

**The Origin of Enantioselectivity in the L-Threonine-derived
Phosphine–Sulfonamide Catalyzed aza-Morita–Baylis–Hilman Reaction:
Effects of the Intramolecular Hydrogen Bonding**

Supporting information

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Complete citation for Gaussian 09:

Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Cartesian coordinates and energies of optimized intermediates and transition states.

Imaginary frequencies are in parenthesis.

Catalyst

Etotal:-2516.643089
G:-2516.724645
E(RmPW1PW91):-2517.079978
P -2.59099700 -1.77456000 0.00089500
C -1.34049400 -0.71960100 -0.93447300
H -1.64075000 0.33057500 -0.97841500
H -1.32620200 -1.10900200 -1.95926600
C 0.07212500 -0.77530700 -0.33228100
H 0.02805800 -0.42029800 0.70356600
N 0.57509800 -2.17104100 -0.36632800
H -0.17047000 -2.85703300 -0.48735100
C -4.09694400 -1.59292600 -1.05611900
C -6.44362200 -1.52538200 -2.61351500
C -4.31821200 -0.55711400 -1.97811300
C -5.07259700 -2.59725700 -0.93648400
C -6.23891800 -2.56064800 -1.69995600
C -5.47942400 -0.52629800 -2.75275500
H -3.58624900 0.23504400 -2.09791800
H -4.90957200 -3.41763700 -0.24249800
H -6.98160900 -3.34551200 -1.58939400
H -5.63107300 0.28169400 -3.46303100
H -7.34662600 -1.49960700 -3.21653700
C -2.96167500 -0.71410200 1.47478100
C -3.41746200 0.79774400 3.80189800
C -4.00631900 0.22175000 1.52573900
C -2.15679400 -0.89111800 2.61358700
C -2.37664000 -0.13063900 3.76304400
C -4.23373400 0.96872700 2.68219400
H -4.65009700 0.36302500 0.66344300
H -1.35089200 -1.61977000 2.60527900

H -1.73925800 -0.27475200 4.63058300
H -5.05067400 1.68469300 2.70809400
H -3.59658100 1.38012500 4.70121800
O 0.67022700 1.49329800 -0.81432100
Si 1.63108000 2.87530800 -0.93874400
C 1.54685200 3.55426800 -2.70366900
H 1.96313000 2.82815200 -3.40998000
H 2.13049600 4.47597800 -2.80271900
H 0.52297700 3.77218700 -3.01766500
C 3.43500800 2.40256500 -0.60492800
H 3.55806200 1.86502100 0.34017900
H 4.06925000 3.29494000 -0.56337400
H 3.82987600 1.76459300 -1.40306100
C 1.03817500 4.15598100 0.37470900
C 1.62351600 3.75185400 1.75099900
H 2.71648400 3.81490300 1.75134200
H 1.35091400 2.73499900 2.04766200
H 1.26190500 4.43237300 2.53387700
C 1.67191700 5.52250700 0.00286200
H 1.27708700 5.93812600 -0.92833300
H 2.76101600 5.45528800 -0.10563100
H 1.47602400 6.25465200 0.79755800
C -0.51516200 4.34933100 0.50469400
H -0.63367200 5.26720700 1.10490200
C -1.23907900 4.59534100 -0.83112900
H -1.28720800 3.67850700 -1.42934600
H -0.76448000 5.37222800 -1.43752600
H -2.27090200 4.91279700 -0.64554300
C -1.24053400 3.22710700 1.26669500
H -1.11188800 2.26165800 0.77165000
H -2.31396000 3.43899200 1.31362000
H -0.88876400 3.12650300 2.29619600
C 1.07657000 0.14784500 -1.07003800
C 1.19491700 -0.13844300 -2.56673200
H 0.28609900 0.16017600 -3.09648400
H 1.37111300 -1.20457600 -2.73407200
H 2.03286600 0.41492700 -3.00021300
S 1.50428500 -2.76040500 0.92390600
O 1.27076100 -4.20830600 0.90993400
O 1.26903100 -1.96465600 2.13892600
C 3.19705800 -2.45291900 0.41664600
C 5.86208800 -2.03738800 -0.32733000
C 3.71627200 -3.12972200 -0.68994300
C 3.99008000 -1.58270000 1.16242500
C 5.31704100 -1.37912100 0.78186700
C 5.04052800 -2.91307500 -1.05557600
H 3.09074200 -3.81506200 -1.25158000
H 3.56731200 -1.08056600 2.02534300
H 5.93794300 -0.69969900 1.35938600
H 5.44736300 -3.43415500 -1.91810700
H 2.05620200 -0.02872300 -0.60604200
C 7.30648800 -1.83693100 -0.71674300
H 7.43415300 -1.85433300 -1.80323100
H 7.93690700 -2.63384100 -0.30358300
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TS I

(156.75i)

Etot:-3168.292280
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O -2.11934500 0.39660100 1.20484000
O -4.07992000 1.49822900 0.77255100
C -4.76043100 0.32891100 0.50202600
H -5.63514800 1.22218900 -1.22113200
C -5.59697300 0.33788800 -0.59228200
C -5.47077400 -1.90558100 1.07535600
C -6.40862100 -0.78552200 -0.89436300
C -4.69775900 -0.80425900 1.35543300
C -6.34280400 -1.93882900 -0.04634600
C -7.28372100 -0.81096000 -2.01432900
H -4.03166900 -0.78998000 2.20728400
H -7.09642000 -3.93758700 0.29419200
H -5.42306300 -2.77553200 1.72541500
C -8.05293200 -1.92027500 -2.28487600
H -7.33548600 0.06407400 -2.65731100
H -8.71621900 -1.92458900 -3.14519500
C -7.98697200 -3.06004600 -1.44671500
H -8.59951700 -3.92864500 -1.67018900
C -7.15026900 -3.06567800 -0.35308700
C -0.95127400 2.98175400 1.97061800
H -0.47374100 2.15990700 2.50027100
H -0.78439000 3.93114300 2.47924800
P 0.38527900 3.22622400 0.35197100
C 0.19031900 1.76991600 -0.78096300
H 0.47180200 2.11800600 -1.77764500
H -0.88068000 1.54258600 -0.409775600
C 0.98775100 0.49723600 -0.40975700
H 2.05650500 0.72210300 -0.40375800
N 0.61258000 0.03239100 0.92813700
H -0.38987200 0.12646100 1.18185200
C -0.31099000 4.62916700 -0.58401400
C -1.51287100 6.84018800 -1.83388800
C -1.48864900 4.47150900 -1.33645700
C 0.24448200 5.91437100 -0.45365200
C -0.35002500 7.00836600 -1.07874600
C -2.08051300 5.57282800 -1.95745600
H -1.95207300 3.49711100 -1.43435700
H 1.14765900 6.05896600 0.12999200
H 0.09582800 7.99306000 -0.97500400
H -2.98774100 5.43528600 -2.53795600
H -1.97403800 7.69385800 -2.32149000
C 2.19046900 3.55708300 0.46725300
C 4.94430300 4.01477900 0.68328600
C 2.93852200 3.93436800 -0.66337500
C 2.83592100 3.40842400 1.70289000
C 4.20956700 3.63868300 1.80588500
C 4.30828600 4.16072500 -0.55312700
H 2.45021700 4.06409600 -1.62474900
H 2.27923400 3.07827700 2.57315600
H 4.70215200 3.51153600 2.76459700
H 4.87950900 4.45069800 -1.43011400
H 6.01278900 4.19043500 0.76638300

O 1.65439600 -1.71625900 -1.20850600
Si 3.25676500 -2.06615900 -1.61978500
C 4.01620100 -2.85433700 -0.08681900
H 3.96587700 -2.13865400 0.73844600
H 5.07040700 -3.09573700 -0.26034300
H 3.51240000 -3.77177200 0.22672300
C 4.24710800 -0.48604200 -1.96190400
H 3.86662200 0.11443600 -2.79287200
H 5.28822500 -0.73821000 -2.19466700
H 4.26092300 0.13577200 -1.06063400
C 3.38236600 -3.25292100 -3.15426200
C 3.31233700 -2.44082900 -4.47089700
H 4.14841600 -1.73801700 -4.54521000
H 2.39198200 -1.86295400 -4.58043100
H 3.37963600 -3.11374900 -5.33731400
C 4.80646500 -3.87186400 -3.11670700
H 4.97356100 -4.51880200 -2.25252100
H 5.58471900 -3.10000600 -3.10097800
H 4.97547100 -4.47619600 -4.01845000
C 2.33825700 -4.42585200 -3.21345500
H 2.68682600 -5.06836700 -4.03992300
C 2.28899900 -5.31067000 -1.95472100
H 1.83686800 -4.77679400 -1.11206500
H 3.27526700 -5.66350200 -1.64247600
H 1.67113500 -6.19510200 -2.14518000
C 0.90182200 -3.99970200 -3.56405800
H 0.47571900 -3.37213400 -2.77649000
H 0.26448200 -4.88542900 -3.66307900
H 0.84447200 -3.45613300 -4.51127800
C 0.73991700 -0.64976700 -1.43963900
C 0.72348900 -0.19669200 -2.90262100
H 1.63692600 0.33637200 -3.18464900
H -0.13065700 0.45546000 -3.10329000
H 0.62032700 -1.06985000 -3.54881900
S 1.66155800 -0.08853000 2.19511000
O 1.33677300 0.89727800 3.24791600
O 3.02547700 -0.07409300 1.63793200
C 1.27433700 -1.69475900 2.89307500
C 0.77656400 -4.20284000 4.02734200
C 1.26494800 -1.83183600 4.28149300
C 1.04048300 -2.79030400 2.05903700
C 0.79281900 -4.03364000 2.63485500
C 1.01837300 -3.08570500 4.83737900
H 1.43486600 -0.96405700 4.90831200
H 1.04699300 -2.66266000 0.98173700
H 0.60494300 -4.88881600 1.99083000
H 1.00822000 -3.19582700 5.91845900
H -0.25213000 -1.05720800 -1.20446300
C 0.47257000 -5.55024400 4.63614700
H 0.89655000 -5.64157500 5.64004400
H 0.86879900 -6.36492800 4.02274300
H -0.60993300 -5.70598500 4.72250400

It I

Etot:-3168.293556
G: -3168.389022
E(RmPW1PW91):-3168.808113
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O -2.08954500 0.29646500 1.02993000
O -4.13027100 1.29439500 0.67457100
C -4.75729800 0.09456400 0.44291500
H -5.81963700 0.95756500 -1.18796700
C -5.68131200 0.06786600 -0.58094000
C -5.29457300 -2.18907100 1.02434400
C -6.45181300 -1.09419600 -0.83856600
C -4.56462400 -1.04971800 1.26468100
C -6.25254100 -2.25596000 -0.02320900
C -7.41395900 -1.15262100 -1.88383700
H -3.83267400 -1.01128000 2.05939300
H -6.86256100 -4.29959400 0.33621900
H -5.14566800 -3.06492000 1.65107100
C -8.14008300 -2.29958500 -2.11387800
H -7.56710800 -0.27163000 -2.50221000
H -8.87090500 -2.32769600 -2.91730300
C -7.94181500 -3.44737200 -1.30798000
H -8.52135600 -4.34601800 -1.49862300
C -7.01827500 -3.42197700 -0.28666000
C -1.00001300 2.93835700 1.79851400
H -0.52784500 2.13767400 2.37376800
H -0.92443000 3.86647200 2.37420900
P 0.13164800 3.22413300 0.30020100
C 0.10334600 1.76068600 -0.82321700
H 0.39271700 2.13972500 -1.80634900
H -0.94541600 1.45069600 -0.87544600
C 0.98645600 0.55207800 -0.42471300
H 2.03602900 0.85457100 -0.39558300
N 0.60554500 0.07465200 0.90455200
H -0.41779100 0.11102000 1.12227600
C -0.58253500 4.59897700 -0.65600900
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C -1.76738300 4.39667800 -1.38677900
C -0.02105100 5.88489500 -0.59678500
C -0.62496800 6.94610900 -1.26930200
C -2.36564600 5.46548000 -2.05476800
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H 0.88713500 6.05799500 -0.02984900
H -0.18035300 7.93535500 -1.21981400
H -3.28021100 5.30033100 -2.61582600
H -2.26377900 7.56559300 -2.52466000
C 1.87480700 3.64854100 0.63419400
C 4.55458100 4.26046100 1.15204500
C 2.74509900 3.97242900 -0.42294100
C 2.36017800 3.62708800 1.94921500
C 3.69822800 3.93479100 2.20182800
C 4.07848600 4.27672200 -0.16216300
H 2.38081600 3.99957800 -1.44593600
H 1.71668500 3.32908400 2.76838600
H 4.06922200 3.90458300 3.22112800
H 4.74557800 4.52471300 -0.98211100
H 5.59563600 4.49473200 1.35303000
O 1.82272900 -1.60696100 -1.22022200
Si 3.45200000 -1.84957000 -1.60140100
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H 4.11066800 -1.87630000 0.77099700

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H 5.40167000 -0.38843800 -2.13188800
H 4.28474100 0.42138200 -1.03577900
C 3.68136100 -3.02562100 -3.13085800
C 3.59988100 -2.21671300 -4.44885200
H 4.40578500 -1.47818800 -4.50850400
H 2.65738200 -1.67893700 -4.57434700
H 3.71175600 -2.88488900 -5.31424800
C 5.13482600 -3.56770900 -3.05676600
H 5.31294000 -4.20685700 -2.18900300
H 5.87044700 -2.75590100 -3.02023000
H 5.35899000 -4.16033200 -3.95424900
C 2.70454000 -4.25407000 -3.21496700
H 3.11262300 -4.87976400 -4.02687200
C 2.66651400 -5.13375100 -1.95214400
H 2.16560000 -4.61785400 -1.12609100
H 3.66077400 -5.43382300 -1.61120000
H 2.09984200 -6.04966100 -2.15220300
C 1.25782000 -3.91048200 -3.61075800
H 0.77002500 -3.31227200 -2.83629900
H 0.67658400 -4.83135900 -3.73162200
H 1.19846100 -3.36838700 -4.55871700
C 0.84104900 -0.60553900 -1.46431200
C 0.82241000 -0.14659800 -2.92602100
H 1.69938600 0.45488000 -3.18602100
H -0.07424300 0.43972300 -3.14414000
H 0.79979600 -1.02109300 -3.57789700
S 1.63291800 -0.02813900 2.18813500
O 1.22820900 0.90636200 3.25977200
O 3.00628100 0.08162200 1.66361500
C 1.32879000 -1.67356100 2.83529100
C 0.95219000 -4.23800100 3.88728700
C 1.26906600 -1.84708500 4.21740700
C 1.20325700 -2.76020900 1.96602500
C 1.01543400 -4.03122800 2.50028200
C 1.08259100 -3.12957200 4.73247400
H 1.35275100 -0.98676700 4.87129300
H 1.24546900 -2.60247600 0.89356200
H 0.91101800 -4.87934300 1.82834500
H 1.03180500 -3.26849500 5.80900100
H -0.12494100 -1.08026700 -1.24900500
C 0.72496900 -5.62188900 4.44581300
H -0.30611100 -5.95209600 4.27154500
H 0.90514200 -5.65404900 5.52351100
H 1.38244000 -6.35646700 3.96929400

TS IIR

(242.80i)

