

Supporting Information

Mechanistic Insight into Conjugated N–N bond Cleavage by Rh(III)- Catalyzed Redox-Neutral C–H Activation of Pyrazolone

Weirong Wu,^{a,b} Yuxia Liu,^{*a} and Siwei Bi^{*a}

^a College of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165, P. R. China.

E-mail: siweibi@126.com; liuyuxia2008@163.com; Fax: +86-537-4456305; Tel: +86-537-4458308

^b Key Laboratory of Inorganic Chemistry in Universities of Shandong, Department of Chemistry and Chemical Engineering, Jining University, Qufu273155, Shandong, China

Cartesian coordinates and electronic energies for all of the calculated structure

R1

SCF done: -571.80596980

C	-1.43969700	-1.36050000	0.00011200
C	-2.81779600	-1.56376300	0.00025100
C	-3.69904800	-0.48131000	0.00017500
C	-3.18211900	0.81451800	-0.00008500
C	-1.80618000	1.04217500	-0.00035400
C	-0.92847500	-0.05372400	-0.00021600
H	-0.75458200	-2.19794500	0.00021100
H	-3.20140700	-2.58020800	0.00045800
H	-4.77238700	-0.64559500	0.00034000
H	-3.85397800	1.66827200	-0.00011900
H	-1.40980100	2.04768300	-0.00059000
N	0.47772000	0.14003600	-0.00040200
C	1.19799700	1.33425500	0.00011800
C	2.53697900	-0.59777500	-0.00010200
C	2.66185200	0.89718300	-0.00001700
H	3.18149300	1.28999200	-0.88149000
N	1.31002700	-0.98767600	-0.00036600
O	0.75794000	2.46955000	0.00053100
H	3.18233100	1.29044800	0.88068800
C	3.66884400	-1.57104200	0.00024900
H	3.28410700	-2.59280300	0.00002000
H	4.30640900	-1.43141600	-0.88100500
H	4.30592700	-1.43144800	0.88182600

K

SCF done: -956.65494723

Rh	0.06475000	-0.10091300	-0.00168800
C	1.56901100	1.52752200	-0.07912000
C	1.68797700	0.77043800	1.13839600
C	1.74283000	0.62608500	-1.18076100
C	2.05568800	-0.59500700	0.78164900
C	2.08324600	-0.68711300	-0.64002500
C	1.16751600	2.96692000	-0.16846100
H	1.61386600	3.54850800	0.64266300
H	1.48144000	3.40842400	-1.11709400
H	0.07430400	3.03928600	-0.09367100
C	1.57937100	1.31529300	2.53016500
H	1.21430700	0.55499600	3.22508800
H	2.55688800	1.65916800	2.89301700
H	0.88752300	2.15955700	2.56835900
C	2.32901800	-1.68922900	1.76696800

H	2.30404300	-2.67259500	1.29413200
H	3.31913500	-1.55581000	2.22022200
H	1.58764200	-1.68855200	2.57013800
C	2.40197700	-1.89379900	-1.46855600
H	3.40451700	-1.80630400	-1.90545600
H	2.37309800	-2.80871900	-0.87379100
H	1.68604200	-2.00769200	-2.28679000
C	1.69490200	0.97560900	-2.63711300
H	2.70209800	1.19000200	-3.01757200
H	1.28484800	0.15199300	-3.22701500
H	1.07103800	1.85393400	-2.81462600
O	-1.14469300	-1.51659600	1.09187000
C	-1.63535500	-1.96189600	0.00066500
O	-1.14188600	-1.53368400	-1.09431200
C	-2.77156000	-2.93888500	0.00823600
H	-3.69051300	-2.34589000	0.00283800
H	-2.74555300	-3.56586800	-0.88526300
H	-2.74695000	-3.55141000	0.91175900
O	-1.43287000	1.33029200	-0.00559400
C	-2.73891200	1.19097700	-0.00981800
O	-3.37538600	0.14490700	-0.01226700
C	-3.44800500	2.54768100	-0.01305300
H	-3.14858000	3.13229400	0.86257600
H	-3.16186900	3.11955700	-0.90158600
H	-4.52862300	2.39929100	-0.00460100

0

SCF done: -1528.47552313

Rh	1.79274300	-0.28504900	0.09206600
C	2.45680500	-1.92384500	-1.20235100
C	2.88149500	-2.17973900	0.15944700
C	1.01506100	-1.87470200	-1.20013400
C	1.71515500	-2.27174700	0.99117500
C	0.55239900	-2.06851700	0.14939900
C	3.35421100	-1.83509500	-2.39977100
H	4.32211900	-1.40077200	-2.13802400
H	3.53764200	-2.83014100	-2.82504000
H	2.91372600	-1.21423100	-3.18320000
C	4.30453600	-2.30794400	0.60629100
H	4.40773900	-2.12067300	1.67654000
H	4.67376800	-3.32056500	0.40059500
H	4.94951900	-1.60086200	0.07904600
C	1.65457400	-2.49000900	2.47047800
H	1.08517100	-3.39726600	2.70223400

