C 4.33079600 -2.09992700 -1.80276500
 C 3.03020900 -1.98499800 -2.26898400
 C 1.16452600 1.07188000 -2.73901300
 C 2.40562100 1.60013400 -2.24589000
 H 5.17857400 1.16296900 -1.37165500
 H 4.76035800 -3.09201100 -1.69156700
 H 2.44990600 -2.86304100 -2.52228800
 H 0.47034000 1.61585100 -3.36717600
 H 2.73861300 2.54265900 -2.65730700
 N 1.26506100 -0.27972600 -2.87787500
 C 6.50959400 -1.18369300 -0.92149100
 H 7.10647300 -1.82581000 -1.57699600
 H 7.03721300 -0.23304200 -0.80812600
 H 6.46879300 -1.66379300 0.06276300
 C 0.23743500 -1.11987600 -3.48136600
 H -0.32165300 -1.64546900 -2.70108300
 H -0.46031100 -0.43557600 -3.97457100
 C 0.78384700 -2.08303500 -4.49864200
 C 0.33359700 -3.32661300 -4.62973800
 H 1.54123400 -1.69281600 -5.17613100
 H 0.69894200 -3.98299600 -5.41254500
 H -0.43307000 -3.72720700 -3.97048900
 C 2.67426700 2.77570500 -0.27210700
 H 3.55837700 3.05275500 -0.83629500
 C -3.38278700 0.64749300 3.00870300

C -3.39740300 -0.28634500 1.97874700
 C -2.33430600 1.24953700 0.53071100
 C -2.32934600 2.18034500 1.57006500
 C -2.86804400 1.90712500 2.83044700
 H -1.86979800 3.15176800 1.42213300
 H -2.86081000 2.63984400 3.62773900
 O -3.97773700 0.12164100 4.10822100
 O -4.01633700 -1.42189900 2.40566500
 C -4.19448900 -1.25430500 3.80897800
 H -5.21523500 -1.52752500 4.08007100
 H -3.45810000 -1.86402600 4.34668500
 C -4.65557700 -1.97777100 -1.98415800
 C -4.31972900 -1.07609300 -0.98174300
 C -2.19138900 -2.10648000 -0.69696500
 C -2.55117900 -3.01000400 -1.70089100
 C -3.78252700 -2.96237700 -2.37473900
 H -1.86788600 -3.80741800 -1.97074500
 H -4.03525100 -3.67277300 -3.15326700
 O -5.88622900 -1.67030800 -2.48120800
 O -5.32688000 -0.16319500 -0.84353900
 C -6.42016200 -0.71134700 -1.57505900
 H -7.11108600 -1.20706300 -0.88122100
 H -6.91567300 0.08241700 -2.13431300
 C -2.89006100 -0.04286100 0.72144200
 C -3.10472100 -1.08046700 -0.33010300
 P -1.43982500 1.74153200 -0.96777100
 C -2.29179800 1.01486500 -2.41878700
 H -3.36878300 1.18541000 -2.33208600
 H -1.93390900 1.51997100 -3.32228100
 H -2.11599800 -0.05538600 -2.50747900
 C -1.86953800 3.50448100 -1.23659200
 H -1.46376800 3.81200800 -2.20557200
 H -2.95552300 3.63622100 -1.24128600
 H -1.43219300 4.15186500 -0.47641100
 P -0.50847100 -2.11619000 0.06641600
 C 0.21387800 -3.68594300 -0.60561500
 H 0.39943200 -3.62695500 -1.68253100
 H 1.18181200 -3.81859300 -0.11103900
 H -0.40108700 -4.56858100 -0.39857600
 C -0.86863200 -2.71933000 1.77734800
 H -1.58872100 -3.54277800 1.77078400
 H 0.07357900 -3.05915000 2.22032800
 H -1.23749700 -1.89391400 2.38557300
 C 2.89804300 1.79820500 0.83257000

H 3.74981200 1.14146900 0.60956100
H 3.15590300 2.35262700 1.74963200
C 1.70922700 3.87595600 -0.12517700
C 1.63279400 4.85618100 -1.13234200
C 1.00112800 4.08224900 1.07553300
C 0.87980200 6.00595700 -0.95260300
H 2.18968400 4.72224200 -2.05662800
C 0.27668500 5.25249000 1.26150900
H 1.05123000 3.35026800 1.87486800
C 0.20708200 6.21124100 0.25215300
H 0.83711100 6.75463500 -1.73655000
H -0.23141200 5.41654800 2.20635000
H -0.36348400 7.12166800 0.40550400

TS4^R

ΔE = -5023.830455 au

ΔG = -5023.921594 au

Cu -0.69508300 0.22939700 0.84764800
C -3.13652700 -0.15020800 1.04632400
C -2.27862900 0.42845300 2.14113800
H -3.49369600 0.68557500 0.42472200
H -2.74911400 1.19931800 2.73992200
H -1.82013400 -0.33168000 2.78671400
N -2.12033700 -0.96834400 0.34690300
C -4.33258100 -0.90467100 1.57968000
C -5.61337000 -0.36617200 1.46885000
C -4.16122500 -2.15345200 2.17962700
C -6.71532800 -1.07062500 1.94340900
H -5.75044500 0.59708100 0.98294400
C -5.26055000 -2.85788200 2.65600900
H -3.16564500 -2.58599100 2.23073900
C -6.53980700 -2.31784500 2.53671000
H -7.71089800 -0.64941600 1.84151000
H -5.12278000 -3.83224500 3.11475700
H -7.39923200 -2.86975200 2.90492400
S -2.26682000 -0.99595300 -1.28744800
C -3.94758000 -1.48448400 -1.55621100
C -4.86155300 -0.55178900 -2.02881800
C -4.35134600 -2.75770800 -1.15855600
C -6.20738600 -0.89904800 -2.08692900
H -4.51835200 0.43088900 -2.33460300
C -5.69640900 -3.08229200 -1.21507200
H -3.62182800 -3.47052800 -0.78894400
C -6.64479800 -2.15563800 -1.66599400
H -6.92987500 -0.17581700 -2.45474900

H -6.02337400 -4.06612000 -0.89055500
C -8.10711400 -2.51336900 -1.66419800
H -8.27802700 -3.48370500 -2.14097400
H -8.70723200 -1.76572900 -2.18942900
H -8.47903000 -2.58457600 -0.63533200
O -1.34259400 -2.01739600 -1.78040800
O -2.10653600 0.36386300 -1.83767700
C -1.38510900 3.26497700 -0.19366000
C -1.91169800 2.99357600 1.07233400
C -3.18383700 3.45303500 1.40992200
C -3.91872800 4.17841400 0.47651900
C -3.36407700 4.41503200 -0.79588100
C -2.10232900 3.96848200 -1.15564900
C 0.20518100 2.09193400 0.88924200
C -0.93528300 2.14446500 1.77063400
H -3.60365100 3.26262900 2.39452100
H -3.94959700 4.97025300 -1.52336700
H -1.70022000 4.14366200 -2.14666400
H 1.23899300 1.95369900 1.18539100
H -0.75741300 2.17316700 2.83912500
N -0.09235300 2.73434100 -0.26733600
C -5.28470200 4.71881900 0.81435100
H -5.25067900 5.80506900 0.95379000
H -5.67471300 4.27782500 1.73590700
H -6.00080400 4.51510800 0.01197300
C 0.83644000 2.94736900 -1.36992400
H 1.01621400 4.02470400 -1.46640200
H 1.78507400 2.49138600 -1.06219700
C 0.34263800 2.36776600 -2.66925100
C 0.58448200 2.93391900 -3.84814700
H -0.22865300 1.44441200 -2.59603000
H 0.24790800 2.47284400 -4.77091900
H 1.12624500 3.87360500 -3.93835700
C 5.16104400 -2.57395400 -1.96426400
C 4.71555800 -2.16799900 -0.71201500
C 4.77829700 0.11596900 -1.39831200
C 5.22739400 -0.31012200 -2.64747900
C 5.42111900 -1.66419700 -2.96174100
H 5.43663700 0.41949700 -3.42183700
H 5.76059400 -1.97937300 -3.94147400
O 5.23419100 -3.93153100 -2.00363600
O 4.47687800 -3.26692300 0.06453700
C 5.02276400 -4.36683800 -0.66546200
H 5.98063000 -4.65901400 -0.21833800