Ettotal:-4387.912059

G: -4388.029987

E(RmPW1PW91):-4388.539103

C 0.90067200 1.82802400 -0.39318500

O -0.19501900 1.67092100 0.16129100

O 1.32953300 3.08446000 -0.77773900

C 0.52910400 4.20686900 -0.61047200

H 1.00826500 4.83475600 -2.58706000
C 0.48057400 5.08206900 -1.67113000
C -0.83519800 5.67250900 0.72808400
C -0.23785200 6.30095700 -1.56696900
C -0.12790000 4.49884100 0.61190100
C -0.91766500 6.60360000 -0.34219900
C -0.30822000 7.23324700 -2.63753300
H -0.06304100 3.79752300 1.43215500
H -2.15221900 8.04867200 0.69165900
H -1.34176200 5.90410100 1.66147400
C -1.01659100 8.40617600 -2.50557400
H 0.21010000 7.00434100 -3.56510100
H -1.06108600 9.10976100 -3.33189300
C -1.68934000 8.70492400 -1.29532900
H -2.24379900 9.63425600 -1.20369800
C -1.63920600 7.82254200 -0.23974600
C 1.49782500 -0.61062300 -0.54544000
H 0.95748100 -0.80578600 0.38428300
H 2.39871200 -1.23928600 -0.52663200
P 0.46280600 -1.24095700 -1.92429100
C -1.24610500 -0.53896400 -1.92972200
H -1.65375500 -0.81998200 -2.90284300
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H -2.39713500 -2.06531200 -0.89581900
N -1.75706900 -0.65790700 0.50017800
H -1.15905800 0.17888500 0.57801000
C 1.22628400 -0.75559700 -3.50558000
C 2.50775100 -0.06454600 -5.89474500
C 0.50064400 -0.16245100 -4.55067300
C 2.60244600 -0.99807400 -3.66266300
C 3.23367800 -0.64703100 -4.85490900
C 1.14224800 0.17708400 -5.74175400
H -0.55718800 0.05175500 -4.44939300
H 3.20007200 -1.42859800 -2.86206500
H 4.29982700 -0.82119100 -4.95596900
H 0.57398900 0.63793500 -6.54387700
H 3.00607700 0.20873300 -6.82008900
C 0.33793800 -3.05763600 -1.90657900
C 0.08744200 -5.83996000 -1.89709500
C 0.10104400 -3.74887100 -3.10713100
C 0.45767600 -3.76764300 -0.70207700
C 0.32930400 -5.15720900 -0.70578800
C -0.02605700 -5.13554700 -3.09815200
H 0.03331100 -3.20876600 -4.04643600
H 0.63679000 -3.25269300 0.23536000
H 0.41822000 -5.70073000 0.22912800
H -0.20496700 -5.66573500 -4.02849600
H -0.00870800 -6.92160200 -1.89290000
O -4.61233100 -0.85799800 -0.20188500
Si -5.65387600 -2.19297700 -0.22690700
C -5.69756400 -2.82579800 1.54609400
H -4.68569800 -3.11604100 1.84023300
H -6.34028300 -3.70901100 1.62540100
H -6.06141900 -2.08412400 2.26098200
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C -7.44132100 -1.74279000 -0.84926500
C -7.50932900 -1.78602300 -2.39598600
H -7.28785100 -2.78978200 -2.77289400
H -6.81908200 -1.09650900 -2.88691600
H -8.52165100 -1.53091100 -2.73936300
C -8.37219100 -2.88602500 -0.35863400
H -8.45194100 -2.94189400 0.72914500
H -8.03239100 -3.86657100 -0.71147200
H -9.38549000 -2.73839000 -0.75623500
C -8.03442500 -0.37862400 -0.34203200
H -9.09357700 -0.40389500 -0.64929800
C -8.01962000 -0.19570300 1.18636100
H -7.00001600 -0.04275200 1.55582300
H -8.45047400 -1.04447400 1.72339800
H -8.59943300 0.69225200 1.46109200
C -7.42114400 0.87805700 -0.98414500
H -6.37171700 0.99322600 -0.69853100
H -7.95582400 1.77017600 -0.63973300
H -7.48617700 0.86734500 -2.07555500
C -3.63753600 -0.29140500 -1.06683800
C -4.09885100 -0.25159300 -2.52769800
H -4.12019800 -1.24542000 -2.98617800
H -3.45455700 0.39409400 -3.13077900
H -5.10373900 0.16988000 -2.57405100
S -1.58416900 -1.77309700 1.71321500
O -0.15884600 -1.96060800 2.05102200
O -2.35622600 -2.96189900 1.31321800
C -2.32637400 -0.96672400 3.13165300
C -3.48993400 0.19051700 5.39609300
C -1.69763700 -1.09778300 4.36993500
C -3.52724300 -0.26475300 3.00197900
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H 2.52551300 1.07191700 -1.53156300
C 3.48252000 0.98912200 0.66185600
H 3.89524200 1.83223000 0.10435400
C 2.84883000 1.35928100 1.95853300
C 1.71814400 2.10305200 4.42086600
C 2.68044600 2.71196900 2.28812500
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C 1.88533000 0.75353500 4.10064300
C 2.12126700 3.08230700 3.51161100
H 2.99875000 3.47560300 1.58405300
H 2.60073300 -0.66295200 2.63714200
H 1.58017300 -0.01369900 4.80652300
H 2.00845100 4.13496500 3.75575100
H 1.28378900 2.38932900 5.37466800

N 4.13602800 -0.19279900 0.64337500
S 5.13495400 -0.46463000 -0.62959500
O 5.35734100 0.73415500 -1.47480900
O 4.68562700 -1.70393000 -1.32215500
C 6.69614500 -0.87187300 0.14902900
C 9.11572100 -1.48277500 1.38714200
C 7.72054500 0.07944000 0.17678800
C 6.87993800 -2.12446800 0.73006400
C 8.08841100 -2.43585200 1.35342200
C 8.92671000 -0.22607800 0.79198200
H 7.56272800 1.04303600 -0.29467900
H 6.08385100 -2.85930300 0.68487600
H 8.21899000 -3.41429700 1.79951900
H 9.74101500 0.49002500 0.82387400
O 10.33450100 -1.68202900 1.96680300
C 10.58668300 -2.93051000 2.59240700
H 9.88642600 -3.11956800 3.41587600
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TS IIS

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Etotal:-4387.906878

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C 0.91114500 3.72424100 -1.18645400
H 1.21397800 3.82661300 -3.29138600
C 0.80610400 4.32588300 -2.41794900
C -0.19970600 5.57314300 -0.12031900
C 0.18078300 5.59370600 -2.54537100
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C -0.34141300 6.23075100 -1.37258100
C 0.04973600 6.25194400 -3.79806400
H 0.52939600 3.85680300 0.94163700
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H -0.58296600 6.06085300 0.77216200
C -0.56959000 7.47810500 -3.88928500
H 0.44891000 5.76942600 -4.68653500
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P 0.30344900 -1.79837900 -1.52883900
C -1.30993900 -0.92545700 -1.74381100
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C -2.39372000 -1.06669600 -0.64529200
H -2.62821200 -2.12324700 -0.49255500
N -1.92129700 -0.50740600 0.62407900
H -1.23544200 0.26222900 0.55736400
C 1.18037800 -1.69846000 -3.11902500
C 2.64234000 -1.56899500 -5.50114700

C 0.52243300 -1.47548600 -4.34027300
C 2.57635300 -1.85828400 -3.10259900
C 3.30125300 -1.78144700 -4.29037900
C 1.25403000 -1.41997200 -5.52579200
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H 3.12220300 -2.01554500 -2.17882700
H 4.38146400 -1.86299200 -4.24191500
H 0.73873200 -1.24660900 -6.46556400
H 3.20905700 -1.50753100 -6.42543500
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C -0.08450600 -4.01332600 0.15221000
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H -0.41316400 -5.70329300 1.43279200
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H -0.81730600 -7.28282000 -0.44343600
O -4.75431500 -0.65295300 -0.16858100
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C -6.04138000 -2.18668800 1.85758400
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H -6.06820400 -4.28337500 -0.61582600
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H 2.65213600 0.33637500 -1.36437000
C 3.39985000 0.48358900 0.89207200
N 4.61962500 0.52816700 0.29941800
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O 5.31071000 -0.68704400 -1.83540500
O 4.38360100 -2.06218700 0.05909200
C 6.80691800 -1.02804900 0.30415500
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C 7.82980600 -0.18009700 -0.13876800
C 7.06506300 -2.00081900 1.26440800
C 8.34876900 -2.13587800 1.79900900
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H 8.53640200 -2.90121900 2.54227900
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Etotal:-4387.915405

G: -4388.032782

E(RmPW1PW91):-4388.565536

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C -0.02967000 6.28864800 -1.56065500
C 0.05712400 4.60750100 0.71519300
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H -1.17430300 6.06325600 1.67253500
C -0.80610600 8.33404200 -2.62166500
H 0.44194300 6.88438300 -3.58805300
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C -1.49574500 8.69352000 -1.43786100
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C 1.50177900 -0.58439600 -0.36482900
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C 2.72809200 1.29811400 2.10750800
C 1.70648200 1.94208100 4.65110900
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C 2.31146000 0.28880300 2.98608100
C 1.80032400 0.60954800 4.24329800
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H 2.09192700 3.99348500 4.10613600
H 1.31671100 2.18852000 5.63500500
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S 5.00279000 -0.55191000 -0.44414100
O 5.27300100 0.63134400 -1.31535100
O 4.55415300 -1.76662500 -1.20885500
C 6.55103600 -1.06474000 0.31907900
C 9.03184200 -1.76037300 1.39333100
C 6.97417200 -0.49521800 1.52413400
C 7.36288400 -1.98468300 -0.33938000
C 8.60583400 -2.33740900 0.19081700
C 8.20730100 -0.84120000 2.05956400
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H 7.01095500 -2.43683500 -1.25996300
H 9.22180600 -3.05897800 -0.33247500
H 8.55396200 -0.41909500 2.99717100
O 10.22502800 -2.03266900 2.00343600
C 11.10087100 -2.95567000 1.37922700
H 10.64776500 -3.95191000 1.29248200
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G: -4388.028837
E(RmPW1PW91):-4388.562238
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H -0.67876600 3.67153600 -2.43245900
C -0.90359900 4.17243800 -1.49556800
C -1.39752200 5.46679400 0.94206800
C -1.90496100 5.17840200 -1.44487800
C -0.43013600 4.49278200 0.87242400
C -2.16250700 5.83632200 -0.19799700
C -2.66022600 5.55348800 -2.58803800
H 0.16771000 4.22256100 1.73384800
H -3.35817500 7.33783200 0.80012500
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H -2.46065900 5.05715400 -3.53425400
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H -4.64789100 7.94865500 -1.21881400
C -3.16609600 6.83982900 -0.14658400
C 1.58476800 -0.60996000 -0.07702400
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H 2.51707700 -1.19146800 -0.10271000
P 0.67868300 -1.21792100 -1.53293300
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H -0.88766200 0.57415600 -1.64322300
C -2.14806800 -0.97416900 -0.73806200
H -2.37416800 -2.02389300 -0.93106400
N -1.78032300 -0.87036800 0.67019400
H -1.23106400 -0.05749800 0.96235700
C 1.61764100 -0.70730400 -3.01248100
C 3.15840600 -0.03076700 -5.24546100
C 1.01121800 -0.13732700 -4.14188900
C 3.00667400 -0.93619600 -3.00247300

C 3.76450100 -0.59557700 -4.12216500
C 1.78259800 0.19953800 -5.25387700
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H 3.50763300 -1.36082600 -2.13224400
H 4.83547400 -0.77099600 -4.10710100
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H 3.75725700 0.23298600 -6.11207200
C 0.59894500 -3.02975400 -1.48355600
C 0.52112600 -5.81942700 -1.49500300
C -0.42290900 -3.70426000 -2.17232200
C 1.59596300 -3.75749200 -0.81231100
C 1.54550800 -5.15148000 -0.82486400
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H 2.31451900 -5.71102600 -0.30243900
H -1.25875300 -5.61189700 -2.69866600
H 0.48775000 -6.90475900 -1.49197500
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C -5.83343200 -2.87623600 1.08217000
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H -5.54184300 -4.15983500 -1.89163200
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C -7.22540200 -1.29665800 -2.85088000
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H -6.46309100 -0.58623200 -3.17826400
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C -8.32228000 -2.60212400 -1.05943500
H -8.52176500 -2.77661600 0.00015500
H -7.96888100 -3.54852600 -1.48452800
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C -7.91997000 -0.12965800 -0.69936000
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C -8.05583000 -0.13481900 0.83402300
H -7.07652500 -0.06539700 1.31967200
H -8.56054800 -1.02614200 1.21506900
H -8.63876000 0.73366300 1.15946300
C -7.20758500 1.16828700 -1.11807000
H -6.18807800 1.19987400 -0.72379900
H -7.74415600 2.03423900 -0.71510200
H -7.16620500 1.29404200 -2.20349400
C -3.45466100 -0.14993300 -0.99220800
C -3.76519800 0.11666700 -2.46915400
H -3.83312200 -0.80681800 -3.05292600
H -3.01123900 0.76262000 -2.92764300
H -4.72024900 0.63861400 -2.54236600
S -1.62184000 -2.20222200 1.66428700
O -0.20777300 -2.46496400 1.97512900
O -2.41655800 -3.27347400 1.04072600
C -2.38002800 -1.62867600 3.18236300
C -3.57254600 -0.85095200 5.58822500
C -1.76868800 -1.96426100 4.39089400

C -3.57788900 -0.91025600 3.15218200
C -4.16174400 -0.52741800 4.35632500
C -2.37248600 -1.57373800 5.58470200
H -0.83158000 -2.50917500 4.38792800
H -4.03134100 -0.65008300 2.20187000
H -5.09083300 0.03632700 4.34026700
H -1.89913500 -1.83111500 6.52815600
H -3.29734800 0.82203800 -0.50467800
C -4.20207700 -0.40032200 6.88380100
H -3.91179400 0.63041100 7.12188300
H -3.88946200 -1.02968900 7.72137500
H -5.29445700 -0.42422500 6.82720300
C 1.96614100 0.87656600 -0.04779000
H 2.40409100 1.19573300 -0.99463300
C 3.18658000 1.03021900 1.01323300
N 4.38240900 0.52798600 0.39661200
S 4.85524600 -0.94178300 0.77555400
O 4.35942000 -1.99027300 -0.20658400
O 4.64992400 -1.34775400 2.19084700
C 6.62418200 -0.84937400 0.48361200
C 9.37935200 -0.82856600 0.04054500
C 7.14415900 -0.20230800 -0.64355300
C 7.47784900 -1.47637100 1.38411500
C 8.85936800 -1.47042900 1.16890000
C 8.51372800 -0.19044100 -0.86289300
H 6.47112000 0.30673500 -1.32406600
H 7.05653400 -1.95816600 2.25970000
H 9.50953700 -1.95992000 1.88414000
H 8.94372300 0.31070800 -1.72413000
O 10.70961600 -0.76022300 -0.27044000
C 11.63272600 -1.37919200 0.60953900
H 11.59642200 -0.93681100 1.61349900
H 12.62109800 -1.20966500 0.17913300
H 11.45548000 -2.45954300 0.69043600
H 2.88327900 0.46205500 1.90493600
C 3.35053600 2.48599000 1.43114400
C 3.62933400 5.17178800 2.21836400
C 2.71752000 2.96176300 2.58630300
C 4.13759800 3.36934900 0.68276600
C 4.27084500 4.70205200 1.06937000
C 2.85683700 4.29532500 2.98095400
H 2.12689500 2.27823500 3.19158300
H 4.66420200 2.98533200 -0.18430500
H 4.88659600 5.37547400 0.47915600
H 2.37553200 4.64239800 3.89162400
H 3.74333500 6.20813000 2.52386600