H	2.64984200	-2.59440300	2.90679700
H	1.15869800	-1.63744500	2.94651700
C	-0.86392900	-2.10312500	0.63232900
H	-1.14632000	-3.12380400	0.91843300
H	-0.98512600	-1.45973200	1.50813800
H	-1.56469100	-1.76668300	-0.13261700
C	0.14230900	-1.63321300	-2.39216100
H	-0.22067400	-2.59071800	-2.78678300
H	-0.72810500	-1.02149600	-2.14208300
H	0.68951500	-1.12717400	-3.18980800
O	0.96402800	0.55415600	1.82066900
C	0.78239900	1.80790900	2.13607800
O	1.01172200	2.78634300	1.42014000
C	0.16097300	1.99642300	3.51706200
H	0.40712400	1.17356900	4.19133200
H	0.49261600	2.94737500	3.93907700
H	-0.92648200	2.03694900	3.39108500
O	1.55402800	1.48723200	-1.15054100
C	2.63474800	1.97505700	-0.67409100
O	3.34404600	1.23111000	0.07713400
C	3.03876000	3.38980500	-0.96134100
H	2.67972300	3.70412900	-1.94370800
H	2.56700700	4.01127500	-0.19433900
H	4.12262500	3.50134500	-0.89589000
C	-4.48569500	-0.44123000	1.09787400
C	-5.37245500	-1.50110900	1.28440500
C	-5.78230700	-2.29774000	0.21420400
C	-5.29373400	-2.01920700	-1.06324400
C	-4.40819700	-0.96407500	-1.27447600
C	-3.99663900	-0.16845600	-0.19180900
H	-4.17377100	0.17757700	1.92739400
H	-5.74578100	-1.70090600	2.28507300
H	-6.47389600	-3.11987600	0.37229200
H	-5.60579600	-2.62399800	-1.91041500
H	-4.03567100	-0.74061300	-2.26554200
N	-3.09250800	0.89545100	-0.41795500
C	-2.61960000	1.85418300	0.48097700
C	-1.81479200	2.11799900	-1.70349500
C	-1.71755800	2.75165700	-0.35136200
H	-2.07658300	3.78736900	-0.32782500
N	-2.57800100	1.07825400	-1.71523500
O	-2.88344100	1.93309500	1.67023000
H	-0.69177300	2.75913300	0.04644300
C	-1.08767100	2.57068000	-2.92383100

H	-1.37938600	1.96690500	-3.78622900
H	-1.30098200	3.62468500	-3.13707200
H	-0.00984700	2.47305400	-2.75402700

TS0-1

SCF done: -1528.4359223

Rh	0.70464100	-0.33855700	-0.38684300
C	2.20809600	-1.91120600	-0.69970600
C	1.61462600	-2.03901700	0.60155700
C	1.15547700	-2.02658300	-1.67664100
C	0.19538900	-2.34368700	0.42513800
C	-0.06849800	-2.37247500	-0.97112600
C	3.66116700	-1.71480100	-0.99340200
H	4.14593600	-1.13617800	-0.20774200
H	4.14876300	-2.69547100	-1.07168100
H	3.80852800	-1.19333900	-1.94160700
C	2.33846000	-1.95147900	1.90634100
H	1.64418300	-1.75326300	2.72445300
H	2.85757200	-2.89527500	2.11766600
H	3.06530800	-1.13765500	1.87110000
C	-0.76500700	-2.59703700	1.54521400
H	-1.80159500	-2.56262500	1.20713900
H	-0.57934800	-3.57969600	1.99645200
H	-0.64780100	-1.83863600	2.32379300
C	-1.34346300	-2.74175800	-1.65640200
H	-1.22353000	-3.72590000	-2.12789200
H	-2.18325200	-2.79040800	-0.96528400
H	-1.59238400	-2.02356600	-2.44108300
C	1.32652500	-2.01492200	-3.16541900
H	1.58683800	-3.01582200	-3.53428300
H	0.40683600	-1.70619700	-3.66784800
H	2.12274200	-1.33088800	-3.46764200
O	0.33476700	0.71877400	1.47108900
C	0.72074900	1.87004000	1.84467500
O	0.70443200	2.93635600	1.15069900
C	1.26912100	1.98829500	3.25155600
H	2.33330700	1.73376100	3.20486500
H	1.16227800	3.00720300	3.62581300
H	0.77399500	1.27828000	3.91708700
O	1.98194100	1.20831600	-0.95177600
C	3.02338000	1.51981900	-0.22713900
O	3.43027500	0.90717000	0.76409900
C	3.71692800	2.79151500	-0.70114600
H	3.72259500	2.86291700	-1.79170200

H	3.15681900	3.64618600	-0.30759400
H	4.73592600	2.82844300	-0.31254500
C	-3.36279800	0.23248700	1.66139500
C	-4.34579000	-0.64050000	2.12580200
C	-4.99742900	-1.51067500	1.24791500
C	-4.67311400	-1.48677000	-0.11077500
C	-3.70459800	-0.60309900	-0.58892000
C	-3.03340800	0.24699800	0.29889800
H	-2.85425200	0.91178700	2.33334400
H	-4.59930400	-0.64378500	3.18212600
H	-5.75913000	-2.19151700	1.61648600
H	-5.19035900	-2.14269400	-0.80606000
H	-3.46845000	-0.55354300	-1.64575200
N	-2.06681400	1.16414200	-0.16703000
C	-2.12144400	2.55407500	0.06326300
C	-0.70515800	1.98816100	-1.67103000
C	-1.04850300	3.07928800	-0.81043300
H	-1.07123000	4.11384300	-1.13770100
N	-1.19929800	0.83071200	-1.22563100
O	-2.86400300	3.10870900	0.85785500
H	-0.06139600	2.97326600	0.10927000
C	0.10377400	2.05734600	-2.92112800
H	0.27340300	1.05962600	-3.33037600
H	-0.43840900	2.65728300	-3.66235600
H	1.07095400	2.52546900	-2.73197100

1

SCF done: -1528.4598023

Rh	-0.83651700	-0.27417600	0.02741500
C	-2.84620400	-1.30975300	-0.22971000
C	-1.98241200	-1.69112200	-1.28411700
C	-2.20980000	-1.66446500	1.02744000
C	-0.81587900	-2.35199700	-0.69148300
C	-1.00414300	-2.39914700	0.72210500
C	-4.21514800	-0.71979000	-0.34918100
H	-4.34127500	-0.17431700	-1.28205700
H	-4.95632700	-1.52924800	-0.30042000
H	-4.42822700	-0.03246300	0.47319900
C	-2.22103000	-1.48011900	-2.74686500
H	-1.27724800	-1.44414700	-3.29517700
H	-2.82116600	-2.29822700	-3.16557300
H	-2.74351200	-0.53607200	-2.91220700
C	0.30053500	-2.95918400	-1.48212300
H	1.17778000	-3.15218000	-0.86394200