H 4.31018400 -5.19225800 -0.65993100
 C 4.47697200 0.11388700 3.26490200
 C 4.86888000 -0.22355900 1.97256800
 C 2.60417700 -0.41236900 1.29495500
 C 2.22699700 -0.07249700 2.59734700
 C 3.15076200 0.19701800 3.61521700
 H 1.16861400 -0.02663500 2.84871600
 H 2.84111900 0.45649500 4.62039500
 O 5.57008300 0.34755300 4.02861200
 O 6.22798800 -0.20590500 1.89538500
 C 6.69278300 -0.02842700 3.23206500
 H 7.10362000 -0.97325300 3.60540700
 H 7.43693400 0.76850800 3.25489100
 C 4.49465400 -0.84666100 -0.39416200
 C 3.97911900 -0.48771200 0.95385700
 P 4.44793600 1.88468200 -0.98944800
 C 6.11629900 2.42502700 -0.39772000
 H 6.37512700 1.87345900 0.51002000
 H 6.88960300 2.23922300 -1.15020700
 H 6.09345800 3.49373400 -0.16273300
 C 4.40108300 2.69158600 -2.65226600
 H 4.22789600 3.76196700 -2.49923900
 H 5.32803600 2.58187200 -3.22450200
 H 3.56536900 2.29813800 -3.24068600
 P 1.21256500 -0.83792100 0.18697900
 C 0.97680000 -2.63039400 0.43708100
 H 0.67404400 -2.82463700 1.46915900
 H 0.18679900 -2.96521600 -0.24013100
 H 1.91653100 -3.15412400 0.23598700
 C 1.61328000 -0.68734600 -1.58325500
 H 2.36473600 -1.41721600 -1.88854200
 H 0.68127200 -0.89310800 -2.11707700
 H 1.96697500 0.31351800 -1.83199400

TS4^s

ΔE = -5023.817486 au

ΔG = -5023.907957 au

Cu 0.48604300 0.52349400 1.52140100
 N 1.50786300 -0.82266500 0.69782600
 S 1.19813500 -2.43900800 0.68453900
 C 2.69608200 -3.11478000 0.00892600
 C 3.03214400 -2.81213300 -1.31017000
 C 3.51670900 -3.91420200 0.79478300
 C 4.21291600 -3.31182400 -1.83518400
 H 2.37646400 -2.18902500 -1.90925100

C 4.69625200 -4.41192500 0.24933600
 H 3.22662800 -4.14397600 1.81469900
 C 5.06271900 -4.11586300 -1.06455700
 H 4.48279900 -3.07903100 -2.86154400
 H 5.33929500 -5.04260600 0.85654900
 C 6.34931700 -4.63723300 -1.64913600
 H 6.17752600 -5.10895400 -2.62188800
 H 7.06400100 -3.82091100 -1.80365500
 H 6.81898200 -5.37430000 -0.99270900
 O 1.06033800 -2.94220900 2.05951000
 O 0.10720900 -2.67163500 -0.24933300
 C 1.21643900 3.47731300 0.15607900
 C 2.09995400 3.14326500 1.18831000
 C 3.45167200 3.46686700 1.08208300
 C 3.90987300 4.11818800 -0.05635800
 C 2.99636900 4.42263800 -1.08486700
 C 1.64922400 4.11028400 -1.00575800
 C -0.03837200 2.48512700 1.74398600
 C 1.31887400 2.43350100 2.20226500
 H 4.15002600 3.21346300 1.87500900
 H 3.36604700 4.92467500 -1.97461800
 H 0.96167500 4.37441700 -1.80116700
 H -0.90861000 2.54038800 2.38342500
 H 1.51682700 2.47825600 3.26587000
 N -0.07124600 3.08444300 0.51940000
 C 5.35797300 4.50876700 -0.19478700
 H 5.50004600 5.57402700 0.02016600
 H 5.98962900 3.93770800 0.49067000
 H 5.71826700 4.32473200 -1.21112200
 C 2.82215000 -0.43969700 1.21954000
 H 3.37643900 -1.27274800 1.68357700
 C -1.27519300 3.38039100 -0.23897800
 H -1.12869800 3.03398900 -1.26334100
 H -2.07887400 2.76887000 0.18077100
 C -1.63087700 4.84025200 -0.22240300
 C -1.86169600 5.54003100 -1.32797400
 H -1.71807100 5.30694200 0.75725100
 H -2.14919700 6.58566300 -1.29199500
 H -1.77936000 5.08740300 -2.31429200
 C 2.43895500 0.49139900 2.33332200
 H 3.18155300 1.23653300 2.59176000
 H 2.05148300 -0.02461400 3.21685600
 C 3.70902900 0.18046900 0.15512800
 C 5.07723300 0.30443500 0.39453300

C 3.17639600 0.64853400 -1.04432000
 C 5.90800200 0.89005600 -0.55484200
 H 5.50141300 -0.07622900 1.32161500
 C 4.00765900 1.23530000 -1.99338600
 H 2.11246300 0.53409100 -1.23068300
 C 5.37331400 1.35471000 -1.75423700
 H 6.97402500 0.97197300 -0.36558600
 H 3.58481100 1.59986600 -2.92496000
 H 6.02250700 1.80161100 -2.50126800
 C -3.51739600 -3.71507300 -0.18028100
 C -3.68632300 -2.40538300 -0.61478100
 C -2.40266800 -1.60187200 1.20393200
 C -2.24410900 -2.91957700 1.63503100
 C -2.80248000 -4.00640000 0.95423800
 H -1.62917400 -3.14120600 2.49709200
 H -2.66191400 -5.02352800 1.29826400
 O -4.17499600 -4.55954000 -1.01329500
 O -4.46182900 -2.39456500 -1.73451300
 C -4.61379800 -3.76121200 -2.10876400
 H -5.66618100 -3.96734900 -2.30939700
 H -3.98923400 -3.97170200 -2.98552500
 C -5.20576400 1.75481100 -0.71769200
 C -4.69876100 0.59205900 -0.15048500
 C -2.78415700 0.68008600 -1.56867400
 C -3.33055300 1.82541600 -2.15200300
 C -4.54457900 2.39485000 -1.73688600
 H -2.80300400 2.31802200 -2.96130900
 H -4.94390600 3.28865800 -2.20169500
 O -6.38092800 2.08366300 -0.11174600
 O -5.55110500 0.15570600 0.82256700
 C -6.72887600 0.94638600 0.66930200
 H -7.49380000 0.36005200 0.14508700
 H -7.07758700 1.27175100 1.64997800
 C -3.15001400 -1.31354200 0.03244200
 C -3.49694100 0.02637500 -0.52531900
 P -1.58008400 -0.28752300 2.14360500
 C -2.89409400 0.89711300 2.63964100
 H -3.81455100 0.35378900 2.86826200
 H -2.57585200 1.44303400 3.53403900
 H -3.11568000 1.61060800 1.84366400
 C -1.14115900 -1.03785100 3.75940400
 H -0.78201600 -0.24207300 4.42103000
 H -2.00753100 -1.51536300 4.22648900
 H -0.33976800 -1.76956100 3.62263300

P -1.06216300 0.12970400 -1.95537000
 C -0.66471500 1.12033100 -3.47282100
 H -0.50562000 2.17920700 -3.24376600
 H 0.28109500 0.73367000 -3.86670800
 H -1.42223100 1.03476300 -4.25948900
 C -1.31065500 -1.51347100 -2.77009200
 H -2.18917200 -1.51715800 -3.42211200
 H -0.41770000 -1.73277900 -3.36458700
 H -1.39024100 -2.29025800 -2.01013200

Int6^R

ΔE = -5023.889137 au

ΔG = -5023.983486 au

Cu -0.72852400 0.62691800 -0.12425600
 C -2.66024700 -1.60534500 -1.31576100
 H -1.85079400 -1.33585200 -2.01091300
 N -2.55300500 0.63929400 -0.45575900
 S -3.04932400 1.70446900 0.65294400
 C -3.89328900 3.00595200 -0.20514300
 C -5.07806400 3.50829100 0.31811800
 C -3.34987900 3.52409300 -1.38053200
 C -5.72302100 4.54689800 -0.34613500
 H -5.48839400 3.08546500 1.22843600
 C -4.00657700 4.55740400 -2.02963400
 H -2.43226200 3.10932500 -1.78626500
 C -5.20043100 5.08700000 -1.52172500
 H -6.64970800 4.94223900 0.05974300
 H -3.59092300 4.96290100 -2.94820900
 C -5.89283800 6.21920300 -2.23416300
 H -6.03468600 5.99061100 -3.29541600
 H -5.29749500 7.13715800 -2.17431400
 H -6.87293100 6.42690300 -1.79741800
 O -1.72361300 2.22447100 1.11213200
 O -3.96117700 1.17211400 1.65609500
 C -2.06570100 -1.62015300 2.28011200
 C -2.81649200 -2.13399600 1.22679500
 C -4.11137600 -2.56940400 1.45704900
 C -4.65142700 -2.46531100 2.74193700
 C -3.86522400 -1.93920700 3.77759800
 C -2.56123900 -1.50952400 3.57120800
 C -0.73644200 -1.36624600 0.45710300
 C -1.97256200 -2.11017000 -0.02047000
 H -4.70241700 -2.99089900 0.64970500
 H -4.29353500 -1.85818500 4.77232900
 H -1.97103200 -1.09059900 4.37794200