TS III R

(1609.89i)

Ettotal:-4387.872548

G: -4387.991732

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O 1.77893600 2.48637700 0.69596700
C 1.33348500 3.76296900 0.35016300
H 3.10068000 4.01871700 -0.80281300
C 2.18419600 4.48618600 -0.45204200

C -0.19010400 5.61207100 0.54068900
C 1.85948100 5.82412600 -0.79460400
C 0.13866200 4.31663700 0.86864600
C 0.64582300 6.40109300 -0.29415500
C 2.70349700 6.61305000 -1.62331000
H -0.50021700 3.71707800 1.50280900
H -0.59427500 8.17505200 -0.26318300
H -1.10596700 6.05058700 0.92856000
C 2.36387700 7.90766500 -1.94386100
H 3.62254000 6.17199800 -1.99899500
H 3.01737300 8.49941400 -2.57837700
C 1.16408100 8.47763900 -1.45034800
H 0.90855100 9.50080900 -1.71059200
C 0.32643100 7.74032100 -0.64457100
C 0.97575200 -1.09948400 1.00739500
H 0.18676300 -0.90034100 1.74101700
H 1.65665600 -1.83429500 1.45084600
P 0.17661100 -2.00763600 -0.38556400
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H -2.91473100 -1.89088000 -0.53101700
N -2.41918900 -0.25045400 0.65485500
H -1.66818200 0.44567700 0.76446100
C 1.41535900 -2.49635200 -1.62146400
C 3.44462800 -3.19953600 -3.40867800
C 1.80862300 -1.60513200 -2.63139600
C 2.05127100 -3.74419200 -1.50979600
C 3.05710500 -4.09301900 -2.40787100
C 2.82618200 -1.95465700 -3.51627100
H 1.35552800 -0.62403000 -2.71799200
H 1.76093200 -4.44148600 -0.73130500
H 3.54145900 -5.06078100 -2.32079100
H 3.15600000 -1.23579700 -4.25670600
H 4.23780000 -3.47026500 -4.09909200
C -0.61830100 -3.53247000 0.20641400
C -1.86866000 -5.88824000 1.04594300
C -1.19938600 -4.40132000 -0.73567100
C -0.66862700 -3.85346000 1.56969900
C -1.29296300 -5.03184000 1.98180600
C -1.82298300 -5.57222200 -0.31477100
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H -0.25931700 -3.18231100 2.31415100
H -1.33568500 -5.26925200 3.03965500
H -2.26990900 -6.23778800 -1.04660400
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O -4.79139500 -0.20420300 -1.10626700
Si -6.07243000 -1.29459200 -1.29782100
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C -8.70404100 -1.41892900 -2.27743400
H -9.12426900 -1.16626900 -1.30151000
H -8.56871300 -2.50652300 -2.30305300
H -9.46027600 -1.17434300 -3.03563900
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H -8.56308000 1.00031100 -3.21815700
C -8.06798300 1.43959900 -1.18598700
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H -2.37254300 -0.06489500 -3.47468400
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C -5.49871900 2.24674900 4.11162200
C -3.78912000 0.51720500 4.21981300
C -4.80723500 1.08207500 2.08526200
C -5.59360100 2.03421800 2.72748900
C -4.58840100 1.47387200 4.84348900
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H -6.29254000 2.62678000 2.14282000
H -4.49808300 1.62504300 5.91566800
H -3.19294300 0.97692900 -1.44833800
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H -5.90749100 4.30250200 4.63156300
H -6.40250700 3.13877500 5.86407000
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C 3.29904300 0.20413500 0.91597100
H 3.55209800 1.23155000 1.18950000
C 3.79245800 -0.73410600 2.00158500
C 4.64611900 -2.46073400 4.05366000
C 3.58193700 -0.40630900 3.35006700
C 4.43882500 -1.93789100 1.69726400
C 4.86331900 -2.79397500 2.71664500
C 4.00338800 -1.26029300 4.36778700
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H 4.61649500 -2.17479200 0.65363700
H 5.37272400 -3.72031500 2.46411500
H 3.83639400 -0.98710800 5.40612100
H 4.98047800 -3.12483700 4.84577600
N 3.75719700 -0.12796000 -0.46901900
S 4.83903300 0.84450000 -1.22131100
O 4.80540700 2.24208100 -0.72262400

O 4.66065900 0.60572400 -2.66866000
C 6.48367900 0.23632100 -0.80163700
C 9.00229200 -0.75386200 -0.11822700
H 2.40066600 0.03888700 -0.59497600
C 7.23017700 0.86131300 0.20275300
C 6.99939900 -0.87530000 -1.46492300
C 8.25795300 -1.37653000 -1.12935400
C 8.48288400 0.36845200 0.54326900
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H 8.64830700 -2.23613100 -1.66131000
H 9.08355700 0.83872000 1.31475400
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C 10.82925200 -2.27759200 -0.34989900
H 10.22782700 -3.18575700 -0.21312400
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TS III5

(1666.70i)

Etotal:-4387.864233

G: -4387.981241

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H -1.76961800 4.71200500 -0.07346900
C -1.45506100 4.57328400 0.95607500
C -0.68063800 4.14205100 3.61849100
C -1.08161400 5.68627600 1.75363300
C -1.05079300 3.07643800 2.83268400
C -0.68068800 5.47009500 3.11274000
C -1.09169200 7.01415900 1.24663100
H -1.05244800 2.06608800 3.22064900
H -0.00419500 6.41843800 4.93623600
H -0.38583800 3.97586100 4.65149700
C -0.72263300 8.07551000 2.04171100
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H -0.73564300 9.08494300 1.64080000
C -0.32587200 7.86141600 3.38458600
H -0.03826100 8.70756900 4.00179900
C -0.30635400 6.58730500 3.90560000
C -1.06160000 -1.10110600 -0.64264700
H -0.25847100 -0.92046300 -1.36686800
H -1.74866800 -1.81533700 -1.10901500
P -0.30882500 -2.09401600 0.70788800
C 1.32294500 -1.57048000 1.38965300
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H 1.09144400 -0.70597600 2.01391700
C 2.51359900 -1.22334100 0.46455500
H 2.72575300 -2.04640300 -0.22203400
N 2.20232600 -0.02698800 -0.32871100
H 1.43640800 0.55227200 0.03479600
C -1.41997700 -2.21060900 2.15400000
C -3.15960600 -2.49382300 4.33167000
C -0.95332200 -2.01966100 3.46397600
C -2.76807300 -2.54380500 1.94118600

C -3.62715900 -2.68377100 3.03089200
C -1.82240600 -2.16047800 4.54563700
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H -3.16823500 -2.68459300 0.94006000
H -4.66671400 -2.94069100 2.85248400
H -1.45025100 -2.00775400 5.55400100
H -3.83417500 -2.60358600 5.17552400
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C 0.16532100 -6.36304800 -1.03938100
C 1.08296900 -4.50561400 0.20393900
C -1.15862700 -4.36144200 -0.70944600
C -1.01811300 -5.64826000 -1.22719200
C 1.21513300 -5.78993700 -0.32267500
H 1.91548000 -4.08458500 0.75469100
H -2.09582600 -3.83680100 -0.87528200
H -1.84086800 -6.08613800 -1.78322900
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H 0.26965700 -7.36225200 -1.45130000
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Si 6.04419000 -2.03738900 -0.17619300
C 6.36196400 -1.45892000 -1.93759800
H 5.41377900 -1.44155600 -2.48125600
H 7.04168700 -2.14418300 -2.45496700
H 6.79562900 -0.45726800 -1.98853700
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H 5.03757200 -4.21629200 0.68294300
H 5.97147200 -4.45048900 -0.79236700
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H 8.42814000 -3.73464200 -0.48540300
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H 9.01841600 -0.03492200 -0.55489200
H 9.00393700 1.16432600 0.73619300
C 7.47952400 -0.16135000 2.56305800
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H 7.99240200 0.73685700 2.92413900
H 7.39854000 -0.84669200 3.41127900
C 3.80395200 -0.96433200 1.31956500
C 3.99968500 -1.90506400 2.51350300
H 3.97123400 -2.96159100 2.22915700
H 3.24343200 -1.73384000 3.28445200
H 4.96991600 -1.70130100 2.96885700
S 2.36454100 0.03844700 -1.98689800
O 1.05644600 0.34348600 -2.59295700
O 3.06881600 -1.18783200 -2.39274700
C 3.38404600 1.48487300 -2.27854500
C 4.98308200 3.70899900 -2.84863000
C 3.04496800 2.32135200 -3.34305500

C 4.51302800 1.73615900 -1.49618300
C 5.29977400 2.84742300 -1.78772800
C 3.84898500 3.42527200 -3.62032300
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H 4.76556700 1.07167800 -0.67722500
H 6.17624700 3.05101900 -1.17800500
H 3.58646300 4.07907800 -4.44753600
H 3.69395000 0.05384900 1.71583900
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H 6.87994300 4.74966800 -2.89609800
H 5.49805500 5.77998700 -2.52112400
H 5.75575400 5.23092300 -4.17853300
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O -4.81393000 -1.30454800 -2.93721000
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C -8.77756900 -1.71291800 -1.24869900
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H -5.85341600 -1.08294900 1.23059100
H -7.24288100 -1.76219500 -2.77052700
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H -8.20287000 -1.19510600 2.06169200
O -10.27738500 -1.59095400 0.68090800
C -11.39507100 -1.79979100 -0.16902300
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C -3.28292700 4.55671900 -2.82496400
C -1.98981800 2.52256800 -2.60585700
C -4.21134500 2.63916600 -1.67209800
C -4.33216300 3.95234400 -2.13134200
C -2.10941700 3.83436500 -3.06203800
H -1.07530200 1.96430700 -2.79344400
H -5.02078100 2.15694300 -1.13564700
H -5.25083900 4.50334700 -1.94824500
H -1.28961900 4.29166100 -3.60986000
H -3.38032300 5.57672500 -3.18692700

It IIR

Etotal:-4387.919234

G: -4388.039022

E(RmPW1PW91):-4388.561028

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O 1.59053600 2.53908600 0.74312100
C 1.00939400 3.74798700 0.41864800
H 2.60571500 4.15173000 -0.93221300
C 1.69286400 4.53315500 -0.48375800
C -0.65228200 5.46926700 0.73145500

C 1.22020800 5.82983700 -0.81123000
C -0.17405500 4.21892000 1.04494000
C 0.01660500 6.31021800 -0.19839700
C 1.89911800 6.67113900 -1.73473400
H -0.68825900 3.58079600 1.75040600
H -1.37049000 7.96512300 -0.06658700
H -1.55979000 5.83380100 1.20643700
C 1.41200300 7.92192000 -2.04047400
H 2.81418200 6.30773000 -2.19497500
H 1.94241600 8.55337000 -2.74771100
C 0.22145900 8.39540800 -1.43602700
H -0.15176500 9.38479200 -1.68457200
C -0.45773500 7.60555100 -0.53563500
C 0.93674300 -1.08324300 1.19386800
H 0.04783400 -1.05274600 1.83179400
H 1.60451700 -1.84897500 1.60193500
P 0.33654600 -1.84535400 -0.41823000
C -0.98587700 -0.87494300 -1.26735900
H -0.99185100 -1.25482500 -2.29216400
H -0.64439100 0.16502800 -1.27206800
C -2.41587200 -0.93802100 -0.67748800
H -2.77200300 -1.97114000 -0.67128800
N -2.40915000 -0.43814900 0.69972200
H -1.69132100 0.28785700 0.90128000
C 1.71697700 -1.91272500 -1.60430500
C 3.94605900 -1.96122000 -3.30038900
C 1.90472900 -0.90016200 -2.55823400
C 2.66228200 -2.94610300 -1.50341600
C 3.76814900 -2.96919100 -2.35072300
C 3.01534200 -0.92774700 -3.40291900
H 1.19482500 -0.08558700 -2.64753600
H 2.53406700 -3.73411700 -0.76832700
H 4.49257300 -3.77318200 -2.26596800
H 3.15365900 -0.13580100 -4.13186900
H 4.81078700 -1.98015400 -3.95642000
C -0.26548800 -3.55590700 -0.21383400
C -1.25524600 -6.15596700 0.07808300
C -0.38043900 -4.40045200 -1.33327300
C -0.65459900 -4.02267800 1.05086900
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Si -5.96000200 -1.44110800 -1.44227600
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H -9.01036800 -1.50768300 -1.64027700
H -8.30071400 -2.73541700 -2.68666900
H -9.23489900 -1.41676600 -3.38989900
C -7.63298400 0.70857900 -2.67975600
H -8.47333100 0.81621700 -3.38636000
C -8.15303600 1.15512200 -1.30146000
H -7.34289100 1.19043200 -0.56525900
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H -5.68510900 1.67263600 -2.46270800
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C -3.40040300 -0.08608300 -1.54359700
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H -3.28850400 -1.29889300 -3.37163000
H -2.26521300 0.15133400 -3.39012100
H -4.00444200 0.31001600 -3.57144200
S -2.96976500 -1.28903100 1.99833200
O -1.86609500 -1.59656600 2.93285200
O -3.76100500 -2.41660800 1.47539600
C -4.01970500 -0.11373600 2.85424200
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C -3.96097300 -0.05986000 4.24679300
C -4.90254600 0.69708600 2.13702700
C -5.73336400 1.56826200 2.83575100
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H -4.92424000 0.64792000 1.05356600
H -6.41442500 2.21018900 2.28293100
H -4.75472200 0.86918400 6.01138300
H -3.18621700 0.96144900 -1.29448500
C -6.62962300 2.57275700 4.97872800
H -6.73842500 3.52779000 4.45570500
H -6.26818300 2.77737700 5.99004300
H -7.63249900 2.13751300 5.06925000
C 1.63345600 0.23113600 1.05324900
C 3.12129900 0.37946600 1.31001100
H 3.27185700 1.34781700 1.79291500
C 3.68853300 -0.67988100 2.24754900
C 4.63951200 -2.62056400 4.05456000
C 3.45902400 -0.55292700 3.62569100
C 4.40398900 -1.79251500 1.79013200
C 4.87571500 -2.75595400 2.68728000
C 3.92827800 -1.51144300 4.52138200
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H 4.60156000 -1.88634000 0.72778600
H 5.43519900 -3.60986600 2.31413800
H 3.74448600 -1.39079600 5.58534700
H 5.00974800 -3.36641000 4.75220300
N 3.88054700 0.41084300 0.00804500
S 5.17086100 1.49854900 -0.16988300
O 5.34570400 2.26488600 1.06984500
O 4.95235000 2.16602900 -1.46600200