H	-0.02579200	-3.90332500	-1.93646600
H	0.61176500	-2.28785500	-2.28645600
C	-0.15593400	-3.08022300	1.74883800
H	-0.75094400	-3.83077600	2.28268000
H	0.69646300	-3.58821100	1.29706400
H	0.22158500	-2.36241000	2.48440700
C	-2.87412400	-1.60036800	2.36958600
H	-3.61076900	-2.41008200	2.46054500
H	-2.15397100	-1.71563000	3.18128800
H	-3.40379200	-0.65655200	2.51821800
O	0.43623200	0.41319400	-1.67184400
C	0.83180500	1.55647500	-1.94278100
O	0.53854300	2.62439400	-1.24210000
C	1.68523600	1.82280100	-3.15176100
H	1.03920700	2.16339700	-3.96855500
H	2.40392200	2.61580700	-2.93742500
H	2.19638800	0.91023800	-3.45606500
O	-1.47863500	1.76356700	0.17685400
C	-2.40708100	2.24044000	-0.63903900
O	-2.87754200	1.64621200	-1.60248900
C	-2.82307400	3.66339200	-0.29035500
H	-3.07959000	3.73973100	0.76986800
H	-1.98318600	4.34339800	-0.46867600
H	-3.66861100	3.96835600	-0.90796300
C	3.82077100	0.29543000	-0.56248200
C	4.76201500	-0.59213300	-1.08124000
C	4.76219500	-1.93833600	-0.70785300
C	3.81720700	-2.38577400	0.21697200
C	2.87609000	-1.50536400	0.75196500
C	2.85882500	-0.16182400	0.35468700
H	3.84241900	1.34489700	-0.82424500
H	5.50462100	-0.22430000	-1.78425900
H	5.49727000	-2.62367500	-1.11946700
H	3.82407600	-3.42312200	0.54322900
H	2.16704200	-1.83190100	1.49900900
N	1.92253100	0.74853900	0.89133700
C	2.33238900	2.00006300	1.46712300
C	0.37494800	1.27198000	2.36995900
C	1.28876800	2.28872200	2.41791200
H	1.27845100	3.15009400	3.06919400
N	0.72886100	0.27854700	1.47451900
O	3.37044900	2.58753100	1.17487700
H	-0.11014400	2.37450200	-0.51591200
C	-0.87928500	1.17173900	3.17890600

H	-0.97348800	0.18333600	3.63750900
H	-0.86341700	1.91744100	3.97776900
H	-1.75841000	1.35375900	2.55484000

2

SCF done: -1299.3654903

Rh	0.94012500	-0.11259000	0.06554200
C	0.45565200	0.24441000	-2.08027100
C	1.74917300	0.77249800	-1.73027400
C	0.46878200	-1.16117200	-1.80571800
C	2.60840900	-0.35336400	-1.36909100
C	1.82653500	-1.53548800	-1.40885900
C	-0.67639600	1.04369300	-2.63939000
H	-0.49757400	1.22578700	-3.70699800
H	-1.63069500	0.52693500	-2.53762300
H	-0.76787000	2.01433600	-2.14586600
C	2.19122600	2.19355800	-1.90337200
H	3.03452500	2.43173900	-1.25044300
H	2.51065900	2.37480100	-2.93801000
H	1.37915800	2.88899700	-1.67694600
C	4.05099100	-0.22675300	-0.98712200
H	4.44218600	-1.15646300	-0.57040800
H	4.65565300	0.03207600	-1.86475900
H	4.19008200	0.55843800	-0.23882700
C	2.26154000	-2.93320700	-1.09289100
H	2.35141400	-3.52638200	-2.01141200
H	3.22850600	-2.95047200	-0.58644100
H	1.53561600	-3.42990300	-0.44366000
C	-0.65074100	-2.13152700	-2.02102700
H	-0.64283300	-2.91715900	-1.26201100
H	-1.62529100	-1.64393600	-1.97586500
H	-0.54801400	-2.61106200	-3.00344900
O	2.12258300	0.23322500	1.86638300
C	1.58722700	-0.75691200	2.47005000
O	0.76312300	-1.48686500	1.84194300
C	1.90629300	-1.01662400	3.91965000
H	2.92079000	-0.68859900	4.15441700
H	1.20916000	-0.44341200	4.54070200
H	1.78077400	-2.07529600	4.15358100
C	-2.29853300	-1.18176900	1.20557800
C	-3.05091800	-2.35590400	1.17629900
C	-4.12720800	-2.49782000	0.29850500
C	-4.44633400	-1.44006600	-0.55550700
C	-3.69879400	-0.26242800	-0.55274600

C	-2.61017000	-0.12804100	0.33153400
H	-1.46585900	-1.08382300	1.88786700
H	-2.79347500	-3.16189500	1.85857400
H	-4.71256000	-3.41269500	0.28586700
H	-5.28869700	-1.52597000	-1.23697300
H	-3.96533900	0.56899000	-1.19071400
N	-1.83862200	1.05386300	0.31908400
C	-2.34482100	2.36213800	0.05251100
C	-0.30108700	2.44981600	1.05929600
C	-1.30349200	3.22997700	0.54371800
H	-1.36721700	4.30804600	0.55531600
N	-0.59401700	1.10247600	0.97115000
O	-3.43676300	2.60624900	-0.46300500
C	0.95945800	2.95109100	1.69880200
H	1.84830700	2.72717400	1.10250700
H	0.89210900	4.03475200	1.82412200
H	1.11701600	2.48968400	2.67583500