H 0.23823000 -1.56840400 0.01331700
 H -1.60237400 -3.12640000 -0.22871800
 N -0.78462100 -1.28688200 1.79813300
 C -6.07321600 -2.88487800 3.00966000
 H -6.43120000 -3.58991500 2.25431900
 H -6.73847700 -2.01371000 2.99517900
 H -6.17316500 -3.35764300 3.99110900
 C 0.34020600 -0.93078900 2.65554200
 H 0.48859700 -1.74571300 3.37283700
 H 1.23022500 -0.90887500 2.01489300
 C 0.13669900 0.37996300 3.37055400
 C 0.56781300 0.59707200 4.60970000
 H -0.37577300 1.16409500 2.81370100
 H 0.44295900 1.56311800 5.08761500
 H 1.05883300 -0.17986500 5.19258700
 C 6.01347700 2.42464700 0.14746400
 C 5.22941900 1.56839500 -0.61642600
 C 4.86926100 0.16379200 1.27759500
 C 5.66162200 1.03259400 2.02683900
 C 6.24422400 2.18731900 1.48187700
 H 5.84402100 0.82678100 3.07565600
 H 6.84978700 2.85722100 2.08094100
 O 6.42245900 3.47185600 -0.61993700
 O 5.11044000 2.06994800 -1.88305500
 C 6.07373200 3.12191800 -1.95411500
 H 6.96457800 2.76290000 -2.48430200
 H 5.63122000 3.98462200 -2.45246200
 C 3.59417500 -2.26788200 -2.52036300
 C 4.32422300 -1.44439000 -1.66737200
 C 2.37788400 -0.19198600 -1.15737900
 C 1.65809800 -1.02341200 -2.02116700
 C 2.24844400 -2.08056500 -2.72543700
 H 0.59650100 -0.83915900 -2.17295600
 H 1.67796700 -2.71413600 -3.39387200
 O 4.40532900 -3.21714900 -3.04395400
 O 5.61912700 -1.86327200 -1.63561600
 C 5.72922600 -2.86693600 -2.64324200
 H 6.27447200 -2.46269800 -3.50339800
 H 6.22628600 -3.74469600 -2.22874700
 C 4.62743200 0.44590400 -0.09231600
 C 3.76686700 -0.40008100 -0.96174400
 P 4.03507500 -1.31992600 1.99157200
 C 5.35427400 -2.59896100 1.76873200
 H 5.53575700 -2.75063900 0.70139500

H 6.29391000 -2.29560500 2.24151800
 H 5.02255300 -3.54654700 2.20441700
 C 4.15738100 -1.02267000 3.81272600
 H 3.69217400 -1.87258200 4.32280500
 H 5.18438700 -0.93311200 4.18190100
 H 3.59896400 -0.12068700 4.08444500
 P 1.39050800 1.16899400 -0.45053600
 C 1.52485700 2.48933000 -1.71299800
 H 1.07721100 2.15143500 -2.65111200
 H 0.99608000 3.38349700 -1.36901600
 H 2.57847100 2.72793200 -1.88977900
 C 2.13610000 1.95145200 1.02210700
 H 3.08011000 2.45308300 0.80309600
 H 1.40555200 2.69050200 1.36824000
 H 2.29114200 1.22992600 1.82550000
 C -3.46430200 -2.70929900 -1.98441100
 C -2.77868400 -3.77695900 -2.57250400
 C -4.85879200 -2.70696900 -2.03995900
 C -3.46098300 -4.82127900 -3.18339100
 H -1.68966900 -3.78732200 -2.55753100
 C -5.54761900 -3.75155100 -2.65400300
 H -5.42688400 -1.88929700 -1.60747000
 C -4.85350800 -4.81227600 -3.22367700
 H -2.90785400 -5.63966400 -3.63370700
 H -6.63252800 -3.72964000 -2.68829400
 H -5.39106100 -5.62508300 -3.70140300
 C -3.45560900 -0.32729000 -1.03639100
 H -3.87335100 0.04357000 -1.98181400
 H -4.28533600 -0.53732900 -0.35121800

Int6^S

ΔE = -5023.913598 au

ΔG = -5024.000789 au

Cu 0.63869600 0.33389000 0.17408400
 N 2.10665800 -0.88200900 0.63684500
 S 1.62617900 -2.33036400 1.15109400
 C 1.62604000 -3.40826700 -0.27455500
 C 2.21872100 -3.01919800 -1.46797500
 C 1.02536500 -4.66132700 -0.15950400
 C 2.20484600 -3.88891600 -2.55704100
 H 2.67052900 -2.03577200 -1.55405300
 C 1.01185000 -5.51426000 -1.25336900
 H 0.55904300 -4.95527700 0.77530000
 C 1.60217000 -5.14419800 -2.46865000
 H 2.67173800 -3.58367800 -3.49016700

H 0.53686200 -6.48765600 -1.16514200
 C 1.60523300 -6.09448900 -3.63765600
 H 2.36394200 -6.87312500 -3.49883600
 H 0.63872000 -6.59642800 -3.74499700
 H 1.82772900 -5.57837700 -4.57568900
 O 2.56177000 -2.91784600 2.11038600
 O 0.21606300 -2.21543600 1.55570700
 C 2.11214300 2.06296200 -1.70966000
 C 3.32834700 1.79876100 -1.09134600
 C 4.45738900 1.58794100 -1.86476400
 C 4.36487300 1.65413500 -3.26084800
 C 3.12871100 1.95211000 -3.84647100
 C 1.98219900 2.16292800 -3.08304700
 C 1.64054200 1.96941900 0.52498500
 C 3.14141500 1.86841700 0.40475900
 H 5.41569800 1.38209300 -1.39495400
 H 3.06019800 2.02683000 -4.92772500
 H 1.03644700 2.40468000 -3.55775000
 H 1.20298000 2.47959900 1.37507200
 H 3.51493000 2.85329400 0.72327000
 N 1.08640900 2.19952100 -0.71643200
 C 5.57865400 1.39519600 -4.11601300
 H 5.47537800 1.84915900 -5.10510600
 H 6.48476900 1.79519900 -3.65202400
 H 5.72987200 0.31903600 -4.25845200
 C -0.00503000 3.17735000 -0.91117400
 H -0.44982500 2.99862700 -1.88930800
 H -0.77423900 2.95205300 -0.16976900
 C 0.50913900 4.58115500 -0.78760600
 C 0.48177400 5.46026200 -1.78328400
 H 0.91956500 4.86118500 0.18207000
 H 0.85380300 6.47197300 -1.65840500
 H 0.07488200 5.20524600 -2.75900400
 C 3.81418500 0.79635700 1.28283600
 H 4.89750400 0.95431500 1.18509900
 C -4.55463900 -2.12602800 1.49593000
 C -4.32910600 -1.14134900 0.54104500
 C -2.40067300 -0.40997800 1.71509200
 C -2.62998200 -1.40793000 2.65968100
 C -3.71135800 -2.29441700 2.56761100
 H -1.94218600 -1.53173300 3.48684800
 H -3.87059000 -3.07507500 3.30159300
 O -5.64661500 -2.85461100 1.14758900
 O -5.26510000 -1.23901300 -0.44421900

C -6.22405600 -2.18073800 0.03395700
 H -7.12795000 -1.64982400 0.35629100
 H -6.44551000 -2.90361800 -0.75241600
 C -4.03092500 2.53838800 -1.81598400
 C -4.01131100 1.69838800 -0.70533700
 C -2.14611800 0.52333200 -1.58976000
 C -2.18967200 1.35732800 -2.70621500
 C -3.13565000 2.38581000 -2.84603600
 H -1.47643000 1.21686200 -3.51165300
 H -3.16624700 3.01956200 -3.72464300
 O -5.02764400 3.44887500 -1.67907400
 O -4.99727100 2.06472200 0.15615300
 C -5.78327100 3.02562800 -0.54591900
 H -6.71538200 2.55789700 -0.88365100
 H -5.97540100 3.88064000 0.10296300
 C -3.25923900 -0.27312000 0.59310700
 C -3.09539200 0.68084200 -0.54128600
 P -0.96223900 0.68852900 1.87463200
 C -1.72753000 2.33662500 2.18292000
 H -2.31604700 2.30922200 3.10482800
 H -0.95251100 3.10320000 2.29525600
 H -2.39186400 2.62381000 1.36434600
 C -0.20186300 0.34242500 3.49493200
 H 0.59010300 1.07975900 3.66149100
 H -0.93011600 0.41636300 4.30837600
 H 0.25522600 -0.64805300 3.47928400
 P -0.77005100 -0.66682200 -1.39191600
 C -0.07963600 -0.85714100 -3.07677200
 H 0.50032600 0.01779200 -3.37799500
 H 0.59935700 -1.71284100 -3.05056600
 H -0.86499900 -1.05531900 -3.81250500
 C -1.53208100 -2.30670300 -1.09587600
 H -2.49818200 -2.37368900 -1.60380700
 H -0.85810000 -3.07054700 -1.49313300
 H -1.64643800 -2.48374000 -0.02640400
 C 3.53045200 -0.59275400 0.70189200
 H 3.98272400 -0.62993300 -0.29918400
 H 4.04890300 -1.34623400 1.30011600
 C 3.44771400 0.97342900 2.75825400
 C 3.29910900 2.25049800 3.31578400
 C 3.30628300 -0.12658900 3.60935800
 C 3.00569100 2.42457900 4.66554800
 H 3.43395600 3.14202900 2.70866900
 C 3.02132900 0.04529800 4.96118100