C 6.63250600 0.47688800 -0.35245900
C 8.92031800 -1.08385900 -0.64434100
C 7.31214100 0.02442100 0.78489100
C 7.09584800 0.16022400 -1.62630900
C 8.24239500 -0.62109200 -1.78007300
C 8.44888900 -0.75589800 0.63758400
H 6.95442300 0.29700900 1.77102600
H 6.57144100 0.54600600 -2.49328800
H 8.60097800 -0.84898000 -2.77653700
H 8.99893800 -1.11691400 1.49986700
O 10.04635100 -1.84935900 -0.67615500
C 10.60384300 -2.18137200 -1.93924100
H 9.90938800 -2.77794100 -2.54444800
H 11.49454400 -2.77418300 -1.72753700
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It IHS

Etot:-4387.917144

G: -4388.037171

E(RmPW1PW91):-4388.553190

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C -1.91026700 3.94145500 1.55051900
C -0.37157200 3.65068100 3.87527300
C -1.53474500 5.10184300 2.27551100
C -0.75271000 2.53793500 3.16382500
C -0.74391500 4.95859500 3.46259300
C -1.91270500 6.40842100 1.86142800
H -0.46685600 1.54268700 3.47621000
H 0.23173300 6.00756000 5.08368400
H 0.22284700 3.53789600 4.77870700
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H -2.51139400 6.51672600 0.96074500
H -1.82600400 8.50867600 2.25224400
C -0.74914600 7.37445400 3.75580500
H -0.45406800 8.25668900 4.31658800
C -0.36698000 6.12262500 4.18328100
C -1.00128100 -1.53986400 -0.41161700
H -0.33008300 -1.34629500 -1.26010300
H -1.67131300 -2.34807700 -0.73425500
P 0.09293400 -2.41652300 0.81697100
C 1.72865300 -1.72874800 1.34637700
H 2.19406700 -2.57600900 1.85752300
H 1.47745000 -0.95656600 2.07480500
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H 3.05580800 -1.95835200 -0.36460900
N 2.14409700 -0.07485100 -0.44886900
H 1.32676100 0.37696900 0.00810300
C -0.80440200 -2.74293100 2.36140800
C -2.26918500 -3.24004700 4.69445300
C -0.16088300 -2.76459100 3.61018600
C -2.18650000 -2.97694400 2.29271500
C -2.91451100 -3.21929900 3.45835700
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C 1.12743200 -4.01520100 -1.23503500
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C 0.44641800 -6.43863900 -0.01838600
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Si 6.29125300 -1.19935500 -0.64286400
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C 3.88912800 2.10933600 -1.79251700
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H 2.40487300 3.99947300 -4.83910700
H 3.73494000 0.30216800 1.52126300
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H 5.44875200 5.24449300 -4.16181200
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O -4.56079600 -2.73123400 -0.03352700
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C -3.64437100 3.43786600 -2.96253100
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TS IVR

(192.64i)

Ettotal:-4387.916473

G: -4388.035159

E[(RmPW1PW91):-4388.548945

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H 1.54601000 -1.85572900 1.92707000
P 0.29279400 -1.97278000 -0.31681100
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C -1.41451600 -5.48049200 0.96366000
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H -0.89650100 -6.40687000 -2.26931600
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Si -5.96657100 -1.30361500 -1.51063700
C -6.87753800 -1.58642700 0.11357700
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H -8.41692400 2.41055800 -1.48167700
C -6.38368600 1.86932400 -3.21282200
H -5.53310400 1.80558800 -2.52855600
H -6.74101800 2.90498100 -3.19913000
H -6.03012300 1.66601000 -4.22738400
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H -3.89900500 0.38395400 -3.57454500
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O -1.97445900 -1.72363100 2.92937800
O -3.87843200 -2.42133800 1.42118500
C -4.06373300 -0.14790800 2.86019800
C -5.70297300 1.63142900 4.26258700
C -4.03478900 -0.14111400 4.25499100
C -4.89914100 0.71794300 2.15082600
C -5.71022500 1.59980600 2.85980800
C -4.85675700 0.74805400 4.94516500
H -3.36861700 -0.81418300 4.78223300
H -4.90474600 0.69725700 1.06615700
H -6.35986600 2.27917500 2.31403400
H -4.83582700 0.75811700 6.03154200
H -3.10230100 0.98066900 -1.27576600
C -6.56380500 2.61717800 5.01467500
H -6.77076000 2.27411400 6.03210500
H -7.51972000 2.78096400 4.50827700
H -6.06666700 3.59200400 5.09228000
C 1.65916600 0.19973700 1.34187000
C 3.16803200 0.32827800 1.48738000
H 3.35704800 1.28594200 1.97969500
C 3.78778500 -0.75401800 2.36629800
C 4.86175700 -2.72365100 4.06751100
C 3.64480800 -0.65664500 3.75825200
C 4.48070600 -1.84945500 1.84033900
C 5.01312400 -2.82782300 2.68560400
C 4.17458600 -1.63037000 4.60224500
H 3.11158300 0.19223300 4.17865400
H 4.61264500 -1.91967700 0.76632000
H 5.55297100 -3.66963400 2.25998000
H 4.05726600 -1.53356900 5.67794300
H 5.27935000 -3.48163300 4.72407400
N 3.83690200 0.38496500 0.14677600
S 5.06298600 1.51732700 -0.13058200
O 5.29691900 2.28599200 1.09717200
O 4.72327600 2.17686300 -1.40447100
C 6.54362900 0.55308400 -0.42669400

C 8.85860900 -0.92314100 -0.89173200
C 7.29991100 0.09092500 0.65752600
C 6.94367900 0.28776300 -1.73329600
C 8.10343600 -0.45132900 -1.97351300
C 8.45011200 -0.64686300 0.42393200
H 6.99063200 0.32224500 1.67031600
H 6.35951000 0.67943100 -2.55826200
H 8.41147500 -0.63959600 -2.99477400
H 9.05870000 -1.01417800 1.24311500
O 10.00416700 -1.64934400 -1.00873700
C 10.49628500 -1.93362900 -2.31039300
H 9.78563800 -2.53751200 -2.88877200
H 11.41539000 -2.50263500 -2.16570500
H 10.72323500 -1.01515600 -2.86570700
H 3.16796600 0.48716300 -0.60984700

TS IVS

(168.03i)

Ettotal:-4387.915728

G:-4388.034825

E(RmPW1PW91):-4388.565497

C 1.26117100 0.68204700 0.24173800
O 0.09075900 1.08276400 0.31195200
O 2.21615000 1.53252300 -0.34583400
C 1.77537900 2.76036200 -0.83677300
H 2.48785800 3.82650800 0.86377200
C 2.02226600 3.90056300 -0.11392800
C 0.80940200 4.03131500 -2.64292400
C 1.66538400 5.17010300 -0.64144900
C 1.16485400 2.81471500 -2.11151300
C 1.04528900 5.23941100 -1.93206000
C 1.90252200 6.37714700 0.06959900
H 0.99355200 1.89079400 -2.65353500
H 0.22143900 6.55890900 -3.43603800
H 0.34255900 4.08232400 -3.62292000
C 1.54475900 7.59340500 -0.46678700
H 2.37106100 6.32360000 1.04872500
H 1.73128700 8.50791100 0.08865200
C 0.93319100 7.66201800 -1.74237400
H 0.65639300 8.62783500 -2.15460400
C 0.69046100 6.51061200 -2.45663000
C 0.93202500 -1.37737600 1.46825600
H 0.12799200 -0.89462400 2.01545200
H 1.41425700 -2.15589800 2.05673500
P -0.34847200 -2.70935200 0.24204700
C -1.33931300 -1.65585400 -0.93084800
H -1.55638800 -2.28466800 -1.79754500
H -0.66722200 -0.85604800 -1.25932000
C -2.64461500 -1.04316500 -0.37340500
H -3.31329800 -1.84068400 -0.04037900
N -2.35506200 -0.18316100 0.77868000
H -1.46645700 0.34164600 0.74225700
C 0.76214400 -3.65755400 -0.85356300
C 2.62450300 -5.05962200 -2.41732000
C 1.37098300 -3.04405300 -1.96144900
C 1.11290700 -4.98114600 -0.53118000
C 2.03057300 -5.67674400 -1.31500400
C 2.29722100 -3.74282200 -2.73575800

H 1.14898600 -2.01397800 -2.21428600
H 0.66148800 -5.47106100 0.32531600
H 2.28757500 -6.70008800 -1.05776200
H 2.78655200 -3.24031300 -3.56304100
H 3.35269000 -5.59741800 -3.01626200
C -1.52425200 -3.94922100 0.92388100
C -3.32728700 -5.80677300 1.99445200
C -1.80761300 -3.94912500 2.29669400
C -2.15594200 -4.88938200 0.08900900
C -3.05321400 -5.81087000 0.62358300
C -2.70648700 -4.87749800 2.82641500
H -1.36005100 -3.20534800 2.94663100
H -1.93439900 -4.91212800 -0.97382400
H -3.53691000 -6.53282700 -0.02785200
H -2.92594500 -4.86236000 3.88927000
H -4.02772100 -6.52584300 2.40897800
O -4.68334700 0.15609300 -0.98546600
Si -6.22442700 -0.53754600 -0.95553700
C -6.93594400 -0.13136400 0.74040300
H -6.28379600 -0.55605000 1.50864300
H -7.93108100 -0.57424500 0.85554700
H -7.02531100 0.94162800 0.92710700
C -6.14914100 -2.42785900 -1.07656900
H -5.74471700 -2.80284900 -2.02057700
H -7.15797500 -2.84326200 -0.96905800
H -5.54754400 -2.83234400 -0.25560800
C -7.36349600 0.14648100 -2.37692900
C -7.15232300 -0.66320900 -3.68010200
H -7.43463700 -1.71191300 -3.54291800
H -6.12241200 -0.65130400 -4.04476000
H -7.78559500 -0.26202900 -4.48382200
C -8.82718800 -0.13517200 -1.94084800
H -9.12459700 0.41485100 -1.04527200
H -8.99158400 -1.19992800 -1.73831500
H -9.51909600 0.14635100 -2.74640500
C -7.23069600 1.67910500 -2.69353200
H -8.06543100 1.89631000 -3.38153900
C -7.40603300 2.60510500 -1.47641900
H -6.54970300 2.53244100 -0.79741000
H -8.31114700 2.38991000 -0.90275100
H -7.46927500 3.64793400 -1.80624000
C -5.94005600 2.08115900 -3.42884200
H -5.06181200 1.91353000 -2.79953700
H -5.97097100 3.14774700 -3.67793100
H -5.80454700 1.53629000 -4.36718000
C -3.39171700 -0.20782700 -1.45989500
C -3.43424000 -0.86094600 -2.84478100
H -3.84585500 -1.87444000 -2.81655800
H -2.43607600 -0.90983600 -3.28798400
H -4.05313800 -0.25521900 -3.50892200
S -2.94836500 -0.43208700 2.30028600
O -1.86122300 -0.79481300 3.23394900
O -4.09230100 -1.35099300 2.17807000
C -3.49487900 1.20244900 2.79759200
C -4.42088500 3.70108300 3.64797200
C -3.26246600 1.61083000 4.11091200
C -4.18377900 2.02048800 1.89924600
C -4.63915700 3.26237600 2.33317800

C -3.72942400 2.85684000 4.52604500
H -2.71320500 0.96440700 4.78561500
H -4.34840800 1.68628900 0.88036400
H -5.17102300 3.90566900 1.63690100
H -3.54827000 3.17958000 5.54777600
H -2.83676300 0.73555400 -1.55176600
C -4.89375200 5.06402800 4.09220900
H -4.99582100 5.11820500 5.17954200
H -5.86025400 5.31656600 3.64560600
H -4.18362000 5.84337900 3.78941900
C 1.79146400 -0.55954300 0.68079400
C 3.24397300 -0.99830000 0.48332200
N 3.70296600 -0.71634700 -0.89069600
S 5.00049100 -1.48714400 -1.59750600
O 4.81515800 -1.30449600 -3.04395000
O 5.06956000 -2.81915700 -0.98561200
C 6.51996700 -0.62787700 -1.18327600
C 8.86671400 0.72405000 -0.53108700
C 6.96800600 0.41896800 -1.99897500
C 7.24486700 -1.00346800 -0.05441200
C 8.42085800 -0.33080700 0.27629700
C 8.13513100 1.09258100 -1.67248100
H 6.41205200 0.67981700 -2.89272900
H 6.89324900 -1.82253900 0.56156000
H 8.97365600 -0.63530900 1.15627100
H 8.50986500 1.90255300 -2.28898800
O 9.99587000 1.44788500 -0.30006900
C 10.78773400 1.12245000 0.83384700
H 10.22543700 1.24559200 1.76767400
H 11.62590100 1.82024800 0.82383100
H 11.17121400 0.09620200 0.77719300
H 3.25282500 -2.08850300 0.55654800
C 4.16545900 -0.48048500 1.59655600
C 5.78679700 0.39480900 3.72891800
C 4.54623500 -1.35799800 2.62005500
C 4.62119200 0.84454000 1.65279100
C 5.42446100 1.27594400 2.70707100
C 5.34533600 -0.92686400 3.68116300
H 4.22037300 -2.39479300 2.58158800
H 4.34725400 1.53835500 0.86620700
H 5.77048400 2.30578100 2.73068100
H 5.62627500 -1.62614100 4.46394700
H 6.41034600 0.73541800 4.55066100
H 3.55816800 0.23320300 -1.21802000

Product

Ettotal:-1871.293746

G: -1871.358947

E(RmPW1PW91):-1871.494175

C -2.11587400 -1.36005500 1.55988700
O -0.01876900 -1.85090800 0.62370300
C -0.69063200 -1.76311400 1.80393100
O -0.21715300 -2.00222000 2.89314600
C -2.97972600 -1.53556200 2.56601600
H -2.63867400 -1.95267900 3.50715500
H -4.02852700 -1.28004700 2.46586900
C 1.33693400 -2.15634700 0.48869900
C 1.90140500 -1.70361200 -0.68389700

C 2.07616500 -2.92138400 1.42464900
C 3.26040700 -1.98362000 -0.97385700
H 1.29151300 -1.13589800 -1.38078000
C 3.39731700 -3.19788300 1.15274400
H 1.60758600 -3.26189200 2.33578700
C 4.03024700 -2.74473300 -0.03451600
C 3.88490100 -1.53208400 -2.16884000
H 3.97646100 -3.78137600 1.86351100
C 5.39308100 -3.02068900 -0.32575300
C 5.20738400 -1.81732900 -2.42013700
H 3.29814900 -0.95736300 -2.88011800
C 5.96959100 -2.56806900 -1.49058900
H 5.97372800 -3.59856100 0.38865500
H 5.67337000 -1.46745700 -3.33661600
H 7.01196100 -2.78623100 -1.70325900
C -2.46752300 -0.70016600 0.22558100
H -1.87700800 -1.17921900 -0.55837300
C -3.94444000 -0.81760300 -0.15255000
C -4.49261700 -2.10054500 -0.31157500
C -4.76389300 0.29182000 -0.37646200
C -5.82717400 -2.26842400 -0.67009800
H -3.86672700 -2.97394800 -0.14874000
C -6.10532400 0.12390700 -0.73415600
H -4.35705000 1.29476600 -0.31488800
C -6.64261000 -1.15260700 -0.87806900
H -6.23081700 -3.26965800 -0.79015100
H -6.72384000 0.99935500 -0.90871800
H -7.68383100 -1.28101600 -1.15860100
N -1.92845200 0.67142700 0.32494100
H -2.45800700 1.28457200 0.93976200
S -1.40177400 1.49847000 -1.05778000
O -2.44242900 2.40069200 -1.57324200
O -0.82239500 0.46804500 -1.92957700
C -0.11394600 2.53047700 -0.37285000
C 0.99362700 1.95134900 0.24715200
C -0.20456600 3.91909700 -0.52123400
C 2.01716400 2.75860200 0.73616800
H 1.06104800 0.87477600 0.35291700
C 0.81370500 4.72616000 -0.03508500
H -1.06903200 4.34812400 -1.01470200
C 1.92950800 4.15272200 0.59593000
H 2.87031900 2.29643200 1.21662600
H 0.77163400 5.80538600 -0.13331600
O 2.86842900 5.02877000 1.03584700
C 4.03126200 4.51799900 1.67748100
H 4.63549400 5.38832600 1.93491900
H 3.7775300 3.96959800 2.59273100
H 4.60434400 3.86361800 1.00978800