TS2-3

SCF done: -1299.336809

Rh	-0.63370000	0.07041200	0.04836000
C	-1.40003500	-0.30434100	-2.03828700
C	-2.50313800	-0.40533100	-1.13762400
C	-0.82769500	1.01796100	-1.91322700
C	-2.65864600	0.88686200	-0.48754000
C	-1.66612200	1.77136500	-0.99551700
C	-0.89471000	-1.35908100	-2.97670700
H	-1.03072500	-1.03018300	-4.01389100
H	0.17046000	-1.56001400	-2.82801300
H	-1.43425600	-2.29949000	-2.85378000
C	-3.42076300	-1.57248000	-0.92985100
H	-3.62204800	-1.72599500	0.13414300
H	-4.38364300	-1.40624400	-1.43011000
H	-2.99601000	-2.49736700	-1.32428800
C	-3.72763500	1.19982800	0.51512000
H	-3.57893000	2.18040800	0.97185800
H	-4.71592700	1.19710000	0.03909600
H	-3.73642100	0.45295000	1.31445400
C	-1.56161400	3.24309300	-0.73147000
H	-2.16544100	3.79351900	-1.46472400
H	-1.92930000	3.50659000	0.26296000
H	-0.53213100	3.59471600	-0.81368400
C	0.27301900	1.57736100	-2.76560900
H	0.85533800	2.32750400	-2.22533700

H	0.96270100	0.79289100	-3.08563500
H	-0.13628000	2.05163900	-3.66736300
O	-1.31570900	-0.71467000	1.93926000
C	-0.63798300	-0.56904900	3.00512300
O	0.44425500	0.07880700	3.09032600
C	-1.15663700	-1.24280500	4.26108900
H	-2.21656800	-1.48223300	4.16645600
H	-0.59678800	-2.17164300	4.41387700
H	-0.98098300	-0.60298500	5.12825600
C	1.12621200	1.15094000	0.78453700
C	1.21139300	2.54437200	1.03102200
C	2.36049600	3.26948700	0.75437200
C	3.47581700	2.60603500	0.20651500
C	3.45384200	1.24606200	-0.06861000
C	2.27320400	0.52430500	0.19714600
H	0.74369000	0.57984200	1.88148300
H	0.36953700	3.03901400	1.50964400
H	2.41443600	4.32996500	0.98263000
H	4.38223200	3.16844400	-0.00272300
H	4.30186700	0.72404500	-0.49399000
N	2.13740100	-0.80350000	-0.11701100
C	3.06473800	-1.76952200	-0.64242500
C	0.98580700	-2.66084200	-0.27607100
C	2.26447500	-2.95858200	-0.72222400
H	2.64303100	-3.92810600	-1.00909300
N	0.88293200	-1.36845500	0.11342800
O	4.24027500	-1.51072400	-0.90967900
C	-0.18591200	-3.58468900	-0.13690600
H	-0.64449800	-3.80494000	-1.10764200
H	0.13459400	-4.53988400	0.28991500
H	-0.94299700	-3.14740100	0.51797500

3

SCF done: -1299.3545971

Rh	0.59294100	-0.10330000	-0.00073800
C	2.15660600	1.01281400	-1.31237400
C	2.87692300	0.43343700	-0.25709200
C	1.39861500	-0.05032000	-1.98175000
C	2.64287900	-1.01535200	-0.28766400
C	1.82816900	-1.31494100	-1.41011500
C	2.14344900	2.44571500	-1.75051100
H	2.70076200	2.55272600	-2.68993200
H	1.12556800	2.80031500	-1.93290200
H	2.60523100	3.10567200	-1.01405200

C	3.75630000	1.11519800	0.74803100
H	3.47895100	0.83147800	1.76829400
H	4.80756700	0.83617700	0.60237000
H	3.68863300	2.20269600	0.67274000
C	3.30104600	-1.98854000	0.64419700
H	2.84679900	-2.97952800	0.57781300
H	4.36847800	-2.09361300	0.41001400
H	3.22164800	-1.65179400	1.68164200
C	1.52718000	-2.66851700	-1.97785500
H	2.20206300	-2.87011300	-2.81979600
H	1.67472900	-3.46259200	-1.24258200
H	0.50154400	-2.73891200	-2.34402300
C	0.61850700	0.12153200	-3.25150800
H	-0.10106700	-0.68858000	-3.38693400
H	0.06089300	1.06130800	-3.25083800
H	1.28797000	0.12906600	-4.12234100
O	0.74243300	-0.10976900	2.34396200
C	-0.13224000	-0.39597200	3.16352400
O	-1.27729600	-0.97356500	2.85176800
C	0.00650300	-0.10589800	4.63448900
H	1.01607200	0.23930200	4.85383700
H	-0.71538700	0.66848900	4.91330100
H	-0.22995000	-0.99885900	5.21875700
C	-1.09967800	-1.26241000	-0.13803400
C	-1.20795200	-2.66012000	-0.11848700
C	-2.42642400	-3.29815100	-0.38282400
C	-3.55722200	-2.53443700	-0.68705300
C	-3.50034800	-1.14195000	-0.69485200
C	-2.27837200	-0.51656800	-0.40312100
H	-1.31363900	-1.11865700	1.87205900
H	-0.33472700	-3.26682400	0.10865400
H	-2.48798600	-4.38262000	-0.35370500
H	-4.50097300	-3.02715900	-0.90456200
H	-4.36314300	-0.52457400	-0.91449600
N	-2.12904700	0.85831700	-0.32432100
C	-2.99135900	1.94070400	-0.65023300
C	-0.99025400	2.65522900	0.20619900
C	-2.20070400	3.09424700	-0.29301500
H	-2.55655000	4.11276500	-0.33928100
N	-0.92402600	1.29344400	0.21723800
O	-4.13123300	1.80383000	-1.10338800
C	0.10740400	3.47136600	0.81930300
H	0.35280700	4.33791900	0.19795800
H	-0.20204800	3.85233600	1.79954400

H	1. 00952500	2. 87337700	0. 96699000
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I