H 3.39252300 -1.13773600 3.22984400
 C 2.86405000 1.31828100 5.49747300
 H 2.90261100 3.42795300 5.06809100
 H 2.91730400 -0.83095900 5.59360000
 H 2.64244300 1.44987000 6.55187400

Int7^R

$\Delta E = -5023.897102$ au

$\Delta G = -5023.990089$ au

Cu -0.70925300 -0.03992700 -0.06464300
 C -3.37200700 0.22480600 1.37257600
 C -2.46332100 0.75658500 2.48956700
 H -4.13073700 0.98976300 1.16078700
 H -3.07889200 1.06384700 3.34081700
 H -1.80256400 -0.03849600 2.85612700
 N -2.52837300 0.04061700 0.20880400
 C -4.08078900 -1.06461400 1.75706300
 C -5.46627800 -1.15751900 1.65038300
 C -3.35679500 -2.19943100 2.13086500
 C -6.12065200 -2.36024600 1.90586500
 H -6.03968900 -0.28771100 1.33937200
 C -4.00522200 -3.39928700 2.39515000
 H -2.27156000 -2.15282900 2.19572900
 C -5.39177900 -3.48357800 2.28028000
 H -7.20012100 -2.41849600 1.80500200
 H -3.43030600 -4.27321200 2.68721800
 H -5.89878200 -4.42231300 2.48151200
 S -3.07524300 0.20392200 -1.30245700
 C -4.20456600 -1.13237700 -1.56897400
 C -5.51659200 -0.85110400 -1.92623500
 C -3.79801000 -2.43646100 -1.28976700
 C -6.43657200 -1.89281100 -1.99156500
 H -5.80941000 0.17223500 -2.13368900
 C -4.72681300 -3.46001900 -1.35658100
 H -2.77378700 -2.63978300 -0.99494900
 C -6.06194800 -3.20292000 -1.69393600
 H -7.46584900 -1.67821100 -2.26454000
 H -4.42184600 -4.47615400 -1.12304200
 C -7.06910200 -4.32182000 -1.69135800
 H -6.67272500 -5.21580900 -2.18249600
 H -7.99418100 -4.03487600 -2.19799200
 H -7.32177400 -4.59889200 -0.66090000
 O -1.80261000 -0.04253600 -2.04958800
 O -3.79066800 1.44526900 -1.56404400
 C -1.53658200 3.39790500 0.17738100

C -2.32499100 3.01526700 1.25729300
 C -3.55234800 3.62276400 1.46440500
 C -3.98609600 4.61198900 0.57829100
 C -3.16127000 4.97702600 -0.49683000
 C -1.92709500 4.38192300 -0.72012400
 C -0.42290400 1.65198600 1.11018500
 C -1.60426800 1.93961300 2.02484500
 H -4.17809700 3.33429600 2.30530000
 H -3.50541100 5.74322800 -1.18532200
 H -1.31343400 4.66113800 -1.56856500
 H 0.52212000 1.29587900 1.51994100
 H -1.14080600 2.38052000 2.92310900
 N -0.35053200 2.63864500 0.19802800
 C -5.33248700 5.26547300 0.74938700
 H -5.26971700 6.34778100 0.60077000
 H -5.74581900 5.08281000 1.74493100
 H -6.04484800 4.87428800 0.01403900
 C 0.79445800 2.88824500 -0.66999300
 H 1.13182200 3.91667300 -0.50047000
 H 1.60273100 2.23122500 -0.32726100
 C 0.48179600 2.66054300 -2.12667300
 C 0.99826800 3.40782200 -3.09788400
 H -0.18489300 1.83002900 -2.35917300
 H 0.78970500 3.19849900 -4.14189800
 H 1.64708800 4.25557000 -2.88652800
 C 5.60988000 -2.06381100 -2.16185700
 C 4.95331100 -1.94315400 -0.94300400
 C 4.97750100 0.43440000 -1.12972400
 C 5.63829600 0.29351400 -2.34952600
 C 5.96081500 -0.95735600 -2.89853500
 H 5.91976000 1.17558200 -2.91377200
 H 6.46402800 -1.04872500 -3.85391100
 O 5.76962900 -3.38168600 -2.46354200
 O 4.66538500 -3.18939200 -0.45760700
 C 5.41760600 -4.08420200 -1.27785700
 H 6.32840700 -4.38553800 -0.74538100
 H 4.80049400 -4.94540800 -1.53469500
 C 3.91360000 -0.65096200 3.31852900
 C 4.53720700 -0.64384700 2.07365200
 C 2.43648600 -0.75306000 0.98330000
 C 1.82327500 -0.76515200 2.23996200
 C 2.54632600 -0.71632200 3.43905500
 H 0.73887900 -0.83700100 2.30070500
 H 2.05801900 -0.73139600 4.40587300

O 4.84569100 -0.57340500 4.29743300
O 5.88491800 -0.56020900 2.24550300
C 6.10948700 -0.69803800 3.64741400
H 6.52965400 -1.68882900 3.85311900
H 6.77354900 0.09699000 3.98881000
C 4.60060200 -0.72579400 -0.40367400
C 3.84999600 -0.68906300 0.88022500
P 4.47661100 2.06789900 -0.43133900
C 5.96798200 2.48223000 0.58456100
H 6.08415500 1.74120300 1.37971700
H 6.88000000 2.48613500 -0.02127600
H 5.83678400 3.46756300 1.04253000
C 4.71998900 3.21615600 -1.85969800
H 4.46602000 4.22722500 -1.52499100
H 5.74653400 3.23839100 -2.24039000
H 4.03941000 2.95114900 -2.67522200
P 1.27564600 -0.94507300 -0.40878900
C 1.11358000 -2.76060200 -0.58682700
H 0.67068800 -3.18468500 0.31806300
H 0.46620300 -2.98961900 -1.43896500
H 2.10014500 -3.20934600 -0.74099000
C 1.95993900 -0.44407500 -2.02590000
H 2.78605100 -1.07935900 -2.35009200
H 1.13496200 -0.53183700 -2.74103900
H 2.28850700 0.59634400 -2.01541000

Int7^S

$\Delta E = -5023.917076$ au

$\Delta G = -5024.004877$ au

Cu 0.15366100 0.33988600 0.72395400
N 1.81662200 -0.65981300 0.94750900
S 1.56677000 -2.20630400 1.35844600
C 2.66871500 -3.15885700 0.33314600
C 2.80861100 -2.84027300 -1.01551800
C 3.34203800 -4.24426300 0.87979900
C 3.62566900 -3.61991100 -1.81971400
H 2.30064200 -1.97046200 -1.41765900
C 4.15600000 -5.01950500 0.06014200
H 3.22799500 -4.47067800 1.93430900
C 4.31022800 -4.72260200 -1.29527600
H 3.74323200 -3.36853100 -2.87044900
H 4.68062200 -5.87093900 0.48448100
C 5.21305700 -5.54917600 -2.17381500
H 4.77531100 -5.69604500 -3.16597600
H 6.18019500 -5.05189800 -2.31160500

H 5.40466400 -6.53264700 -1.73654900
O 1.93025600 -2.49602400 2.74884700
O 0.18398500 -2.51381000 0.95911400
C 1.25151300 3.07115100 0.11102900
C 2.41133800 2.91454700 0.85346000
C 3.59801300 3.46390800 0.39537100
C 3.62047200 4.14036300 -0.82541200
C 2.43163100 4.26118000 -1.55999500
C 1.22742900 3.73552700 -1.10421500
C 0.63510800 1.80200200 1.90974200
C 2.10367200 2.11595100 2.09747000
H 4.51712900 3.33630500 0.95874100
H 2.45192900 4.78348500 -2.51227400
H 0.31355300 3.85537400 -1.67792700
H -0.01443000 1.75784000 2.77733300
H 2.14305600 2.78515200 2.97147500
N 0.15033400 2.44442400 0.78794300
C 4.90138100 4.73413900 -1.35009700
H 4.94167100 5.81256200 -1.15881500
H 5.77177700 4.27351400 -0.87615500
H 4.99043600 4.58568500 -2.43030500
C 3.12973900 -0.15001900 1.32707600
H 3.70180200 -0.95588200 1.80631500
C -1.16731500 3.12101600 0.76744400
H -1.41059300 3.33759700 -0.27238400
H -1.90852200 2.40331100 1.11901900
C -1.14767300 4.36847200 1.59989200
C -1.30525100 5.58609000 1.09243700
H -0.99426500 4.23402000 2.67010200
H -1.29679000 6.47021600 1.72173000
H -1.45895900 5.74421000 0.02770200
C 3.01486800 0.92347100 2.42608200
H 4.01001200 1.31176500 2.66771800
H 2.62782100 0.43533700 3.32716100
C 3.95211600 0.31403000 0.13052700
C 5.32415400 0.52436300 0.27839400
C 3.37368400 0.56013500 -1.11040700
C 6.09134800 0.99209300 -0.78425500
H 5.80261500 0.31653900 1.23338900
C 4.13179500 1.02815500 -2.17756900
H 2.31072700 0.39666600 -1.22469200
C 5.49622100 1.24956800 -2.01736700
H 7.15844400 1.14426000 -0.65266100
H 3.65517800 1.22315900 -3.13443000