Catalyst-W

Ettotal:-2593.061640

G: -2593.146003

E(RmPW1PW91):-2593.506131

P -2.27578200 -1.90946900 0.15436100
C -1.19784500 -0.82669600 -0.94514200
H -1.60814900 0.18448100 -1.00747100
H -1.23584300 -1.26877200 -1.94756100
C 0.25988200 -0.69717300 -0.47692900

H 0.26278600 -0.41453300 0.58089500
N 0.97809800 -1.97967900 -0.63155600
H 0.44213500 -2.76451300 -1.03334600
C -3.90273000 -1.83018900 -0.72215800
C -6.42502300 -1.90251600 -1.97393400
C -4.26088600 -0.86072000 -1.67277100
C -4.83130300 -2.84029400 -0.41837500
C -6.08355500 -2.87290500 -1.03038700
C -5.51007300 -0.89956500 -2.29542600
H -3.56944200 -0.06648700 -1.93415600
H -4.56551000 -3.61084600 0.30076900
H -6.78729300 -3.66104800 -0.77879100
H -5.76773000 -0.14276800 -3.03096400
H -7.39607300 -1.93106000 -2.45961100
C -2.52724300 -0.80930700 1.62495400
C -2.77983400 0.79424400 3.92194400
C -3.55720300 0.13942300 1.72480100
C -1.63189300 -0.95074400 2.69884500
C -1.75283400 -0.14613400 3.83395800
C -3.68354500 0.93215900 2.86630500
H -4.26939100 0.25374100 0.91368600
H -0.83086300 -1.68247700 2.64689100
H -1.04882700 -0.26528800 4.65250700
H -4.48993800 1.65740700 2.93111200
H -2.88080100 1.41170500 4.80994800
O 0.39159200 1.67484300 -0.93663300
Si 1.06924900 2.89703400 0.01059400
C 2.68460000 3.48184900 -0.78640200
H 3.38331300 2.64252800 -0.88222900
H 3.17599900 4.23809600 -0.16456900
H 2.53941400 3.90929600 -1.78173900
C 1.51862400 2.19293900 1.70885400
H 0.65567100 1.75239700 2.21695600
H 1.93712200 2.96514600 2.36457400
H 2.27751700 1.40849900 1.61035000
C -0.24934700 4.29047900 0.19145900
C -1.26601600 3.86823500 1.28101200
H -0.78507000 3.78654300 2.26049300
H -1.74673300 2.90831400 1.07531400
H -2.05905000 4.62353500 1.37353400
C 0.48883200 5.54414300 0.73073800
H 1.21192000 5.95510000 0.02086600
H 1.02910500 5.32911100 1.66023500
H -0.23510100 6.33770800 0.95940700
C -1.02217300 4.68877000 -1.11620800
H -1.56256300 5.61313100 -0.85063700
C -0.11953900 5.02947900 -2.31509200
H 0.35918900 4.13025100 -2.71697200
H 0.66342300 5.75181100 -2.06729000
H -0.71792700 5.46436400 -3.12303400
C -2.08530000 3.67162900 -1.56999100
H -1.62549300 2.71006700 -1.81293100
H -2.59393900 4.04310100 -2.46677900
H -2.85129700 3.50355800 -0.80856200
C 1.02269500 0.42658100 -1.23115900
C 1.08702200 0.24052300 -2.74394400
H 0.09195100 0.32138100 -3.19102700
H 1.50936700 -0.73644700 -2.99490500

H 1.71663000 1.01634100 -3.18836500
S 1.93863100 -2.57330000 0.59838800
O 1.93985200 -4.03785200 0.41737900
O 1.55853900 -1.98879500 1.89398000
C 3.58940300 -1.97706100 0.22826500
C 6.19078200 -1.09879000 -0.31469200
C 4.20964000 -2.35647300 -0.96591300
C 4.25123900 -1.17612100 1.15611900
C 5.54724300 -0.73947400 0.87473700
C 5.50056200 -1.91310800 -1.22864200
H 3.68654500 -2.98741500 -1.67651700
H 3.75420700 -0.90720000 2.08130700
H 6.06519800 -0.11257400 1.59529600
H 5.98459800 -2.20327400 -2.15741600
H 2.05016300 0.41440800 -0.83851800
C 7.59935500 -0.64325100 -0.60859300
H 7.68681600 -0.24935100 -1.62640300
H 8.30682400 -1.47669300 -0.52399500
H 7.92164200 0.13648900 0.08614400
O -0.43241900 -4.45808900 -1.14454000
H -1.12625600 -4.20200700 -0.51388900
H 0.30252100 -4.75207500 -0.57855400

TS I-W

(169.17i)

Ettotal:-3244.717836

G: -3244.816720

E(RmPW1PW91):-3245.238014

C 2.47450400 2.26000800 -0.71528300
C 1.65283800 3.37995000 -0.96384000
H 1.93980700 4.32668300 -0.52431500
O 2.27378300 1.06957200 -1.04975300
O 3.61558700 2.59774100 -0.01299300
C 4.62734700 1.66642700 0.17426800
H 4.63599400 2.04300600 2.26987900
C 5.10533700 1.50375600 1.45289900
C 6.28561400 0.15276100 -0.69924600
C 6.20855700 0.64674100 1.70405100
C 5.22230100 0.99425800 -0.92320800
C 6.81106400 -0.04943400 0.60587100
C 6.73540000 0.45208000 3.00941100
H 4.83610200 1.13937100 -1.92500400
H 8.36574900 -1.43525500 0.02194300
H 6.74169700 -0.36965800 -1.53570900
C 7.80378700 -0.39019700 3.22046800
H 6.27874400 0.98090600 3.84211500
H 8.19555800 -0.52948500 4.22397900
C 8.39901200 -1.07853000 2.13524200
H 9.24186400 -1.73944600 2.31493000
C 7.91189500 -0.91005100 0.85850700
C 0.51187300 3.28740900 -1.78988900
H 0.44051800 2.43816300 -2.46424000
H 0.14160600 4.21344600 -2.22343300
P -1.29784300 2.85093200 -0.56001800
C -0.90565100 1.35352100 0.45861800
H -1.49914700 1.36225100 1.37699600
H 0.14777700 1.46086100 0.73781600
C -1.11880000 0.01513600 -0.27162000

H -2.16208300 -0.05432700 -0.59226800
N -0.29985500 0.00903400 -1.48363600
H 0.67961200 0.32648100 -1.41054300
C -1.35879800 4.23496900 0.62662000
C -1.25799900 6.49371300 2.29745500
C -0.55090400 4.23873300 1.77619300
C -2.10094700 5.38971600 0.31743700
C -2.05547700 6.50495800 1.15041400
C -0.50563400 5.36122000 2.60507900
H 0.04222800 3.36897600 2.03403400
H -2.72432100 5.41262300 -0.57108900
H -2.64212300 7.38449800 0.90242200
H 0.11990700 5.34600000 3.49247500
H -1.22262900 7.36444800 2.94518300
C -3.00439600 2.64961800 -1.20703200
C -5.56542400 2.29231500 -2.28696300
C -4.14554600 2.84399700 -0.40760900
C -3.16270400 2.27362600 -2.54949300
C -4.43928000 2.09221900 -3.08365600
C -5.41782200 2.66782600 -0.94860100
H -4.04004900 3.13955700 0.63133900
H -2.29395300 2.10678600 -3.17726800
H -4.54694400 1.78927100 -4.12009000
H -6.29357500 2.82121500 -0.32491900
H -6.55833300 2.15408300 -2.70459500
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Si -3.32369100 -1.89511700 1.79618600
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H -3.01274500 -3.72744700 0.06955400
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H -4.73353500 -1.51671700 4.48925300
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H -3.83050500 -2.61724100 5.52862900
C -4.76185000 -3.85050800 3.21408800
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C -2.28291200 -3.90363800 3.73208100
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C -1.79751200 -4.76430100 2.55234100
H -1.27749500 -4.15812200 1.80240100
H -2.61205400 -5.29541600 2.05158900
H -1.08482900 -5.51802500 2.90396400
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C -0.84185900 -1.19972000 0.66099500
C 0.56627300 -1.22220500 1.25109500
H 0.67036500 -0.45322200 2.02213700
H 1.32707000 -1.04820700 0.48555700

H 0.76189400 -2.18975600 1.71979700
S -0.69089400 -0.78167600 -2.88548500
O 0.08600700 -0.09620100 -3.93221200
O -2.15859300 -0.83652300 -2.95053500
C -0.10298400 -2.47974500 -2.80043400
C 0.77562200 -5.13245300 -2.65240200
C 1.26657700 -2.75315300 -2.89094300
C -1.03607000 -3.50700100 -2.65629400
C -0.58862200 -4.82620600 -2.58239500
C 1.68785100 -4.07764800 -2.81271000
H 1.99237200 -1.95501700 -3.04035000
H -2.09342500 -3.27268800 -2.61839200
H -1.31372500 -5.62881900 -2.47713400
H 2.75012100 -4.29574800 -2.88623000
H -0.97896900 -2.09480500 0.04010300
C 1.26154300 -6.55818300 -2.55440500
H 0.43344800 -7.26951900 -2.61104800
H 1.78507500 -6.73113200 -1.60658000
H 1.96719500 -6.79375300 -3.35785000
H 2.92059100 0.24791900 -2.59901300
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It I-W

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O 2.38725000 0.44031700 -0.82503800
O 4.20336100 1.56984600 0.01374000
C 4.95728200 0.41813600 0.08852300
H 5.33759800 0.76058400 2.15507500
C 5.54608200 0.12660700 1.29855600
C 6.05690200 -1.46456000 -0.94714700
C 6.42359000 -0.98043400 1.42972400
C 5.21921800 -0.38070600 -1.05585300
C 6.68265600 -1.80152200 0.28393400
C 7.05263400 -1.30977400 2.66110100
H 4.75851300 -0.13555900 -2.00525400
H 7.74842100 -3.53160200 -0.45591100
H 6.25421300 -2.07974800 -1.82109800
C 7.89379400 -2.39561900 2.75720700
H 6.85743900 -0.68688300 3.53055400
H 8.36648900 -2.63416200 3.70588900
C 8.14944600 -3.20661900 1.62465200
H 8.81554500 -4.06001100 1.71275200
C 7.55567000 -2.91311600 0.41723900
C 1.18929000 3.02787900 -1.58662900
H 0.91817600 2.20306800 -2.25119800
H 1.15134700 3.96349700 -2.15461600
P -0.22238100 3.17554600 -0.34102300
C -0.25490700 1.70377500 0.77211600
H -0.70631400 2.02196000 1.71492500
H 0.79813200 1.47072600 0.96050500
C -0.98374200 0.47118500 0.19280600
H -2.02540200 0.73260800 -0.00565500
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H 0.68547300 0.17327500 -1.10538100
C 0.15553300 4.60822300 0.71512700
C 0.89592400 6.84151800 2.23700500
C 1.13274700 4.49003600 1.71927500
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C 1.49578000 5.60478000 2.47516300
H 1.62402400 3.54073900 1.89739700
H -1.17995900 5.96973100 -0.30755400
H -0.53097100 7.92982300 1.03999600
H 2.25132200 5.50399800 3.24801900
H 1.17986200 7.70615300 2.82929600
C -1.87482600 3.43199300 -1.06054400
C -4.41410400 3.75953400 -2.18659800
C -2.96062700 3.82537400 -0.25640500
C -2.07585000 3.19446600 -2.42773100
C -3.34402200 3.36195800 -2.98540500
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TS IIR-W

(228.88i)

Etotal:-4464.329031

G: -4464.448751

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C 1.92540400 0.88157500 4.17021200
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C 6.47916400 -1.92287000 0.62268700
C 7.60984000 -2.48852600 1.21057600
C 8.88948300 -0.50302600 0.64245100
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H 5.54332000 -2.47197800 0.62148700
H 7.53573300 -3.47381100 1.65405000
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C 9.97667900 -3.52621000 2.37122900
H 9.27920500 -3.57293500 3.21702800
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H 9.72003500 -4.31356000 1.65127000
H 3.38379400 -1.63326400 0.99196600
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TS IIR-W2

(192.08i)