SCF done: -1070.2609183

Rh	-0. 45195000	-0. 04172500	-0. 01414300
C	-2. 47007900	0. 48391800	0. 98361200
C	-2. 59153300	0. 90334400	-0. 36029500
C	-2. 18399300	-0. 95115000	0. 99522300
C	-2. 33184400	-0. 24644900	-1. 20072900
C	-2. 17106400	-1. 40482000	-0. 35986000
C	-2. 66676800	1. 31747900	2. 21361000
H	-1. 94303900	1. 05964000	2. 99148700
H	-2. 56723400	2. 38487500	2. 00258500
H	-3. 66899800	1. 15655200	2. 63275700
C	-3. 01630000	2. 25121500	-0. 86449400
H	-2. 45946100	2. 54835300	-1. 75785500
H	-4. 07971700	2. 23777700	-1. 13788000
H	-2. 88408900	3. 03147200	-0. 11260700
C	-2. 40610900	-0. 26370500	-2. 69668200
H	-1. 81144900	-1. 07864100	-3. 11509100
H	-3. 44470600	-0. 40271100	-3. 02803200
H	-2. 04517800	0. 67298600	-3. 12868600
C	-2. 17072300	-2. 82388200	-0. 84855800
H	-3. 17456900	-3. 09621400	-1. 19899800
H	-1. 47666400	-2. 97699700	-1. 67891000
H	-1. 90613400	-3. 52605700	-0. 05570100
C	-2. 11567300	-1. 80509200	2. 22623700
H	-1. 53679200	-2. 71409900	2. 04945400
H	-1. 64292900	-1. 27171400	3. 05468800
H	-3. 12159700	-2. 10255300	2. 55206500
C	1. 12684000	-1. 30296800	-0. 00694600
C	1. 13849900	-2. 70843500	0. 05022800
C	2. 32974800	-3. 43078500	0. 05890500
C	3. 55996600	-2. 75942400	0. 00816100
C	3. 60592000	-1. 37244200	-0. 04177300
C	2. 39288000	-0. 66322500	-0. 04211600
H	0. 20406400	-3. 25627700	0. 09217200
H	2. 30489600	-4. 51647300	0. 10555900
H	4. 48811000	-3. 32417200	0. 01201900
N	2. 33688000	0. 72129600	-0. 06203800
C	3. 34736900	1. 72117000	-0. 03093600
C	1. 25804800	2. 63727700	0. 02221000
C	2. 58506400	2. 95695900	0. 02045500
H	3. 02537000	3. 94182300	0. 05244400

N	1.07400600	1.26431800	-0.02934000
O	4.55377600	1.49932700	-0.04649100
C	0.09081800	3.56493900	0.06650400
H	-0.57979800	3.31299900	0.89373300
H	0.43378900	4.59325500	0.19926700
H	-0.48958500	3.51333700	-0.85952100
H	4.54065300	-0.82697100	-0.07349300

TSR-1'

SCF done: -1528.4219778

Rh	0.35028300	-0.94651400	0.46408000
C	0.96114300	-2.15279200	-1.27304400
C	1.78816500	-2.50365400	-0.12913500
C	-0.39419700	-2.50363000	-0.96378000
C	0.92691600	-3.04303700	0.87865400
C	-0.42896800	-3.02474600	0.38615900
C	1.48227400	-1.60433600	-2.56478600
H	1.97327800	-2.39726300	-3.14353700
H	0.68631300	-1.17044200	-3.17117200
H	2.21880600	-0.81979300	-2.37113800
C	3.28102900	-2.38949400	-0.04141100
H	3.57697400	-1.80865100	0.83504400
H	3.73737200	-3.38577000	0.01122800
H	3.68521700	-1.88441600	-0.92078100
C	1.34935800	-3.51074800	2.23681100
H	2.41307300	-3.33209100	2.40200400
H	0.79826600	-2.97897400	3.01779200
H	1.15656800	-4.58453900	2.34711300
C	-1.60827200	-3.63227900	1.08447400
H	-1.66679400	-4.70854200	0.87480300
H	-1.52904600	-3.51162000	2.16829100
H	-2.54655800	-3.17707500	0.76267000
C	-1.55935600	-2.40345000	-1.89725000
H	-1.62668500	-3.32346200	-2.49325000
H	-2.49914800	-2.28863200	-1.35365400
H	-1.45596600	-1.55706100	-2.57917300
O	0.42611800	-0.47492000	2.54429900
C	0.30828400	0.73417600	2.90700800
O	-0.19453000	1.64370200	2.17227100
C	0.82550100	1.11634400	4.27148800
H	1.90631200	1.26256700	4.17339800
H	0.36461200	2.04194100	4.61814300
H	0.65709800	0.30612100	4.98366000
O	1.50042600	0.72817600	-0.09682400

C	2.57144300	1.04858700	0.57397100
O	3.05287500	0.43489400	1.52932300
C	3.21876300	2.34162700	0.07581800
H	3.27869200	2.35338600	-1.01639900
H	2.59739800	3.18858600	0.38379800
H	4.21542000	2.45147100	0.50638100
C	-1.56269200	0.35584700	0.36924500
C	-2.57479000	-0.30447900	1.10090300
C	-3.88751200	-0.41269200	0.64136000
C	-4.23549200	0.15655500	-0.58649200
C	-3.27961500	0.86324200	-1.31615500
C	-1.97070000	0.96616900	-0.83678400
H	-0.70261800	1.05202200	1.19548100
H	-2.31194600	-0.74377400	2.06022000
H	-4.63610300	-0.93230000	1.23406400
H	-5.25232000	0.07863600	-0.96097700
H	-3.54458000	1.34703000	-2.25094100
N	-1.05793900	1.76028600	-1.59558700
C	-0.59331900	1.49958300	-2.86339500
C	0.19267900	3.50856300	-1.93172200
C	0.33235900	2.67329000	-3.17459400
H	1.35585800	2.31149000	-3.32622200
N	-0.58485400	2.96663700	-1.05991900
O	-0.87110700	0.53486200	-3.56543800
H	0.02818000	3.18833700	-4.09243500
C	0.84660200	4.82849500	-1.68900900
H	0.55560500	5.21187200	-0.70885200
H	1.93869800	4.73883600	-1.72319400
H	0.55808300	5.55818300	-2.45559400

1'