H 6.09530300 1.61109000 -2.84754100
 C -4.41099800 -3.35274500 -0.21225100
 C -4.29474800 -2.04098800 -0.65778300
 C -2.81601000 -1.54155600 1.13141800
 C -2.93061900 -2.86165400 1.56052200
 C -3.72759800 -3.80106100 0.89208100
 H -2.37072900 -3.19584200 2.42522700
 H -3.79770900 -4.82897100 1.22673600
 O -5.22100600 -4.04784600 -1.05117100
 O -5.01876700 -1.88118800 -1.79993200
 C -5.75531100 -3.09267100 -1.96204500
 H -6.81079200 -2.91226700 -1.72683300
 H -5.63217400 -3.45734000 -2.98327000
 C -4.54948000 2.28240300 -1.34961800
 C -4.49221100 1.07782800 -0.65320500
 C -2.29511000 0.67842300 -1.46137400
 C -2.37222400 1.87737700 -2.16978200
 C -3.50510300 2.70673500 -2.13383400
 H -1.53611900 2.19750600 -2.78250300
 H -3.55676600 3.62991900 -2.69908900
 O -5.74105000 2.88683800 -1.11572900
 O -5.64948000 0.89972700 0.03774400
 C -6.52808900 1.93170700 -0.40640700
 H -7.27990100 1.50664500 -1.08125100
 H -6.98956100 2.41088500 0.45769100
 C -3.49608400 -1.10432200 -0.03591700
 C -3.39665800 0.24091100 -0.67246700
 P -1.75292300 -0.36921000 2.02457600
 C -2.98130600 0.80986300 2.73951800
 H -3.65471600 0.27733000 3.41763500
 H -2.47491100 1.59848400 3.30774400
 H -3.58836200 1.27336000 1.95820900
 C -1.19204100 -1.21122300 3.54725100
 H -0.64607200 -0.48024900 4.15291800
 H -2.03622100 -1.58654600 4.13356300
 H -0.50236600 -2.02165500 3.30861000
 P -0.69716100 -0.20370700 -1.36149400
 C 0.25297800 0.39965700 -2.81031700
 H 0.65079200 1.40449200 -2.64299200
 H 1.10331300 -0.27265000 -2.95687200
 H -0.35352300 0.38646900 -3.72114100
 C -0.97865800 -1.95487500 -1.80524000
 H -1.62347400 -2.02949600 -2.68578500
 H -0.00587400 -2.40575800 -2.02011700

H -1.40454500 -2.50344700 -0.96723900

Int8^R

ΔE = -5023.902469 au

ΔG = -5023.995167 au

C -4.71284200 -2.42619600 1.70158600
 C -4.88470200 -1.29462600 0.91201800
 C -2.64603900 -0.62247100 1.33226800
 C -2.48758300 -1.76319500 2.11894500
 C -3.51668500 -2.69360400 2.32055000
 H -1.53798800 -1.95501200 2.60694200
 H -3.37619100 -3.57813000 2.92988500
 O -5.85910200 -3.15281400 1.71423500
 O -6.14555800 -1.28246300 0.40261700
 C -6.82732800 -2.37363300 1.01664500
 H -7.56640500 -1.98858800 1.72868400
 H -7.29909200 -2.98608300 0.24591100
 C -5.41451500 2.92043700 -0.34491400
 C -5.05578700 1.76927500 0.34844700
 C -3.71997200 1.04621700 -1.48111200
 C -4.08596500 2.20609000 -2.16269700
 C -4.93773200 3.17429500 -1.60707400
 H -3.71631000 2.37972700 -3.16698500
 H -5.21055300 4.07234400 -2.14870200
 O -6.22034600 3.68878100 0.43788100
 O -5.61575100 1.79729500 1.59117600
 C -6.55629600 2.86663200 1.55069800
 H -7.56565600 2.45845700 1.41295800
 H -6.48218300 3.44890700 2.46960300
 C -3.88482100 -0.37376700 0.67866200
 C -4.20303300 0.81544300 -0.16310600
 Cu -0.64621600 -0.32600000 -0.98164500
 P -1.18091500 0.42026500 0.99844900
 C -1.72292300 2.16870900 1.18183000
 H -2.13334900 2.54878900 0.24453800
 H -2.47637700 2.27257200 1.96830300
 H -0.84651900 2.76742200 1.44897900
 C -0.14677200 0.23880700 2.51075200
 H 0.60835100 1.03089000 2.49609300
 H -0.73403100 0.33148800 3.42960800
 H 0.37930200 -0.71922500 2.51493600
 P -2.51587500 -0.13020500 -2.19407300
 C -2.26452500 0.42295000 -3.91858200
 H -1.75470700 1.38981900 -3.94639700
 H -1.60629800 -0.31329200 -4.39029500

H -3.19529300 0.48407600 -4.49140100
 C -3.43494700 -1.69848100 -2.40080100
 H -4.40029000 -1.53994900 -2.89006300
 H -2.81603500 -2.37400800 -2.99698700
 H -3.58477400 -2.16892800 -1.42752900
 N 0.89955800 -1.09647000 -1.93888100
 S 0.70727900 -2.67456200 -1.77977500
 C 1.77417600 -3.15411600 -0.41478000
 C 3.04012300 -3.67681700 -0.65942900
 C 1.36298200 -2.90165400 0.89348400
 C 3.90356600 -3.92401700 0.40921700
 H 3.33209600 -3.90972600 -1.67879100
 C 2.23043700 -3.14941100 1.95024500
 H 0.35488300 -2.53711900 1.06859800
 C 3.51436500 -3.66568000 1.72677800
 H 4.88508100 -4.34887300 0.21484100
 H 1.90017300 -2.96743100 2.97057000
 O -0.66950700 -2.82219000 -1.27643700
 O 1.16190000 -3.45274700 -2.92503300
 C 3.47986800 1.57006100 1.61943000
 C 2.50759700 1.75536300 0.64495600
 C 1.80837900 2.95082000 0.58849300
 C 2.08566500 3.94751500 1.52787600
 C 3.07401100 3.72002500 2.50169600
 C 3.79281100 2.53205700 2.56707600
 C 3.42114100 -0.34797300 0.46363100
 C 2.40761500 0.50910200 -0.16979600
 H 1.04714700 3.10609100 -0.17197100
 H 3.28664400 4.50133200 3.22543400
 H 4.56369100 2.38208900 3.31421900
 H 3.69618300 -1.35904600 0.18322900
 H 1.40995500 0.03029200 -0.05798000
 N 4.00850600 0.25553200 1.45277500
 C 5.12662900 -0.29099400 2.23013800
 H 4.87924800 -0.20553300 3.29216900
 H 5.18584300 -1.35372600 1.97641900
 C 6.40049400 0.43397400 1.89283300
 C 7.23170500 0.91136600 2.81234900
 H 6.61893200 0.53108000 0.83037200
 H 8.16099800 1.39689300 2.53388300
 H 7.02628200 0.82162100 3.87691300
 C 1.34279500 5.25823200 1.50416500
 H 0.55889200 5.26062300 0.74245300
 H 0.87595100 5.46240300 2.47318200

H 2.02429900 6.08791500 1.28831000
 C 2.17549500 -0.61934900 -2.43107300
 H 2.14468300 -0.40768000 -3.50759500
 H 2.96630300 -1.37187900 -2.29726500
 C 3.94764700 1.20917300 -2.04426100
 C 5.07068000 0.37479300 -2.06491300
 C 4.13195400 2.57521200 -2.26319200
 C 6.34158100 0.89548600 -2.29278800
 H 4.96226900 -0.69785600 -1.92222900
 C 5.40066700 3.10033600 -2.48940300
 H 3.27085900 3.23875700 -2.25134200
 C 6.51081200 2.26174700 -2.50099600
 H 7.19856900 0.22894900 -2.32212300
 H 5.52131700 4.16550700 -2.65973800
 H 7.50058600 2.66854300 -2.68204900
 C 2.56832900 0.67736000 -1.70606700
 H 1.82226000 1.43566200 -1.97713400
 C 4.42548700 -3.98611200 2.88505400
 H 5.47834400 -3.98130500 2.58626800
 H 4.29602400 -3.27578400 3.70830200
 H 4.20571600 -4.98358300 3.28159600