Ettotal: -4464.329425

G: -4464.448977

E(RmPW1PW91):-4464.96449458

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O 1.24977200	3.15757100	-0.73937800	O -4.70211600	-0.69998900	-0.20745000
C 0.46507300	4.27752400	-0.50900200	Si -5.75391300	-2.02367700	-0.29647400
H 0.95825300	5.00809900	-2.44649500	C -5.77204300	-2.76892400	1.43244100
C 0.43191900	5.21223700	-1.51918200	H -4.75973600	-3.09714700	1.68320800
C -0.88316000	5.68853300	0.90462500	H -6.42987800	-3.64368200	1.46865900
C -0.26806900	6.43423800	-1.34964400	H -6.10453100	-2.06914300	2.20283900
C -0.19252200	4.51268800	0.72600700	C -5.08545100	-3.35988000	-1.46304200
C -0.94783300	6.67908600	-0.11197300	H -4.97859400	-3.03948200	-2.50351100
C -0.32047100	7.42569100	-2.36693700	H -5.75610800	-4.22692000	-1.45894800
H -0.14307500	3.76562300	1.50548700	H -4.11174900	-3.70565100	-1.10068700
H -2.16438000	8.08306300	0.99704200	C -7.54450300	-1.51823800	-0.86397400
H -1.39017500	5.87522000	1.84787400	C -7.62714300	-1.46089300	-2.40931100
C -1.01140400	8.60022000	-2.17201500	H -7.41339100	-2.43928900	-2.85100100
H 0.19749200	7.24061000	-3.30445000	H -6.93732700	-0.74396700	-2.86010900
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H -2.22469200	9.77296100	-0.80740200	H -8.55022000	-2.80514000	0.64619100
C -1.65121400	7.90134500	0.05600700	H -8.16002900	-3.64008900	-0.85650400
C 1.41116000	-0.54516600	-0.64576100	H -9.49921900	-2.49549000	-0.81069200
H 0.90264200	-0.76308400	0.29723600	C -8.11720800	-0.18322300	-0.26528900
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P 0.32796100	-1.19351100	-1.98086600	C -8.08044800	-0.09646400	1.27139600
C -1.34918600	-0.42504300	-1.97033500	H -7.05608000	0.03561900	1.63587200
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H -1.18612200	0.65643300	-1.92157800	H -8.65727400	0.77139300	1.60943600
C -2.35517700	-0.86926800	-0.87984600	C -7.49918700	1.10490100	-0.83717100
H -2.54859000	-1.93904300	-0.98317900	H -6.44129800	1.18403600	-0.57158900
N -1.82054900	-0.63710800	0.46196800	H -8.01054800	1.97973900	-0.42052500
H -1.21363200	0.18884900	0.57466100	H -7.59108700	1.16819800	-1.92489800
C 1.08387400	-0.77820700	-3.58937600	C -3.71412500	-0.11168300	-1.04384100
C 2.34808800	-0.22120000	-6.02537200	C -4.18841400	0.03946000	-2.49301100
C 0.35027100	-0.25256800	-4.66392300	H -4.24891800	-0.92185800	-3.01302100
C 2.45991300	-1.01991300	-3.74362200	H -3.52708400	0.69983200	-3.06081200
C 3.08335500	-0.73770300	-4.95766100	H -5.17885400	0.49650400	-2.50024100
C 0.98255000	0.02131100	-5.87673600	S -1.61237900	-1.84301600	1.58260600
H -0.70824700	-0.03843600	-4.57020200	O -0.18155600	-2.02789200	1.88349300
H 3.06599700	-1.40076000	-2.92664700	O -2.38635100	-3.00186500	1.10692800
H 4.14938100	-0.91464000	-5.05568700	C -2.34522900	-1.16062900	3.07146400
H 0.40628100	0.43148300	-6.70038800	C -3.49355400	-0.21060400	5.43989600
H 2.83881500	-0.00094400	-6.96867000	C -1.73679100	-1.44670500	4.29454200
C 0.13060900	-2.99860300	-1.87940100	C -3.52144000	-0.41113400	3.01084300
C -0.20384700	-5.76860300	-1.77528100	C -4.08269800	0.05862400	4.19586600
C -0.71966300	-3.64287200	-2.79605400	C -2.31754100	-0.97185400	5.46882800
C 0.82223400	-3.74818300	-0.91659800	H -0.82017300	-2.02484400	4.31728300
C 0.64901700	-5.13351500	-0.87533200	H -3.98254100	-0.20263000	2.05148700
C -0.88806000	-5.02275400	-2.73965900	H -4.99544300	0.64728600	4.15325000
H -1.23989800	-3.07388300	-3.56187900	H -1.84677100	-1.19398800	6.42278400
H 1.50413900	-3.29133400	-0.20620400	H -3.54755900	0.89581600	-0.63991000
H 1.18848800	-5.70698600	-0.12877100	C -4.09649300	0.33257600	6.71259400

H -5.18866700	0.36314100	6.65663300	C -0.28893500	5.54068200	-0.05941800
H -3.75256800	1.35669600	6.90339300	C 0.27234200	5.64760500	-2.44609300
H -3.81601700	-0.27280200	7.57900000	C 0.29933300	4.30233800	0.04290900
C 1.78034400	0.90055300	-0.77893800	C -0.32785500	6.24813200	-1.29151900
H 2.43300100	1.17114900	-1.60125000	C 0.24531100	6.35536500	-3.67824800
C 3.46763200	1.00718300	0.65618500	H 0.33376100	3.77305800	0.98544200
H 3.83739500	1.87494600	0.11063800	H -1.38342700	7.98024000	-0.53937700
C 2.78114000	1.30873300	1.93334600	H -0.73116900	6.00028500	0.82070800
C 1.56039900	1.96530800	4.37658500	C -0.34845700	7.59416900	-3.76727300
C 2.64415000	2.64890600	2.32770700	H 0.70478300	5.90086300	-4.55217200
C 2.29643300	0.30013500	2.78045000	H -0.36085700	8.12376900	-4.71555000
C 1.68538800	0.62941200	3.98793200	C -0.94314200	8.18711000	-2.62667600
C 2.04328900	2.97525400	3.54279000	H -1.40703500	9.16565300	-2.70949300
H 3.01878100	3.43554600	1.67914700	C -0.93081300	7.52764700	-1.41814500
H 2.38971200	-0.73895900	2.48755000	C 1.23568100	-1.10034300	-0.25131300
H 1.30460600	-0.16093100	4.62744600	H 0.63927900	-1.09825600	0.66478000
H 1.95620100	4.01704100	3.83770200	H 2.03238600	-1.84166700	-0.11397100
H 1.08973800	2.21689600	5.32269700	P 0.15946600	-1.79953900	-1.57407400
N 4.12231400	-0.15923500	0.55344200	C -1.44062500	-0.89913200	-1.77431800
S 5.16769400	-0.30491300	-0.72616900	H -1.85002300	-1.27405200	-2.71408000
O 5.32424300	0.94156300	-1.50386600	H -1.18491700	0.15602900	-1.91616700
O 4.77149700	-1.52987200	-1.48137300	C -2.52580800	-1.04617400	-0.67776900
C 6.73345000	-0.66900700	0.05952800	H -2.77287500	-2.10228600	-0.54301400
C 9.18845800	-1.21994100	1.24768000	N -2.04534500	-0.51369100	0.60040600
C 7.79566400	0.22565400	-0.10182100	H -1.34697100	0.24685500	0.54441700
C 6.89044900	-1.83648000	0.80820100	C 1.04292700	-1.67675300	-3.15925600
C 8.11863700	-2.11305500	1.40640000	C 2.51297200	-1.51741700	-5.53526900
C 9.02014600	-0.05071900	0.49043200	C 0.39147000	-1.42175600	-4.37741000
H 7.65116600	1.12266900	-0.69328500	C 2.43680600	-1.85320900	-3.14327900
H 6.06107300	-2.52618700	0.93182900	C 3.16587600	-1.76284000	-4.32728400
H 8.22995900	-3.02062000	1.98685800	C 1.12690700	-1.35070400	-5.55991500
H 9.86392700	0.62197300	0.38055300	H -0.68129500	-1.26779600	-4.41952100
O 10.42682400	-1.39790200	1.78582600	H 2.97790300	-2.03262400	-2.22129800
C 10.66590200	-2.56199300	2.56387100	H 4.24478200	-1.86155900	-4.28023800
H 10.01541200	-2.59920600	3.44652400	H 0.61627800	-1.15160900	-6.49708300
H 11.70582700	-2.49806100	2.88665200	H 3.08302400	-1.44428100	-6.45657200
H 10.52602200	-3.47726200	1.97528500	C -0.20273800	-3.55757700	-1.26042500
H 3.68141500	-2.21095500	1.01443200	C -0.80866800	-6.24562600	-0.79486500
O 3.67279000	-3.12129600	0.66769500	C -0.42820600	-4.42776400	-2.34054900
H 4.03853100	-2.96593200	-0.21937900	C -0.27245900	-4.04363400	0.05499000
			C -0.57810100	-5.38644400	0.27900400
			C -0.73262200	-5.76619600	-2.10462300
			H -0.34931400	-4.06626600	-3.36091200
			H -0.09756800	-3.39168800	0.90374900
			H -0.63543400	-5.75451100	1.29808800
			H -0.90207000	-6.43515800	-2.94269500
			H -1.04340200	-7.29017300	-0.61337200
			O -4.88087600	-0.61028900	-0.19132600
			Si -6.05215000	-1.82468600	-0.03203800
			C -6.18592600	-2.15401300	1.81711900
			H -5.21349500	-2.48778000	2.18808400
			H -6.91510300	-2.94698000	2.01479200
			H -6.48679200	-1.27509200	2.39219300
			C -5.47495300	-3.43889700	-0.83845200
			H -5.30373700	-3.36887600	-1.91615100
			H -6.22043100	-4.22608300	-0.67819100
			H -4.54807800	-3.77181200	-0.35948300
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TS IIS-W

(227.33i)

Ettotal:-4464.319539

G:-4464.439312

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O 1.54459900 2.49849800 -1.06376700

C 0.87303600 3.71450500 -1.11172100

H 1.33568800 3.89444900 -3.18162000

C 0.86866200 4.36589800 -2.32256400

C -7.83064700 -1.60339100 -2.29165500
H -7.73257600 -2.67550600 -2.49030500
H -7.05535500 -1.09489000 -2.86917100
H -8.80005800 -1.28909500 -2.70280000
C -8.82522700 -2.25044200 -0.12378800
H -8.92816600 -2.10641600 0.95384500
H -8.58142900 -3.30621600 -0.28980000
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C -8.22187200 0.17666800 -0.51692500
H -9.27440900 0.21068500 -0.84554500
C -8.20417400 0.61356300 0.95895500
H -7.17846300 0.71670200 1.32874100
H -8.73256100 -0.08104500 1.61687100
H -8.68543900 1.59202700 1.06378800
C -7.46942400 1.23318000 -1.34468100
H -6.41625000 1.28260300 -1.05430600
H -7.90625700 2.22281500 -1.17125500
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C -4.23958600 -0.49132000 -2.56203500
H -4.32062100 -1.54846000 -2.83423000
H -3.52764400 -0.01165700 -3.23922700
H -5.20708200 -0.01742700 -2.73264000
S -2.00949600 -1.37558000 2.01232200
O -0.61226700 -1.58497800 2.45143100
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C -2.73688800 -0.25745500 3.20900100
C -3.88751000 1.40638100 5.14008500
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C -4.49315100 2.33079700 6.16793000
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H 2.56493500 0.29975800 -1.33693100
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N 4.52977000 0.41681500 0.39452100
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O 5.16096800 -0.82656100 -1.74352600
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C 6.68326600 -1.22211000 0.38092000
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H 8.41706600 -3.37308200 2.34896400
H 9.79758500 0.14118700 0.28569500

O 10.54454400 -1.73681900 1.79791600
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H 10.31813200 -2.79224700 3.58751000
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H 1.81911400 4.51106200 4.10767600
H 5.58504300 1.89661600 -0.33092500
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It IIR-W

Ettotal:-4464.337553

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H 2.19990800 3.57445200 -2.92259600
C 1.71155000 4.11098400 -2.11535100
C 0.48865900 5.44823500 0.02620200
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C 0.89382400 4.14346500 0.18021300
C 0.67241200 6.14219800 -1.20054600
C 1.49519800 6.15243800 -3.51668300
H 0.75594500 3.61730600 1.11639900
H -0.21668900 8.00473000 -0.55056300
H 0.01957200 5.96849600 0.85676600
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H 1.97560100 5.63385400 -4.34201300
H 1.23590700 7.97711300 -4.59931500
C 0.45889600 8.13337500 -2.58033000
H 0.13938100 9.16364500 -2.70530800
C 0.25984100 7.48916500 -1.38024600
C 1.09004900 -1.32122500 0.10866100
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H -1.42262100 0.32311200 0.58803300
C 1.04330300 -2.34557900 -2.64501400
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C 0.65691800 -1.96392600 -3.93951500
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H 1.20250300 -1.91431100 -6.01662700
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C 3.27023900 -0.04657900 0.66147000
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C 2.89538900 0.31431900 2.09391700
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C 2.84826800 1.66138400 2.48195600
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H 3.12268900 2.43195300 1.76637700
H 2.66079800 -1.71294000 2.78553500
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H 2.46933800 3.07533300 4.06098600
H 1.88083300 1.32164000 5.72757700
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O 4.71293800 -0.64002000 -1.79626000
O 5.22788400 -2.92469700 -0.82454700
C 6.62198700 -0.83539600 -0.00809600
C 9.10702200 0.07561600 0.87829000
C 7.04695200 -1.12213500 1.29510100
C 7.43458800 -0.09172300 -0.85813300
C 8.68007200 0.36904200 -0.42158700
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H 6.39514000 -1.67969300 1.95912200
H 7.08301200 0.13331700 -1.85901400
H 9.29757800 0.95064600 -1.09569000
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O 10.30040600 0.47551000 1.41091900
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H 3.46208400 -2.95751700 1.04304600
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It IIS-W

Etotal:-4464.330914

G: -4464.452718

E(RmPW1PW91):-4464.994364

C 0.68632800 1.66976000 -0.39651100

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C -1.53300000 5.45376400 -0.32051200
C -0.94665500 3.87060200 -2.57587800
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C -1.85182200 6.27351800 0.79614200
H -0.67998000 3.24956500 -3.42472800
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C -2.78935000 7.27513200 0.68954900
H -1.34106600 6.09401100 1.73812900
H -3.02292400 7.89409500 1.55076100
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C -3.16794200 6.73194000 -1.63980000
C 1.47922000 -0.72299400 -0.29923700
H 0.97737900 -0.83964600 0.66562500
H 2.40881600 -1.30236200 -0.23144400
P 0.49032900 -1.62055100 -1.53509200
C -1.19760900 -0.90469600 -1.76504700
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C -2.29245900 -1.13588400 -0.68944600
H -2.54597400 -2.19704400 -0.65923500
N -1.85849800 -0.76255700 0.65278900
H -1.28886700 0.08100800 0.75490100
C 1.32745900 -1.48510400 -3.14932000
C 2.69132500 -1.31972800 -5.58687800
C 0.62741400 -1.61281900 -4.36142600
C 2.71921800 -1.29591300 -3.17080800
C 3.39319500 -1.20001900 -4.38841100
C 1.31072300 -1.53465500 -5.57264600
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H 4.45862500 -1.00100700 -4.36248200
H 0.76241600 -1.63350600 -6.50459300
H 3.21606700 -1.24329200 -6.53462300
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C 0.24675100 -6.08589600 -0.44460100
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C 1.35692400 -3.94145300 -0.23765800
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C -0.72231300 -5.51692400 -1.27350700
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H 2.03767900 -5.74055900 0.70589500
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H 0.19414300 -7.14197000 -0.19761800
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C -5.13833900 -3.54217100 -1.12458100
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C -7.28658400 1.08753000 -1.25305800
H -6.23295500 1.14696800 -0.96643600
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S -1.67415000 -1.86772300 1.88956300
O -0.25120400 -2.09660200 2.18454300
O -2.51635400 -3.02176700 1.53372900
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C -1.68398000 -1.07916900 4.51408700
C -3.53215400 -0.24805600 3.16733600
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H -3.69775200 0.50864500 7.67232900
H -5.05326600 1.09956300 6.69554500
C 1.85591500 0.73887500 -0.58658000
C 3.09603400 1.11831000 0.37680500
N 4.22993400 0.30127700 0.01786000
S 4.57832400 -0.94839700 0.97572300
O 4.19971100 -2.24813300 0.32598500
O 4.10540300 -0.77361100 2.37192600
C 6.37459100 -0.96480700 1.01051700
C 9.16158500 -1.00825300 1.12178600
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C 7.02610300 -0.69439800 2.20864600
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C 8.49831200 -1.28326400 -0.08553800
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H 6.43455200 -0.47551200 3.09067900
H 2.23051600 0.86573200 -1.60349700
H 8.91332100 -0.50447400 3.21491900
H 9.09534400 -1.51401400 -0.96191800
O 10.52618700 -1.05506700 1.06670600
C 11.25328900 -0.79500900 2.25618100
H 11.06409500 0.21776400 2.63481500
H 12.30781500 -0.88724300 1.99148400
H 11.01472100 -1.52052100 3.04449500
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C 3.40665500 2.60588200 0.26815100
C 3.93373200 5.36434600 0.10420600
C 3.00559400 3.47410800 1.29104700
C 4.08562500 3.13625300 -0.83849900
C 4.34334500 4.50395100 -0.91794400
C 3.26683000 4.84473300 1.21268800
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H 4.42868600 2.47143900 -1.62601500
H 4.87151700 4.90122400 -1.78064200
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H 4.14097300 6.42884300 0.03942100
O 5.39822200 0.34996600 -2.49790400
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H 6.28721500 0.69090900 -2.33925300