SCF done: -1528.462915

Rh	-0.96200000	-0.18309400	0.01551900
C	-0.90176300	-2.03952200	-1.17649700
C	-1.80378200	-2.37481400	-0.06507600
C	-1.51780800	-0.99817500	-1.95760400
C	-2.88174100	-1.48744100	-0.10290300
C	-2.68174300	-0.56915300	-1.23843200
C	0.25615600	-2.89909400	-1.57552800
H	-0.12276700	-3.85539400	-1.96303300
H	0.86498300	-2.42785100	-2.34616200
H	0.88665300	-3.10211100	-0.70809800
C	-1.55233000	-3.48798400	0.90661600
H	-2.20165800	-3.41780600	1.78270300

H	-1.74085400	-4.45874600	0.42977700
H	-0.51261100	-3.47792300	1.24220900
C	-4.03776800	-1.39562000	0.84513500
H	-3.92291400	-2.07960200	1.68845500
H	-4.13634100	-0.37999000	1.24147200
H	-4.97642900	-1.64445000	0.33446000
C	-3.69159100	0.44784400	-1.67760700
H	-4.54753600	-0.04214100	-2.16004100
H	-4.07235100	1.01739800	-0.82512500
H	-3.26574300	1.15340800	-2.39358600
C	-1.03791300	-0.48528200	-3.28141700
H	-1.42294900	-1.12481600	-4.08660600
H	-1.38874200	0.53280200	-3.46370000
H	0.05282600	-0.48027600	-3.33059700
O	-2.00435700	1.29020400	1.38033100
C	-1.55501300	1.90738000	2.36565200
O	-0.39954100	1.67980100	2.91426600
C	-2.34926500	3.02272800	2.99733300
H	-2.30944000	2.94729000	4.08640900
H	-1.89350700	3.97771700	2.71476400
H	-3.38087700	3.00185100	2.64657400
O	0.45871000	-0.25187400	1.64165000
C	1.30017800	-1.18938800	2.00360200
O	1.58132100	-2.17945800	1.33185700
C	1.93298000	-0.94035400	3.36773100
H	2.55738700	-0.04325900	3.31643100
H	1.16018200	-0.76007200	4.12170000
H	2.54135200	-1.79638100	3.66168300
C	0.04720300	1.44580600	-0.74810000
C	-0.75120100	2.56177900	-1.06650200
C	-0.21384800	3.75815300	-1.54582600
C	1.16359300	3.88257700	-1.72652800
C	1.97735700	2.79554800	-1.42865200
C	1.43135300	1.59504700	-0.95033100
H	0.06981000	0.87521100	2.42178800
H	-1.82403100	2.50810000	-0.91070100
H	-0.87400300	4.59192100	-1.77342400
H	1.59653300	4.80733300	-2.09650300
H	3.05374200	2.85805700	-1.56072200
N	2.36801500	0.54362900	-0.68495700
C	2.74080200	-0.45004100	-1.56303900
C	4.10046800	-0.29756700	0.33998700
C	3.88040800	-1.17790700	-0.85571100
H	3.53802700	-2.17407100	-0.55116600

N	3.23906200	0.65939200	0.41250800
O	2.25995600	-0.67637000	-2.66531700
H	4.75416900	-1.29726100	-1.50360700
C	5.15979300	-0.48589300	1.37491700
H	5.11750600	0.32239500	2.10838100
H	5.02611500	-1.44262100	1.89418000
H	6.15808700	-0.50082400	0.92124300

2'

SCF done: -1299.3532601

Rh	-0.92830300	-0.08772100	0.31197000
C	-1.62145100	-1.11458900	-1.50878000
C	-2.45859600	-1.67446600	-0.44597000
C	-1.90896700	0.28593600	-1.62908700
C	-3.17300800	-0.61615800	0.13423500
C	-2.80127800	0.62572100	-0.55230200
C	-0.79691400	-1.94451400	-2.44403000
H	-1.44214600	-2.37678400	-3.22132400
H	-0.01513600	-1.35714700	-2.92664000
H	-0.32424400	-2.77771100	-1.91537500
C	-2.47417000	-3.12384400	-0.05981400
H	-3.07331200	-3.29507800	0.83715000
H	-2.89365600	-3.74038700	-0.86439000
H	-1.46229800	-3.48917200	0.14278500
C	-4.12478800	-0.67558300	1.29010100
H	-4.13146400	-1.66039500	1.76118400
H	-3.86044800	0.05893300	2.05696300
H	-5.14648000	-0.45251500	0.95804400
C	-3.48138200	1.94504000	-0.33877700
H	-4.45251700	1.96468300	-0.85126400
H	-3.66750400	2.13510500	0.72244200
H	-2.88525300	2.77199200	-0.72925100
C	-1.39802800	1.20357400	-2.69926800
H	-2.03814100	1.13707900	-3.58877500
H	-1.39717100	2.24268800	-2.36271900
H	-0.37540500	0.94562000	-2.98253500
O	0.58192500	-1.31862000	1.30780800
C	0.31292700	-0.77117800	2.42531600
O	-0.63309700	0.07949100	2.47791400
C	1.13431600	-1.09486900	3.64481100
H	1.25664300	-2.17720600	3.73854900
H	2.12941100	-0.65780200	3.51294200
H	0.67220000	-0.68628500	4.54430600
C	0.38261100	1.49520900	0.22210500

C	-0.13374000	2.74522400	0.61354900
C	0.64479100	3.90318000	0.64407000
C	1.99079600	3.85048000	0.28003100
C	2.53345400	2.62913300	-0.10232000
C	1.74441400	1.46956600	-0.12535900
H	-1.16861000	2.81482700	0.93337800
H	0.19941300	4.84340800	0.96026200
H	2.60835200	4.74367100	0.29826300
H	3.58017500	2.55126700	-0.38220300
N	2.41868700	0.25859300	-0.48874600
C	2.40098900	-0.36913600	-1.70952300
C	3.87011900	-1.33416100	-0.14993100
C	3.35458600	-1.55314500	-1.54475400
H	2.80789700	-2.49784100	-1.65173400
N	3.33018700	-0.31011000	0.41490600
O	1.77273400	-0.03615800	-2.70639200
H	4.13487800	-1.54138200	-2.31347000
C	4.88203900	-2.17892700	0.55138200
H	5.08154300	-1.77306000	1.54541500
H	4.52653200	-3.21123800	0.65768800
H	5.82345000	-2.21987100	-0.01019400