TS5^R

$\Delta E = -5023.888035$ au

$\Delta G = -5023.979500$ au

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 C -4.84492500 -1.44683400 0.53261400
 C -2.59216200 -1.07277400 1.17563500
 C -2.56824500 -2.34556800 1.74530000
 C -3.68244100 -3.19588600 1.72666400
 H -1.66780800 -2.70850500 2.22826200
 H -3.65363700 -4.18351000 2.17031400
 O -6.01217600 -3.31694400 0.95274600
 O -6.06184000 -1.23484300 -0.02893500
 C -6.86661300 -2.35652300 0.33353500
 H -7.63421600 -2.03937300 1.04701600
 H -7.30920400 -2.79079000 -0.56470700
 C -4.88555200 2.93684900 -0.19855500
 C -4.70774400 1.68156900 0.37642200
 C -3.23898600 1.05658100 -1.38730100
 C -3.42694400 2.31651800 -1.95225700
 C -4.25284700 3.28918900 -1.36535000
 H -2.93536000 2.56891900 -2.88498300
 H -4.38993900 4.26560200 -1.81443100
 O -5.70500600 3.68229900 0.58574300

O -5.40067000 1.61423200 1.54470100
 C -6.20290700 2.79411800 1.58272300
 H -7.24395700 2.53623300 1.35608900
 H -6.11101100 3.26211500 2.56362800
 C -3.75844600 -0.59920700 0.51339500
 C -3.88791800 0.71798200 -0.16722900
 Cu -0.18501500 -0.41144500 -0.78407400
 P -1.06195400 -0.08896900 1.18320100
 C -1.47417900 1.63310300 1.62988000
 H -1.77422900 2.20117200 0.74778400
 H -2.28686100 1.64822900 2.36191100
 H -0.58177300 2.09792600 2.05714400
 C -0.09844400 -0.68718000 2.61359200
 H 0.67302800 0.05988600 2.81759900
 H -0.72861300 -0.80365300 3.49984300
 H 0.39697200 -1.63286200 2.38235600
 P -2.05613800 -0.13235900 -2.10520200
 C -1.52888600 0.56709700 -3.70547500
 H -0.98277500 1.50340600 -3.56091100
 H -0.83347300 -0.15392300 -4.14558800
 H -2.36518000 0.73170600 -4.39119100
 C -3.00104500 -1.62424100 -2.56980700
 H -3.91556000 -1.36254500 -3.10908500
 H -2.35421300 -2.24613000 -3.19287100
 H -3.24717200 -2.20048800 -1.67637600
 N 1.13940100 -0.85496800 -2.06825700
 S 1.09264900 -2.46147300 -2.20725500
 C 2.22188600 -3.11558900 -0.98551500
 C 3.56194300 -3.31488300 -1.30599200
 C 1.76397000 -3.34258300 0.30997000
 C 4.45017800 -3.71251100 -0.31079200
 H 3.89871200 -3.17881300 -2.32879300
 C 2.65871800 -3.75331200 1.29037400
 H 0.70632800 -3.22761500 0.52831400
 C 4.01521800 -3.93810800 0.99916600
 H 5.49602400 -3.86973100 -0.56036700
 H 2.29821700 -3.95049600 2.29720600
 O -0.26020400 -2.80308100 -1.72743100
 O 1.55696400 -2.92169800 -3.50568100
 C 2.70002800 1.40619700 2.17206500
 C 2.22830700 1.89733900 0.94336600
 C 1.61257600 3.15222400 0.88660100
 C 1.45132400 3.88740500 2.05346400
 C 1.90938400 3.35051000 3.27796800

C 2.53880100 2.11983900 3.36176900
 C 3.18377700 -0.12124000 0.61579200
 C 2.50309800 0.88937100 -0.05809500
 H 1.27133700 3.55355100 -0.06444400
 H 1.77696100 3.93415100 4.18490400
 H 2.91074800 1.74224700 4.30791100
 H 3.57931900 -1.05230100 0.23064100
 H 1.06273600 -0.05744400 0.00208800
 N 3.27290300 0.16172200 1.93996000
 C 3.85771800 -0.70446800 2.95432100
 H 3.11087400 -0.89876500 3.73377400
 H 4.06876500 -1.65717800 2.45971400
 C 5.11054000 -0.12507500 3.55114400
 C 5.32217800 -0.02084300 4.85866600
 H 5.86679800 0.19784700 2.83808400
 H 6.25178700 0.37452000 5.25469300
 H 4.57618200 -0.33603000 5.58552200
 C 0.81119600 5.25264500 2.03021900
 H 0.34693000 5.45918800 1.06192000
 H 0.04064900 5.34480500 2.80291100
 H 1.55460600 6.03558800 2.21666100
 C 2.37267700 -0.14769900 -2.36742600
 H 2.41896500 0.11027600 -3.43132100
 H 3.26832400 -0.74888400 -2.14848900
 C 3.57263900 2.03899400 -2.01501200
 C 4.90446900 1.72032100 -1.74474200
 C 3.29368400 3.18411400 -2.76002200
 C 5.93444500 2.52984000 -2.21004500
 H 5.13997100 0.83601800 -1.15729100
 C 4.32134000 4.00001400 -3.22451400
 H 2.25982400 3.44166500 -2.98057200
 C 5.64520000 3.67406600 -2.94986800
 H 6.96613700 2.27062700 -1.99281400
 H 4.08651700 4.89087700 -3.79890100
 H 6.44900800 4.30918800 -3.30849700
 C 2.43728200 1.14600500 -1.54436000
 H 1.49906900 1.68903200 -1.73749500
 C 4.97929300 -4.40953200 2.05764600
 H 5.94457300 -3.90058700 1.97521800
 H 4.58662900 -4.24106000 3.06480700
 H 5.16708400 -5.48387600 1.95279100

Int9^R

ΔE = -5023.890176 au

ΔG = -5023.981702 au

C	-4.59585700	-3.01755000	0.06597500	H	-2.58552800	-1.69467700	-2.23596000
C	-4.64057400	-1.65221900	-0.20980000	N	1.21231800	-0.89515800	-1.79333200
C	-2.57529400	-1.34545900	0.91275200	S	1.12791600	-2.50916700	-1.82603000
C	-2.53250200	-2.71519400	1.16841800	C	2.32834400	-3.10235400	-0.64645000
C	-3.54724600	-3.58421100	0.74978300	C	3.66245400	-3.24093600	-1.01897100
H	-1.68836200	-3.14569000	1.69386800	C	1.94308300	-3.31442300	0.67499700
H	-3.50344800	-4.64814500	0.94654800	C	4.61541000	-3.54164100	-0.04938100
O	-5.69191300	-3.61984800	-0.44396700	H	3.94810000	-3.13400700	-2.06048100
O	-5.76585500	-1.36451800	-0.90946800	C	2.90107500	-3.62605800	1.63037900
C	-6.48224500	-2.59327200	-1.04211400	H	0.88845500	-3.27128600	0.92602300
H	-7.43762600	-2.51656100	-0.51545600	C	4.25543800	-3.72427300	1.28870300
H	-6.62652400	-2.81616000	-2.10191600	H	5.65577100	-3.65102500	-0.34256200
C	-4.95370800	2.76779900	0.20638500	H	2.59627500	-3.81158900	2.65769000
C	-4.77252700	1.40690400	0.44327400	C	5.29418300	-4.01628000	2.34106900
C	-2.96108500	1.35937000	-1.09502500	H	5.59002800	-3.09941500	2.86635100
C	-3.15030400	2.72156100	-1.32041200	H	4.91479100	-4.71558500	3.09195400
C	-4.15116300	3.45915000	-0.66757500	H	6.19771600	-4.44706600	1.90195300
H	-2.51808700	3.24896600	-2.02544000	O	-0.20136600	-2.78804700	-1.24518300
H	-4.28753300	4.51854200	-0.84824100	O	1.48955000	-3.04711400	-3.12796300
O	-5.96504200	3.23077900	0.98005900	C	2.17359200	1.55820300	2.14122200
O	-5.65727900	0.98912400	1.38546700	C	1.90653900	1.99687100	0.82492500
C	-6.55875100	2.07923300	1.57599300	C	1.12691400	3.14955400	0.62949400
H	-7.50929100	1.85945600	1.07687100	C	0.65647800	3.85916600	1.72229600
H	-6.69650700	2.25284100	2.64355600	C	0.97534400	3.41288300	3.02759900
C	-3.64945600	-0.77601000	0.17245400	C	1.72389600	2.27147300	3.25894300
C	-3.78583900	0.66559400	-0.16653800	C	3.16816500	0.14628200	0.72608100
Cu	-0.01683100	-0.34531400	-0.44967000	C	2.55991700	1.08279100	-0.06982500
P	-1.14065300	-0.35021100	1.39110600	H	0.92401000	3.50561800	-0.37862600
C	-1.63196700	1.29428500	1.99088600	H	0.62340000	3.99286600	3.87684300
H	-1.83942700	1.98629000	1.17585200	H	1.98060700	1.96554000	4.26827200
H	-2.51803000	1.19376800	2.62514900	H	3.73675700	-0.73325400	0.45010800
H	-0.79961100	1.69073100	2.57846400	H	0.79455100	-0.80793500	0.65459700
C	-0.43801400	-1.11208100	2.88757300	N	2.92691700	0.40730100	2.05538600
H	0.35281400	-0.44250000	3.23821900	C	3.50531300	-0.32234100	3.17060400
H	-1.20281700	-1.21318100	3.66277800	H	2.71976900	-0.55618500	3.89978500
H	0.00777800	-2.08545900	2.67963500	H	3.85981200	-1.27551400	2.76452100
P	-1.56958700	0.47679600	-1.86251200	C	4.62736100	0.42747700	3.83544300
C	-0.83790500	1.61861200	-3.07898200	C	4.69341100	0.65377800	5.14297300
H	-0.41097600	2.49772400	-2.59004900	H	5.41314800	0.78254600	3.17075600
H	-0.03207300	1.07276000	-3.57823000	H	5.53134900	1.18040000	5.58793600
H	-1.57127400	1.93463000	-3.82636800	H	3.91579500	0.31107700	5.82298400
C	-2.24807600	-0.87823800	-2.87552800	C	-0.18918100	5.09560200	1.54535900
H	-3.07109800	-0.51752500	-3.49854900	H	0.27771600	5.96762900	2.01543100
H	-1.44124900	-1.26332400	-3.50496200	H	-0.33846600	5.32730600	0.48682000