TS IIIR-W

(484.65i)

Etotal:-4464.312579

G: -4464.432627

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C 1.16041300 3.98724700 0.37767300
H 2.68423100 4.33990300 -1.06421600
C 1.85556000 4.77336900 -0.51159600
C -0.27043500 5.81732100 0.98897100
C 1.49522000 6.13359200 -0.68645500
C 0.09178400 4.49947000 1.15214500
C 0.40539500 6.66925200 0.07552700
C 2.18124800 6.98440000 -1.59574800
H -0.43057600 3.85379000 1.84374600
H -0.78133200 8.43478800 0.47451700
H -1.09133600 6.22432000 1.57353200
C 1.80652400 8.29993400 -1.74636900
H 3.00729200 6.57505500 -2.17071600
H 2.33814400 8.93947700 -2.44495700
C 0.72835300 8.82950700 -0.99457000
H 0.44359300 9.86967700 -1.12354500
C 0.04541800 8.03167200 -0.10504000
C 0.96372300 -0.83852100 1.17164100
H 0.16267100 -0.47474400 1.82257100
H 1.71944700 -1.30359800 1.81324900
P 0.20289100 -2.27054100 0.27818400
C -1.04286300 -1.77644700 -0.97763600
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C -2.44107000 -1.34150800 -0.48011200

H -2.96307000 -2.19908900 -0.04992200
N -2.34769000 -0.32822300 0.57289400
H -1.62770900 0.40511200 0.51998900
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C 1.86995800 -3.00903300 -1.87723900
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C 2.99014000 -5.17434900 -0.49025500
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C 5.06168600 -2.24727500 2.30784100
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H 5.60161500 -2.16513700 4.39570400
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O 4.58461200 0.62967800 -3.25158100
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C 8.08394200 -1.38868800 -1.57350700
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H 8.46981800 -2.26381600 -2.08211800
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H 9.99723600 -3.22067100 -0.58292500
H 11.57455900 -2.47486600 -0.21379100
H 10.79345800 -2.16604800 -1.78717300
O 1.10993400 -0.15942900 -2.18122800
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TS IIIS-W

(928.43i)
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G: -4464.417723
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H -1.56630600 4.84022500 0.14516700
C -1.13560100 4.71260900 1.13275300
C -0.05268100 4.31935200 3.69520100
C -0.57427200 5.81986100 1.82295500
C -0.60311600 3.26111800 3.01236400
C -0.01726000 5.62256700 3.12877300
C -0.54572500 7.12269900 1.25615400
H -0.63565400 2.26823200 3.44492500
H 0.96482800 6.58050500 4.80232200
H 0.36166300 4.16830200 4.68857000
C 0.00743700 8.17894700 1.94424700
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H 0.99031200 8.82562800 3.76751800
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H 2.64843600 -2.16265800 -0.08436500
N 2.14690100 -0.16695000 -0.41307900
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C -1.34723000 -2.30452900 2.42618600
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C -0.77265300 -2.31174600 3.70918600
C -2.71876600 -2.56089500 2.27669200
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C 0.14081900 -6.21215300 -1.06137400
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C -1.14853000 -4.18996100 -0.71967600
C -1.00196100 -5.44932600 -1.30063100
C 1.14184900 -5.71806500 -0.22525700
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H 0.25039600 -7.18904000 -1.52246700
O 4.89644100 -0.95737800 0.38856600

Si 5.95500000 -2.12932500 -0.22626700
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H 3.69307400 0.12611200 1.58924100
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C -8.76558200 -1.53174900 -1.63049700
C -8.11985500 -1.31328100 0.70260600
H -6.01530600 -1.04409900 1.09149600
H -7.13123100 -1.44024200 -3.04272300
H -2.83111400 0.10394600 1.00703700
H -9.51771200 -1.65573800 -2.39982700
H -8.42318100 -1.26808100 1.74333500
O -10.38894400 -1.58408700 0.19692200
C -11.44494000 -1.74378100 -0.73881500
H -11.50708700 -0.89189600 -1.42747600
H -12.36186000 -1.79750900 -0.15039800
H -11.33443800 -2.66793300 -1.31995300
H -2.51033200 0.11052500 -2.00665200
C -2.80427000 2.14235300 -1.60903300
C -2.61669500 4.78868300 -2.54187600
C -1.65021400 2.58677300 -2.27038100
C -3.86581500 3.03340600 -1.43315100
C -3.77170100 4.34835600 -1.89327100
C -1.55525700 3.89946300 -2.73085100
H -0.82678500 1.89610600 -2.43789100
H -4.77249800 2.68332000 -0.95329200
H -4.60793700 5.02762400 -1.75111900
H -0.65625000 4.22424400 -3.24767100
H -2.54929700 5.80887200 -2.90990700
O -4.00271100 -0.03843400 1.66557700
H -4.40493300 0.22775600 0.18687800
H -4.09506300 0.77603800 2.18080900

It IIR-W

Etotal:-4464.337794
G: -4464.459085
E(RmPW1PW91):-4464.986322
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O 1.46495500 2.50340300 1.16188500
C 0.82830700 3.70522600 0.93643500
H 2.35915200 4.25054700 -0.44668200
C 1.44146400 4.56154200 0.04426600
C -0.86830000 5.35406300 1.41310600
C 0.91197700 5.85653700 -0.19600200
C -0.33756300 4.10699400 1.64209100
C -0.27504400 6.26304700 0.49544100
C 1.52033800 6.76606000 -1.10306000
H -0.79754200 3.41946400 2.33755700
H -1.70763200 7.85948000 0.77676700
H -1.76192100 5.66362000 1.94931800
C 0.97896700 8.01328700 -1.32012200
H 2.42404600 6.45904800 -1.62291200
H 1.45502600 8.69766600 -2.01655800
C -0.19642800 8.41371300 -0.63894100
H -0.61268600 9.40072100 -0.81851700
C -0.80689700 7.55608700 0.24877100
C 0.96516800 -1.14325500 1.64369400
H 0.05206000 -1.09102500 2.24674600
H 1.65001200 -1.84826400 2.12547000

P 0.40198100 -2.05445400 0.08269600
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H -0.60919800 -1.39020000 -1.97173300
H -0.26556300 -0.01244800 -0.93045900
C -2.20701400 -0.96063300 -0.56431700
H -2.64850600 -1.95097000 -0.68956800
N -2.36767200 -0.57176400 0.83585300
H -1.70477600 0.15513100 1.17680400
C 1.80861000 -2.48308700 -0.99661700
C 3.97780600 -3.20328800 -2.61361600
C 2.18623000 -1.66593300 -2.07341500
C 2.53441900 -3.65621300 -0.72957000
C 3.61404100 -4.01170400 -1.53425600
C 3.26527300 -2.03442600 -2.87875000
H 1.66380000 -0.73810000 -2.28313000
H 2.24908500 -4.29884700 0.09708600
H 4.16552800 -4.92248100 -1.32216000
H 3.54487800 -1.40074500 -3.71478900
H 4.81479600 -3.48570600 -3.24526300
C -0.40785200 -3.64539700 0.45315000
C -1.62474000 -6.10876500 0.97114500
C -0.89060100 -4.43415800 -0.60643100
C -0.53772900 -4.10151400 1.77125000
C -1.14330900 -5.33361000 2.02366000
C -1.49992500 -5.65782000 -0.34574900
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H -0.20355700 -3.49345200 2.60202200
H -1.24889400 -5.67573200 3.04801900
H -1.87565300 -6.25929000 -1.16772400
H -2.10224600 -7.06274300 1.17344300
O -4.38256900 -0.19324800 -1.37635500
Si -5.47495500 -1.32115300 -2.00430200
C -6.58517300 -1.81453700 -0.56422100
H -5.96683300 -2.25999900 0.22073900
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H -7.12750000 -0.97140000 -0.12966600
C -4.59894700 -2.90622200 -2.57390300
H -3.83735600 -2.75237600 -3.34390300
H -5.33348300 -3.60999200 -2.98230000
H -4.13121100 -3.39747000 -1.71398300
C -6.50420900 -0.59822400 -3.48385100
C -5.70308200 -0.72330700 -4.80336200
H -5.50643500 -1.77195500 -5.04900400
H -4.73962300 -0.20855000 -4.78040700
H -6.27813500 -0.30041000 -5.63897900
C -7.74219400 -1.52039900 -3.64828100
H -8.41892300 -1.49207800 -2.79107000
H -7.45161100 -2.56650300 -3.79878100
H -8.31936700 -1.21987900 -4.53350400
C -7.00797800 0.88123900 -3.32517500
H -7.70241000 1.03129000 -4.16929200
C -7.80838300 1.15665900 -2.03931600
H -7.15740100 1.15011700 -1.15873300
H -8.61127000 0.43395900 -1.87212200
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H -5.18680800 1.87589100 -2.64573500
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H -5.38010300 1.89452800 -4.40969500
C -2.98059100 0.03999400 -1.48334500
C -2.50597700 0.09473200 -2.93882500
H -2.54380200 -0.88289500 -3.42986300
H -1.48416700 0.47838200 -3.00640400
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S -3.11983800 -1.47640000 1.98835800
O -2.17399500 -1.78679400 3.07837000
O -3.79618000 -2.59096100 1.30106100
C -4.33243900 -0.36260200 2.70645000
C -6.27540000 1.27927100 3.87527300
C -4.52574300 -0.39962600 4.08735700
C -5.09173500 0.48599800 1.89722700
C -6.05315700 1.30013100 2.48982100
C -5.49600200 0.42110100 4.66060600
H -3.90918900 -1.04858500 4.69840500
H -4.92274800 0.51329700 0.82588700
H -6.63819600 1.97025000 1.86500600
H -5.64269000 0.39935100 5.73714100
H -2.81307000 1.03184600 -1.04514900
C -7.33800700 2.15300000 4.49671200
H -7.33329500 3.15777300 4.06255000
H -7.19730500 2.24872400 5.57665100
H -8.33804700 1.73427800 4.32996500
C 1.59926500 0.19163200 1.43842400
C 3.10158500 0.39458800 1.44067600
H 3.30258200 1.35535100 1.92191800
C 3.87469600 -0.66349900 2.21734500
C 5.23425200 -2.58990400 3.75801100
C 3.81303300 -0.63796100 3.61949000
C 4.62885300 -1.66694200 1.60050000
C 5.30436900 -2.62240200 2.36632000
C 4.48332800 -1.59048100 4.38374800
H 3.22966600 0.13772700 4.10913300
H 4.69261200 -1.68827000 0.51865000
H 5.89046300 -3.39085600 1.86917300
H 4.42595800 -1.54988500 5.46794800
H 5.76216400 -3.33051900 4.35208300
N 3.58530600 0.50711500 0.01566300
S 4.72234300 1.67936600 -0.40094600
O 4.97129400 2.60040700 0.71370000
O 4.26258400 2.19794000 -1.71469400
C 6.25406800 0.80729400 -0.70694700
C 8.63860100 -0.54866800 -1.18041300
C 7.20827800 0.70924300 0.31213000
C 6.48951600 0.23920800 -1.95676600
C 7.68239900 -0.44077800 -2.20055800
C 8.39488200 0.03172900 0.07485900
H 7.01959400 1.17542200 1.27229100
H 5.75087800 0.34750200 -2.74282500
H 7.85989300 -0.86750800 -3.18012400
H 9.15495200 -0.05695600 0.84335800
O 9.83311600 -1.18697700 -1.30912700
C 10.15848300 -1.77317900 -2.56158500
H 9.44284500 -2.55741000 -2.83871600
H 11.14673000 -2.21710300 -2.43671900
H 10.19766100 -1.02244900 -3.36048000
H 2.78541000 0.67200900 -0.59810900

O 1.47519700 1.63033100 -2.06884100
H 2.38567100 1.96169300 -2.18751400
H 1.05687200 2.30434300 -1.51404700

It IIIS-W

Etotal:-4464.329538

G: -4464.450606

E(RmPW1PW91):-4464.975080

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C -1.70282800 4.13334200 1.41542000
C 0.16645700 4.16648100 3.50813000
C -1.17794200 5.37802800 1.85156500
C -0.35895900 2.97109800 3.07677500
C -0.21976500 5.39977300 2.91720700
C -1.57156200 6.60896600 1.25951600
H -0.06371200 2.02897100 3.51889000
H 1.02860000 6.66134100 4.15535800
H 0.88794700 4.17970800 4.32129600
C -1.04486000 7.80292800 1.69767600
H -2.29686900 6.58771500 0.45051100
H -1.35441800 8.73605100 1.23555000
C -0.09833800 7.82435700 2.75152300
H 0.30927400 8.77296700 3.08903600
C 0.30297600 6.64899900 3.34567800
C -1.04659200 -1.35371100 -0.22463700
H -0.39746000 -1.13876500 -1.08394200
H -1.73911000 -2.14307900 -0.54509900
P 0.04015700 -2.25383600 0.97840800
C 1.71944800 -1.64516700 1.46484400
H 2.15944200 -2.51446500 1.96172500
H 1.53677200 -0.85871900 2.19763200
C 2.70861500 -1.14088000 0.39298400
H 2.90992600 -1.92927200 -0.33568900
N 2.14532200 0.02366400 -0.30760200
H 1.36015500 0.48448900 0.19423000
C -0.86664500 -2.52345000 2.53034000
C -2.38245400 -2.88511000 4.85597900
C -0.26437000 -2.39866200 3.79186000
C -2.23207500 -2.83793300 2.44350100
C -2.98774300 -3.01382400 3.60401500
C -1.02158800 -2.58393600 4.94819800
H 0.78575500 -2.14832100 3.88536000
H -2.71658000 -2.95093700 1.48002300
H -4.04715100 -3.22540700 3.50694600
H -0.54860300 -2.48347900 5.92021000
H -2.97055800 -3.01704000 5.75934300
C 0.35379100 -3.87990100 0.19946900
C 0.88326300 -6.34045200 -1.03042700
C 0.91454000 -3.92093300 -1.09040300
C 0.06241500 -5.08024400 0.86372700
C 0.32678500 -6.30388600 0.24818500
C 1.17601300 -5.14934500 -1.69670300
H 1.15464500 -3.01043600 -1.63152200
H -0.37756500 -5.06226200 1.85491000

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Si 6.13621900 -1.62134900 -0.79400600
C 6.11232500 -1.00716700 -2.57332800
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H 6.42605800 0.03462600 -2.67232200
C 5.51301700 -3.41130600 -0.82250200
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H 4.57946100 -2.72392900 1.89785900
H 3.86342700 -1.59044100 3.05944000
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O 0.64407100 0.34229700 -2.36280100
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C 2.92061500 1.61691200 -2.40590700
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C 4.77597300 3.12549300 -2.18342800
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H 2.65780100 4.16446400 -4.62406600
H 3.92899100 0.24812800 1.47381500
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H 4.64656500 6.04978500 -3.00185100
H 4.77281600 5.45937200 -4.66011700
H 6.05985500 5.11432700 -3.49169600
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N -4.32097000 -0.40277500 0.53963300