4

SCF done: -1609.7085143

Rh	0.04249500	-0.20099600	0.76435900
C	-0.99691200	0.43100700	2.85179200
C	-0.64939100	-0.96196200	2.89982700
C	0.21463400	1.16294200	2.66718400
C	0.77440500	-1.08696100	2.75595900
C	1.31871600	0.23703800	2.61028200
C	-2.34169700	1.04364200	3.12043200
H	-2.55215900	1.87618200	2.44276900
H	-3.14891600	0.31868700	3.00729800
H	-2.39206400	1.43636200	4.14469100
C	-1.57839400	-2.11950800	3.10821000
H	-2.57988200	-1.78677800	3.38858200
H	-1.66311800	-2.71490900	2.19231100
H	-1.20840700	-2.77455200	3.90395100
C	1.54840100	-2.36285300	2.91054200
H	2.46567100	-2.35421000	2.31898600
H	1.82146500	-2.52057700	3.96243000
H	0.96107900	-3.22449400	2.58511400
C	2.76919200	0.62116700	2.67612800
H	3.01334500	1.01632100	3.67092800

H	3.41764600	-0.23922900	2.50247600
H	3.02923300	1.39063600	1.94319100
C	0.33548600	2.65599000	2.69264900
H	1.26672600	2.99385400	2.23441500
H	-0.49677500	3.14255900	2.17738200
H	0.33060400	3.01588300	3.73010200
C	1.34947000	-1.36124100	-0.33344900
C	2.74113400	-1.35012700	-0.26255600
C	3.51097600	-2.22719700	-1.04057700
C	2.88016300	-3.11344500	-1.91396300
C	1.48956500	-3.14529300	-2.01003300
C	0.73137100	-2.27433500	-1.21090700
H	3.25065700	-0.63366800	0.37177600
H	4.59514100	-2.19838300	-0.97075600
H	3.47059100	-3.78872000	-2.52728100
N	-0.65488200	-2.25452200	-1.23534900
C	-1.58592400	-2.81569300	-2.14706900
C	-2.60798900	-1.54526400	-0.53665200
C	-2.84699500	-2.33096100	-1.64741800
H	-3.81085700	-2.59940800	-2.05376800
N	-1.27766600	-1.51766000	-0.23118300
O	-1.27747000	-3.54351300	-3.09722700
C	-3.63710000	-0.87475900	0.31901500
H	-3.37320300	0.16158200	0.54026000
H	-4.59949300	-0.87449400	-0.19775400
H	-3.76997300	-1.40177100	1.27040600
H	0.96814000	-3.81522200	-2.68278000
C	-0.58922800	1.35928900	-0.70408100
C	0.66431000	1.35330500	-0.71863700
C	-1.89172700	1.79993200	-1.14595500
C	-2.50594300	1.20243600	-2.26251200
C	-2.53825300	2.87265200	-0.50169500
C	-3.73589200	1.67285700	-2.71801100
H	-2.02088500	0.36890700	-2.75680600
C	-3.76765000	3.33641800	-0.96482500
H	-2.05952600	3.35040200	0.34734700
C	-4.37111200	2.73664300	-2.07295500
H	-4.19872600	1.20356800	-3.58099200
H	-4.25181900	4.16975900	-0.46383800
H	-5.32958000	3.09865900	-2.43322500
C	1.95576600	1.83825700	-1.15330200
C	2.67219000	1.18234300	-2.17179400
C	2.48234500	3.02298900	-0.60300700
C	3.88271200	1.70429000	-2.62289900

H	2.27340400	0.27108700	-2.60061600
C	3.69667900	3.53445100	-1.05668600
H	1.91988000	3.54988800	0.16061400
C	4.40166400	2.87556600	-2.06627400
H	4.42258000	1.19058500	-3.41274100
H	4.08755400	4.45233200	-0.62701500
H	5.34714600	3.27569700	-2.42063900

TS4-II

SCF done: -1609.691991

Rh	0.66189300	-0.69168100	-0.27972600
C	2.67330500	-1.13459700	-1.38790700
C	2.32432100	-2.30981300	-0.59729900
C	1.66027500	-0.96164300	-2.37169900
C	1.11553900	-2.84884500	-1.10102500
C	0.65937900	-1.97418300	-2.16247900
C	4.01234200	-0.45559300	-1.35550400
H	3.96497600	0.57527100	-1.71512900
H	4.43440100	-0.43774500	-0.34973300
H	4.72417800	-0.99079300	-1.99880800
C	3.17128300	-2.86313300	0.50920500
H	3.38365600	-2.10051700	1.26416200
H	2.67831700	-3.69426200	1.01667100
H	4.12982600	-3.22828100	0.12006500
C	0.44240500	-4.11788200	-0.67012300
H	-0.63731200	-3.98859600	-0.56052500
H	0.61300500	-4.91298800	-1.40722700
H	0.82453300	-4.46965300	0.29051200
C	-0.50386500	-2.22225800	-3.08064900
H	-0.15373200	-2.56655000	-4.06265600
H	-1.17034100	-2.99193000	-2.68642600
H	-1.09541300	-1.31624600	-3.24255100
C	1.65020300	0.01481400	-3.51134200
H	0.67146000	0.48830500	-3.63194800
H	2.39027000	0.80673200	-3.38103900
H	1.88085400	-0.49876900	-4.45399500
C	-1.17600300	-1.15722600	0.66601900
C	-2.18528000	-1.99031500	0.15485700
C	-3.12830200	-2.57760300	0.99557900
C	-3.09359700	-2.31209000	2.37160300
C	-2.09800400	-1.50801700	2.91681800
C	-1.11508400	-0.96317100	2.06891800
H	-2.27111800	-2.13202800	-0.91740400
H	-3.90469000	-3.21227700	0.57784000