H -1.17714000 4.96969700 2.00418300
 C 2.44374800 -0.23867600 -2.20768500
 H 2.47467700 -0.13896400 -3.29906100
 H 3.33882000 -0.80869200 -1.91890400
 C 3.71563300 1.91688400 -2.18310600
 C 4.97022300 1.97448100 -1.57940300
 C 3.53962200 2.53296900 -3.42467900
 C 6.02696100 2.63171900 -2.20447500
 H 5.12081300 1.51448400 -0.60733200
 C 4.59169900 3.18901100 -4.05287400
 H 2.56427100 2.49578100 -3.90707900
 C 5.84205100 3.23951500 -3.44189600
 H 6.99746800 2.67200000 -1.71922100
 H 4.43600100 3.66343400 -5.01695600
 H 6.66663000 3.75240200 -3.92700300
 C 2.54592700 1.15805200 -1.56973500
 H 1.63688700 1.70324000 -1.85743700

TS7^R

$\Delta E = -5023.885690$ au

$\Delta G = -5023.979537$ au

C -5.02219600 -2.79635300 0.76998900
 C -4.92581300 -1.50013200 0.27098900
 C -2.69675800 -1.33368600 1.06966600
 C -2.80120100 -2.63738000 1.55315500
 C -3.96881800 -3.40065900 1.41170200
 H -1.96190200 -3.09482500 2.06446000
 H -4.03914300 -4.41220600 1.79271700
 O -6.24737700 -3.30122000 0.49139700
 O -6.08865300 -1.16251300 -0.34369600
 C -6.99728500 -2.23100900 -0.07981500
 H -7.75639800 -1.89596900 0.63539100
 H -7.44821500 -2.56355700 -1.01615400
 C -4.69641600 2.90544500 -0.06739200
 C -4.59236500 1.60078800 0.40663600
 C -3.10649500 1.05135900 -1.36492000
 C -3.21960900 2.36064100 -1.82914500
 C -4.01736500 3.32045800 -1.18644300
 H -2.68872900 2.66547300 -2.72384600
 H -4.09872700 4.33489600 -1.55805400
 O -5.50563300 3.62267900 0.75175500
 O -5.32331400 1.47152500 1.54596600
 C -6.06380300 2.68541200 1.66888600
 H -7.11292200 2.50075000 1.41119300
 H -5.96338200 3.06954900 2.68498000

C -3.78507000 -0.73313400 0.37665800
 C -3.80545300 0.64336000 -0.19429200
 Cu -0.18826600 -0.59322700 -0.75308900
 P -1.10896300 -0.45559000 1.22976000
 C -1.46177700 1.22268400 1.85806500
 H -1.65825200 1.91248600 1.03590900
 H -2.32638300 1.20107000 2.52800500
 H -0.58420200 1.57864800 2.40374900
 C -0.22294300 -1.24795100 2.61439300
 H 0.64304900 -0.61698200 2.83228900
 H -0.85113900 -1.32333100 3.50676100
 H 0.14139300 -2.23862400 2.33468000
 P -1.93814700 -0.11238300 -2.13623800
 C -1.29250000 0.70186900 -3.63568700
 H -0.72286600 1.59727000 -3.37114300
 H -0.59969400 -0.00377700 -4.10492700
 H -2.07757600 0.96425400 -4.35070200
 C -2.87744200 -1.54041100 -2.77535600
 H -3.70147200 -1.22632300 -3.42178000
 H -2.18071500 -2.17084500 -3.33487300
 H -3.26657300 -2.13011800 -1.94317900
 N 1.33519800 -0.82374600 -1.87376300
 S 1.39985700 -2.43118900 -2.14927100
 C 2.60843200 -3.07214400 -1.01503200
 C 3.95442500 -3.08050500 -1.37155200
 C 2.20646300 -3.44567500 0.26483100
 C 4.90526800 -3.43116500 -0.41816100
 H 4.24918100 -2.83482900 -2.38676700
 C 3.16709100 -3.80745000 1.19985500
 H 1.14809100 -3.47810000 0.50259900
 C 4.53052200 -3.78761000 0.88106300
 H 5.95618500 -3.44042200 -0.69300800
 H 2.85638500 -4.12025600 2.19357500
 C 5.56766600 -4.12657600 1.92006300
 H 5.85817800 -3.23215600 2.48586000
 H 5.18968100 -4.86023600 2.63762600
 H 6.47380900 -4.53252400 1.46282900
 O 0.07769400 -2.87384300 -1.67221600
 O 1.84746500 -2.70667200 -3.50165500
 C 2.37953900 1.37118200 2.31304300
 C 2.03326200 1.95136000 1.07656300
 C 1.33377800 3.16738500 1.05119500
 C 0.98141100 3.77972300 2.24303200
 C 1.33869400 3.16721600 3.46840200

C 2.03509500 1.97295800 3.52812100
 C 3.16320400 0.04667800 0.69455200
 C 2.53964000 1.08861900 0.04604700
 H 1.08682100 3.63531000 0.10113000
 H 1.06728700 3.66385700 4.39628500
 H 2.32665900 1.54019900 4.47954900
 H 3.68068200 -0.81342300 0.28862800
 H 1.17935500 -0.58897100 -0.22033600
 N 3.05892800 0.19681000 2.05586200
 C 3.66618300 -0.67166600 3.05017500
 H 2.92237400 -0.91762700 3.81777000
 H 3.91639300 -1.60442000 2.53484200
 C 4.88906400 -0.06298900 3.68025300
 C 5.07285500 0.03579300 4.99240600
 H 5.64506700 0.29910400 2.98533300
 H 5.97817500 0.46389800 5.41024000
 H 4.32580200 -0.31438300 5.70204800
 C 0.21858300 5.08067500 2.25920900
 H 0.75288700 5.84604700 2.83205200
 H 0.06623200 5.46713800 1.24765400
 H -0.76649500 4.95608700 2.72398500
 C 2.45373900 0.03346900 -2.23793000
 H 2.39864800 0.26912600 -3.30570800
 H 3.42143500 -0.45785300 -2.06079100
 C 3.41970200 2.33065600 -1.97920300
 C 4.69013600 2.47406700 -1.42398400
 C 3.08274100 3.09571800 -3.09797900
 C 5.60546400 3.36636100 -1.97540700
 H 4.96095400 1.89705200 -0.54447200
 C 3.99482300 3.98662100 -3.65236200
 H 2.09345500 2.99277900 -3.54070800
 C 5.26099900 4.12492300 -3.08964500
 H 6.58870400 3.47345400 -1.52756500
 H 3.71597000 4.57651000 -4.52018300
 H 5.97367600 4.82447000 -3.51505500
 C 2.40589900 1.33737800 -1.42805600
 H 1.40837000 1.77564000 -1.59442300

Int10^R

ΔE = -5023.938498 au

ΔG = -5024.034840 au

C -4.82173800 -2.55261900 1.96340500
 C -4.92251400 -1.59816500 0.95669000
 C -2.84714000 -0.64101100 1.61291200
 C -2.75783600 -1.60733000 2.61434000