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C -6.48759700 -1.56010000 -0.71173500
C -8.72501500 -1.04858400 -2.28869500
C -7.62771600 -0.98683400 -0.13286900
C -6.46756300 -1.88286800 -2.06509000
C -7.58629600 -1.62805900 -2.86117700
C -8.74003400 -0.73356200 -0.91832500
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C -9.91967000 -1.04315300 -4.35833300
H -9.15454000 -0.48655000 -4.91345600
H -10.90836500 -0.72634100 -4.69232000
H -9.79854100 -2.11579400 -4.55432700
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C -3.91273300 4.00318400 -2.00754200
C -2.52477500 2.03487400 -1.74950900
C -4.62445500 2.18061100 -0.57841800
C -4.84653700 3.44296700 -1.13675700
C -2.75071400 3.28870400 -2.31390400
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H -5.75538500 3.98510600 -0.88940500
H -2.01439200 3.71129900 -2.99225100
H -4.08798300 4.98163300 -2.44650400
O -3.85906600 0.49340400 3.22828700
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TS IVR-W

(186.59i)

Etotal:-4464.335067

G: -4464.457048

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C 1.51253800 4.54553600 -0.02518600
C -0.81001100 5.45164100 1.25258700
C 0.98956500 5.81915000 -0.37274300
C -0.28726500 4.22420800 1.58443700
C -0.20312300 6.28208400 0.27178500
C 1.61202300 6.65141400 -1.34202700
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H -1.70759000 5.80576500 1.75301900
C 1.07763400 7.87900800 -1.66264000
H 2.51985200 6.30106900 -1.82583400
H 1.56347600 8.50501400 -2.40550000
C -0.10385000 8.33512600 -1.02837900

H -0.51430500 9.30588700 -1.29045700
C -0.72774200 7.55310100 -0.08241400
C 1.04372700 -0.98056900 1.92397900
H 0.06812400 -0.94633000 2.40368300
H 1.69483000 -1.73643700 2.35673900
P 0.36848300 -2.16319600 0.18457100
C -0.70874300 -1.10843000 -0.89962100
H -0.62963900 -1.51292500 -1.91171200
H -0.23446100 -0.12113100 -0.91386800
C -2.19909000 -0.99646100 -0.50987000
H -2.66425700 -1.98154300 -0.57852300
N -2.34772900 -0.53249300 0.87190400
H -1.68061800 0.19017500 1.18901800
C 1.75554100 -2.63376800 -0.91396200
C 3.93879200 -3.38314600 -2.51396500
C 2.16537100 -1.82026200 -1.98297000
C 2.46596100 -3.81797500 -0.64664300
C 3.54673400 -4.18942000 -1.44232300
C 3.24781200 -2.20149700 -2.77873900
H 1.65350000 -0.88912100 -2.20163300
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H 4.07842700 -5.11208800 -1.22936300
H 3.54417200 -1.56974900 -3.61089300
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C -1.82834500 -6.17476100 0.94468600
C -0.91692300 -4.55634500 -0.60142100
C -0.76664900 -4.17196600 1.78738000
C -1.42300600 -5.38295000 2.01661100
C -1.57650300 -5.75990600 -0.36626600
H -0.70939600 -4.25016400 -1.62264400
H -0.49267700 -3.54645000 2.62868800
H -1.62644100 -5.69618000 3.03568300
H -1.89201000 -6.37491000 -1.20390100
H -2.34416800 -7.11304600 1.12611700
O -4.37074500 -0.24286600 -1.35145700
Si -5.47075300 -1.38012100 -1.94787000
C -6.56922800 -1.84356500 -0.48861000
H -5.94372900 -2.26012500 0.30646300
H -7.30362600 -2.60334700 -0.77782500
H -7.11690400 -0.99302500 -0.07540500
C -4.60608200 -2.97616700 -2.50249200
H -3.86146300 -2.83636800 -3.29131900
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H -4.11761200 -3.45352400 -1.64632500
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C -5.72530800 -0.82886100 -4.75380500
H -5.54027400 -1.88289700 -4.98464700
H -4.75707200 -0.32255400 -4.74832600
H -6.30515000 -0.41411300 -5.59027800
C -7.75787200 -1.59145700 -3.56294600
H -8.42408000 -1.54314800 -2.69834600
H -7.47619300 -2.64204800 -3.69802300
H -8.34317200 -1.30250000 -4.44672400
C -7.00287100 0.81005900 -3.29006700
H -7.70735100 0.94997100 -4.12763300
C -7.78449500 1.11492200 -1.99933900
H -7.12228500 1.11817900 -1.12715500

H -8.59067700 0.40154700 -1.80962100
H -8.23811700 2.11003400 -2.06433500
C -5.90302300 1.87322700 -3.45735600
H -5.16442600 1.80177700 -2.65446000
H -6.34426600 2.87532100 -3.41658200
H -5.38265200 1.79006800 -4.41526600
C -2.96575800 -0.02521200 -1.46605200
C -2.48910500 -0.02133000 -2.92153400
H -2.52856200 -1.01410900 -3.38018000
H -1.46487500 0.35452200 -2.99653100
H -3.12590500 0.64928300 -3.50217500
S -3.10376800 -1.36311000 2.07920900
O -2.15099400 -1.63458900 3.17381100
O -3.81230800 -2.49388500 1.45741100
C -4.28533200 -0.18561100 2.74537700
C -6.19255900 1.55299100 3.82818900
C -4.44127400 -0.11070500 4.12946000
C -5.06698300 0.59442300 1.89020000
C -6.01249200 1.45606600 2.44008100
C -5.39491000 0.75690200 4.65977200
H -3.81413200 -0.71653500 4.77320600
H -4.93000500 0.52908100 0.81565900
H -6.62099100 2.06753500 1.77862100
H -5.51742000 0.81830500 5.73788000
H -2.79444000 0.98174500 -1.06473600
C -7.19957800 2.51603400 4.40909900
H -6.77527900 3.52415400 4.49441200
H -7.51632800 2.20935900 5.40983400
H -8.08999300 2.59253800 3.77785200
C 1.65337000 0.27272900 1.62433200
C 3.15752700 0.46526600 1.49763900
H 3.40042200 1.43153400 1.94894500
C 3.98193100 -0.59142400 2.22219600
C 5.44646300 -2.51697900 3.65948300
C 4.13360500 -0.48689500 3.61274700
C 4.57704900 -1.67120300 1.56211700
C 5.30424500 -2.62718600 2.27694100
C 4.85709400 -1.43989600 4.32697300
H 3.67673500 0.34973700 4.13556900
H 4.47881400 -1.75086900 0.48570600
H 5.76263000 -3.45766500 1.74689200
H 4.96673400 -1.33927300 5.40315300
H 6.01500900 -3.25848400 4.21355500
N 3.51734800 0.54919600 0.04235400
S 4.64328200 1.68896600 -0.47846400
O 4.91709800 2.68275700 0.56632500
O 4.14216600 2.12331700 -1.80690700
C 6.16585800 0.79943700 -0.76491900
C 8.54117000 -0.58009300 -1.21023600
C 7.14704800 0.77229100 0.23278800
C 6.36931300 0.14934600 -1.98003400
C 7.55776100 -0.54267400 -2.20943900
C 8.32908400 0.08280700 0.00957400
H 6.98217600 1.30045400 1.16471600
H 5.60930500 0.20117100 -2.75109400
H 7.71002600 -1.03520300 -3.16188300
H 9.10923900 0.04626600 0.76192500
O 9.73359400 -1.22300700 -1.32777000

C 10.02378900 -1.90064300 -2.54256900
H 9.30161400 -2.70272600 -2.73951600
H 11.01595600 -2.33440400 -2.41352700
H 10.03885600 -1.21096300 -3.39545400
H 2.68486900 0.69475700 -0.53266900
O 1.35540300 1.55129600 -1.97189900
H 2.25312700 1.87304300 -2.18076900
H 0.94171100 2.29584100 -1.51193400

TS IVS-W

(191.50i)

Etotal:-4464.321203

G: -4464.444517

E(RmPW1PW91):-4464.964497

C 1.13868200 0.78774400 -0.32385900
O -0.08304000 1.00065400 -0.37739900
O 1.99807100 1.59030100 -1.09498600
C 1.52475800 2.82649000 -1.54535400
H 2.83265200 3.87779200 -0.23376600
C 2.08891500 3.96254300 -1.01931700
C 0.17264000 4.11534800 -3.06726300
C 1.70503900 5.23833100 -1.51122700
C 0.56078200 2.89031000 -2.57887000
C 0.72562700 5.31992100 -2.55466100
C 2.26331000 6.44100600 -1.00003400
H 0.13575800 1.97129100 -2.96400900
H -0.39727100 6.65675600 -3.83328600
H -0.56863100 4.17461500 -3.85977100
C 1.87190400 7.66506000 -1.49328100
H 3.00637700 6.37595600 -0.20979000
H 2.30620900 8.57651500 -1.09284100
C 0.90363500 7.74576500 -2.52401700
H 0.60411600 8.71766600 -2.90510700
C 0.34522400 6.59890200 -3.04141400
C 0.93232400 -1.09831700 1.13567400
H 0.04192200 -0.68751900 1.59384700
H 1.40984000 -1.84712100 1.76636300
P -0.27871000 -2.52136700 -0.15701100
C -1.68697100 -1.70814800 -1.07951100
H -2.02600900 -2.45243900 -1.80465200
H -1.23842300 -0.87241700 -1.62582600
C -2.90143600 -1.18607900 -0.28308500
H -3.38854700 -2.01097400 0.24325800
N -2.47799600 -0.19078500 0.71086700
H -1.62959900 0.34673300 0.48490500
C 0.77552700 -3.14829900 -1.51220800
C 2.53438000 -4.08164900 -3.49658700
C 0.65448800 -2.70489900 -2.84013800
C 1.80310600 -4.05278200 -1.19289800
C 2.66907200 -4.51896000 -2.17828400
C 1.52824300 -3.17346500 -3.82547500
H -0.12517900 -2.00791900 -3.12502100
H 1.94337900 -4.38366800 -0.16858000
H 3.47156400 -5.19540400 -1.90876800
H 1.41304900 -2.83217900 -4.85056600
H 3.22119000 -4.43528800 -4.25881700
C -1.01062000 -4.00176500 0.64586500
C -2.17833700 -6.19432100 1.94207000

C -1.39715300 -3.90474900 1.99299300
C -1.20876500 -5.21054200 -0.04339500
C -1.78859300 -6.29947400 0.60458600
C -1.98419000 -4.99817800 2.63210700
H -1.25196500 -2.98026100 2.54389800
H -0.90142000 -5.30263900 -1.08007000
H -1.93577700 -7.23049500 0.06499600
H -2.28641300 -4.90948900 3.67086200
H -2.63020200 -7.04487900 2.44391100
O -5.11572000 -0.16696400 -0.53516300
Si -6.59261400 -0.87664600 -0.11227100
C -6.99246100 -0.21953000 1.60669900
H -6.19467800 -0.51846700 2.29120600
H -7.93156900 -0.64898000 1.97133300
H -7.08633400 0.86838500 1.64467000
C -6.43581800 -2.75698900 0.04497400
H -6.19795500 -3.27431800 -0.88824300
H -7.37427700 -3.18077100 0.42095400
H -5.65940700 -2.99197200 0.78064000
C -8.01928100 -0.44045500 -1.36297600
C -8.03716300 -1.43618900 -2.54924400
H -8.23607900 -2.45618500 -2.20501700
H -7.10406000 -1.46409900 -3.11661400
H -8.83810900 -1.17231400 -3.25394800
C -9.35282800 -0.67786000 -0.60152400
H -9.49703000 0.00314600 0.23982300
H -9.41961600 -1.69912300 -0.20896800
H -10.20251800 -0.54305900 -1.28470400
C -8.02979500 1.02836700 -1.92002300
H -8.99215100 1.11850600 -2.45185900
C -8.01446900 2.12810900 -0.84269900
H -7.04159700 2.17915100 -0.34239100
H -8.78108200 1.98669000 -0.07655700
H -8.19206500 3.10540800 -1.30481000
C -6.92970900 1.34324900 -2.94883400
H -5.93861100 1.30570600 -2.48823700
H -7.07075300 2.35464000 -3.34616700
H -6.94297000 0.65951800 -3.80216300
C -3.94640100 -0.54091300 -1.25052300
C -4.25845100 -1.38956500 -2.48734100
H -4.56513100 -2.40693000 -2.22562400
H -3.39504000 -1.45292200 -3.15455300
H -5.06530400 -0.91912900 -3.05059300
S -2.81549300 -0.32746900 2.32808900
O -1.58878500 -0.59364800 3.10806000
O -3.92347200 -1.28789400 2.45602500
C -3.33320500 1.32979200 2.77372700
C -4.19310400 3.87157800 3.56171700
C -2.91667200 1.84615000 4.00135700
C -4.17529800 2.05979300 1.93182500
C -4.59574500 3.32466100 2.33418600
C -3.35252300 3.11242700 4.38632900
H -2.25274400 1.26604400 4.63182500
H -4.48699500 1.63922000 0.98184900
H -5.24709800 3.89998400 1.68148100
H -3.02930700 3.51891200 5.34086400
H -3.49723500 0.40183500 -1.59338500
C -4.62999800 5.25825700 3.96705000
H -3.95476100 6.01743100 3.55335400
H -4.62865600 5.37733000 5.05409600
H -5.63534400 5.48390300 3.59949600
C 1.79281800 -0.24079400 0.40247200
C 3.30400300 -0.41828500 0.53648500
N 3.93069500 -1.16486100 -0.57048800
S 5.07645800 -2.33162700 -0.31097500
O 5.28402600 -2.98050300 -1.61245300
O 4.64393400 -3.09693000 0.87006700
C 6.64200200 -1.57128900 0.12717800
C 9.04897100 -0.33738000 0.79542100
C 7.50121800 -1.12952000 -0.88724100
C 6.98917000 -1.40858400 1.46572700
C 8.19355200 -0.79189900 1.80710600
C 8.69825400 -0.51552000 -0.55367400
H 7.23268900 -1.28652400 -1.92625600
H 6.32602600 -1.77871400 2.23933900
H 2.73915500 -0.74790100 -3.31161600
H 8.45163100 -0.67537600 2.85242700
H 9.38612400 -0.16880500 -1.31740800
O 10.24289000 0.27904200 1.01296900
C 10.65782800 0.49569400 2.35428500
H 9.94890900 1.13213400 2.89814600
H 11.62149700 1.00265400 2.29142100
H 10.78236100 -0.44993200 2.89647100
H 3.43340600 -1.07960800 1.39823100
C 4.01563200 0.89586800 0.90079000
C 5.27709800 3.29024400 1.68336100
C 3.70986300 1.50270000 2.12716400
C 4.96355300 1.50584700 0.07512700
C 5.58965200 2.69311400 0.46205300
C 4.33179900 2.68734900 2.51761200
H 2.96831500 1.04476500 2.77681200
H 5.21819000 1.05535600 -0.87752100
H 6.32374100 3.14942400 -0.19609100
H 4.08073300 3.13811100 3.47387700
H 5.76717200 4.21153600 1.98559700
O 3.33258000 -0.00364200 -3.13531700
H 3.91822100 -0.77889200 -1.52231700
H 2.79824100 0.62555800 -2.61987500

Fig. S1 The B3LYP/6-31G** gas phase geometries of the optimized transition states.