C -3.74155100 -2.58827700 2.80999200
 H -1.90305600 -1.61766900 3.28037600
 H -3.65460200 -3.33478400 3.59023200
 O -5.89739800 -3.37974700 1.91628400
 O -6.06242400 -1.80755200 0.24397300
 C -6.78043600 -2.81772700 0.94932500
 H -7.64024500 -2.36623000 1.45797300
 H -7.09442800 -3.59362200 0.24927600
 C -5.49217100 2.23696300 -1.18336200
 C -5.16767300 1.30080900 -0.20638600
 C -3.55482500 0.31449100 -1.64692600
 C -3.88985600 1.25804500 -2.61662000
 C -4.86556300 2.24508700 -2.40488200
 H -3.39707600 1.24073300 -3.58199100
 H -5.11544700 2.97295000 -3.16746500
 O -6.44523900 3.07942700 -0.70617600
 O -5.90525900 1.53885800 0.91257400
 C -6.86980400 2.51739600 0.53202000
 H -7.84589200 2.03542000 0.39877000
 H -6.91071100 3.29944700 1.29104500
 C -3.96139800 -0.63729200 0.72666800
 C -4.19996600 0.33530700 -0.37867100
 Cu -0.59653800 -0.31641400 -0.49151800
 P -1.44803700 0.50928000 1.34351400
 C -2.14979800 2.20032600 1.32269400
 H -2.58652000 2.41620500 0.34562500
 H -2.91380100 2.33199000 2.09449400
 H -1.32892900 2.90025800 1.50092100
 C -0.49306200 0.48354000 2.90380200
 H 0.26584500 1.26942300 2.83844700
 H -1.11893800 0.66454100 3.78325200
 H 0.02293800 -0.47373600 3.01599000
 P -2.16215400 -0.83604400 -1.92196600
 C -1.77596300 -0.73159000 -3.70532200
 H -1.35874400 0.24821800 -3.95315100
 H -1.00733600 -1.48558300 -3.90283700
 H -2.64231500 -0.93072200 -4.34374800
 C -2.81633500 -2.53458200 -1.73975400
 H -3.76620400 -2.66030700 -2.26721000
 H -2.07006200 -3.22239700 -2.14907900
 H -2.95143100 -2.77485100 -0.68358500
 N 1.30789800 -0.90767500 -0.74160000
 S 1.23449200 -2.61821400 -0.83946600
 C 2.90778600 -3.09812900 -0.52944400

C 3.78761900 -3.26836200 -1.59607100
 C 3.34382300 -3.18074100 0.79186000
 C 5.12774500 -3.51533800 -1.32561700
 H 3.42216700 -3.22339700 -2.61690500
 C 4.68648300 -3.43337700 1.03935200
 H 2.63702700 -3.07320900 1.60851400
 C 5.59885400 -3.59428300 -0.01023000
 H 5.81950600 -3.65826100 -2.15062500
 H 5.03079900 -3.52349800 2.06591200
 C 7.05864900 -3.83863300 0.26625500
 H 7.62272500 -2.90030600 0.20946400
 H 7.21282400 -4.26061700 1.26272800
 H 7.49098100 -4.52544800 -0.46663300
 O 0.40453200 -2.99576300 0.29160100
 O 0.85911000 -2.93257200 -2.20493300
 C 3.22948400 1.79280000 2.16912600
 C 2.45957400 2.14761800 1.04270300
 C 1.49416500 3.16237500 1.15600500
 C 1.30556700 3.79631400 2.37311500
 C 2.08808300 3.40642100 3.48775500
 C 3.04995300 2.41823400 3.40848600
 C 3.86969200 0.49592500 0.47012900
 C 2.88107300 1.30409300 -0.04035400
 H 0.91227000 3.46388100 0.28737400
 H 1.93232600 3.91447900 4.43571100
 H 3.65468200 2.15446500 4.26951000
 H 4.44354000 -0.28784300 -0.01098000
 H 1.78986000 -0.68329900 0.13631900
 N 4.08514400 0.77759000 1.79715400
 C 5.06862400 0.13263600 2.65103400
 H 4.57091300 -0.24747600 3.55126000
 H 5.44229200 -0.73580100 2.09619700
 C 6.20139200 1.04957000 3.02510100
 C 6.59930300 1.25747700 4.27554800
 H 6.69908800 1.54696000 2.19437100
 H 7.43311900 1.91256300 4.50620700
 H 6.10957100 0.77482300 5.11908600
 C 0.28727000 4.89803600 2.53483000
 H 0.75628200 5.81795700 2.89962200
 H -0.20530700 5.13081700 1.58596200
 H -0.48729000 4.62117300 3.25978300
 C 2.04867100 -0.22221000 -1.82386900
 H 1.46899200 -0.29677100 -2.74532700
 H 3.02371200 -0.69700900 -1.99060400

C 2.98701500 1.97795000 -2.52299400
 C 4.35735300 2.22591400 -2.48028700
 C 2.26359400 2.37156600 -3.65158200
 C 4.99366800 2.85322000 -3.54854400
 H 4.92714800 1.94528600 -1.59962700
 C 2.89596900 2.99625700 -4.72010200
 H 1.19007500 2.19242000 -3.68985700
 C 4.26687700 3.23750000 -4.67064700
 H 6.06084000 3.04687800 -3.49899200
 H 2.31955500 3.30114500 -5.58814000
 H 4.76356200 3.72897400 -5.50126500
 C 2.25632900 1.24458700 -1.40766300
 H 1.25648300 1.69535200 -1.32249800

Int11^R

$\Delta E = -1702.884721$ au

$\Delta G = -1702.947086$ au

N -1.18219800 -2.04073300 -1.41179000
 S -2.82915300 -2.20016000 -1.28656600
 C -3.34928400 -0.78161900 -0.33305300
 C -3.32933400 -0.83252300 1.05767800
 C -3.65552400 0.40489000 -0.99681100
 C -3.57931500 0.32814600 1.78528500
 H -3.13206300 -1.77391800 1.55991400
 C -3.91973700 1.54881600 -0.25593900
 H -3.69550600 0.41974200 -2.08114200
 C -3.86326200 1.53532900 1.14348900
 H -3.55722300 0.29048900 2.87100800
 H -4.17139300 2.47278600 -0.77097900
 C -4.09040100 2.80394400 1.92476600
 H -3.21210700 3.45947600 1.86723300
 H -4.94322300 3.36423900 1.52897900
 H -4.28008100 2.59619600 2.98136300
 O -3.35893400 -2.03302000 -2.62726800
 O -3.07186500 -3.38630000 -0.48594300
 C 1.63008000 2.05838400 -0.68440500
 C 2.09120700 0.73090400 -0.79108600
 C 3.42801300 0.49247200 -1.14139200
 C 4.27614800 1.56098700 -1.38315200
 C 3.78054900 2.88038600 -1.26770300
 C 2.47043800 3.15051100 -0.91886300
 C -0.06888300 0.69684100 -0.18593900
 C 0.98439200 -0.13158100 -0.46863400
 H 3.79976000 -0.52732400 -1.20824100
 H 4.45967600 3.70925000 -1.45276000

H 2.11685100 4.17175700 -0.81432100
 H -1.07951300 0.46230200 0.11958700
 H -0.93564500 -1.21308700 -1.94773600
 N 0.29817400 2.01581800 -0.33086600
 C -0.55728600 3.15348200 -0.06811900
 H -0.39857500 3.91027000 -0.84489900
 H -1.58985200 2.80097600 -0.16598400
 C -0.33943700 3.74527800 1.29909300
 C -0.15295900 5.04082600 1.52995400
 H -0.35045300 3.03178300 2.12229100
 H -0.01719700 5.42915700 2.53458000
 H -0.12739500 5.76557400 0.71868600
 C 5.72273500 1.33919800 -1.75168100
 H 6.39582500 1.73931000 -0.98431100
 H 5.94372700 0.27394000 -1.86564600
 H 5.97360700 1.83624800 -2.69577400
 C -0.35620400 -2.26114200 -0.22143000
 H -0.26136700 -3.33762200 -0.06671300
 H -0.81079500 -1.83579900 0.68560200
 C 1.96903900 -2.16083000 0.66417100
 C 2.12822600 -1.49795900 1.88091500
 C 2.65333000 -3.36010900 0.45646600
 C 2.95509400 -2.02364500 2.86936400
 H 1.61410400 -0.55484800 2.04367700
 C 3.48084500 -3.88816000 1.44182400
 H 2.53582600 -3.88428200 -0.48963700
 C 3.63351000 -3.21977200 2.65343000
 H 3.07381500 -1.49418100 3.81029600
 H 4.00788500 -4.82062300 1.26229900
 H 4.28308600 -3.62579700 3.42318700
 C 1.03209900 -1.63508100 -0.41675200
 H 1.41474600 -2.00232000 -1.38006500