H	-3.84466500	-2.74503600	3.02652800
N	-0.03551100	-0.25656700	2.54718100
C	0.12422900	0.47617100	3.76344400
C	1.92904200	0.68580600	2.37366600
C	1.41814400	1.07400400	3.59813500
H	1.91376000	1.67970400	4.34179000
N	1.08899000	-0.16755900	1.72434900
O	-0.71934300	0.49551200	4.66528600
C	3.27081600	1.04695600	1.81845400
H	3.20884200	1.31528800	0.76235300
H	3.67799600	1.90177200	2.36357400
H	3.98402300	0.21998200	1.91992300
H	-2.03824600	-1.29459500	3.97688800
C	-0.06288600	1.25038000	-0.36163300
C	-1.20413500	0.65377800	-0.35103400
C	0.50094400	2.58432700	-0.36548200
C	-0.20869500	3.63019200	0.26168200
C	1.72491000	2.88550700	-0.98854800
C	0.28854300	4.93005700	0.24845600
H	-1.14392900	3.40602900	0.76386400
C	2.21484700	4.18963000	-1.00476400
H	2.28287600	2.08751800	-1.46404300
C	1.50020000	5.21751500	-0.38613800
H	-0.26949500	5.72109800	0.74104300
H	3.15948900	4.40329900	-1.49712700
H	1.88664400	6.23241300	-0.39212900
C	-2.56179700	0.84057600	-0.85739800
C	-3.68543500	0.73407500	-0.01868000
C	-2.74472900	1.22765000	-2.19780500
C	-4.95641900	1.01945100	-0.51102400
H	-3.55083000	0.43702700	1.01543800
C	-4.02146700	1.49937400	-2.68844400
H	-1.87703600	1.32357100	-2.84334200
C	-5.12975600	1.39616700	-1.84603500
H	-5.81556500	0.94615400	0.14924600
H	-4.14876300	1.79583500	-3.72567400
H	-6.12442100	1.61031200	-2.22642100

II

SCF done: -1609.7349186

Rh	1.26046600	0.01780000	-0.14554700
C	2.82403200	1.49719700	-0.27265300
C	3.57508900	0.30210200	0.13416100
C	2.34765000	1.28229700	-1.63223000

C	3.39804500	-0.66446000	-0.86085300
C	2.60923500	-0.07338500	-1.94986500
C	2.85165000	2.82780900	0.41503400
H	1.92075200	3.37680100	0.25185600
H	2.99511100	2.72311200	1.49171600
H	3.67584400	3.44106500	0.02514900
C	4.29727300	0.10796600	1.43518000
H	3.68820300	-0.46404500	2.14499000
H	5.23239600	-0.43916600	1.28182300
H	4.54860400	1.06485400	1.89919000
C	3.90237100	-2.07631800	-0.85597600
H	3.09885700	-2.78765900	-1.07375500
H	4.67789800	-2.21706800	-1.61975900
H	4.32956300	-2.34509800	0.11226900
C	2.28938500	-0.78284700	-3.23055200
H	3.18886100	-0.87704600	-3.85332300
H	1.91245600	-1.79219900	-3.04183700
H	1.53566400	-0.24697300	-3.81118700
C	1.82492200	2.34530900	-2.54746100
H	1.20073200	1.92803000	-3.34132700
H	1.23302300	3.08653200	-2.00813300
H	2.66238300	2.86994900	-3.02639200
C	-0.88424600	-1.76061400	-0.63913400
C	-0.97147700	-2.52372500	-1.82067100
C	-0.50251000	-3.83199400	-1.86939900
C	0.05379200	-4.42478300	-0.72718800
C	0.14990300	-3.69336800	0.45151500
C	-0.29741100	-2.36452200	0.49651500
H	-1.44452200	-2.08118400	-2.69257900
H	-0.58941900	-4.40326900	-2.78952000
H	0.39852700	-5.45417600	-0.75822400
N	-0.19282800	-1.63410400	1.70541200
C	-1.05594900	-1.68667900	2.82054100
C	0.47707700	0.00753200	2.98536000
C	-0.55372200	-0.61623200	3.65442600
H	-0.92930200	-0.37833900	4.63861500
N	0.74875100	-0.61290400	1.79382900
O	-1.97431000	-2.50324500	2.94026600
C	1.25908800	1.20181800	3.43988600
H	1.00115500	2.09209400	2.85605500
H	1.03739600	1.41342800	4.4887100
H	2.33659900	1.03905000	3.34837900
H	0.56001300	-4.13103400	1.35552800
C	-0.68913900	0.65679500	-0.31382300

C	-1.50143800	-0.38882900	-0.56293600
C	-1.11341400	2.05457700	-0.09330600
C	-1.40883100	2.49957000	1.21019600
C	-1.23779200	2.97825500	-1.14734300
C	-1.79571000	3.81837700	1.44625900
H	-1.35582700	1.79070200	2.03032800
C	-1.62220800	4.29928600	-0.90887500
H	-1.05252000	2.64807200	-2.16436700
C	-1.89615600	4.72805700	0.39050700
H	-2.03059200	4.13390200	2.45931500
H	-1.71965700	4.98952600	-1.74279800
H	-2.19869900	5.75448900	0.57699100
C	-2.98923000	-0.34818700	-0.72201200
C	-3.78861300	-1.16964500	0.09544900
C	-3.61812100	0.46807900	-1.67450200
C	-5.17687500	-1.15488400	-0.03220900
H	-3.32448200	-1.80181200	0.84919200
C	-5.00806800	0.47565400	-1.80241100
H	-3.01413500	1.09450800	-2.32227300
C	-5.79247100	-0.33534800	-0.98155100
H	-5.77894200	-1.78515700	0.61646800
H	-5.47617300	1.11292500	-2.54801100
H	-6.87447500	-0.32996300	-1.08093400

TSII-III

SCF done: -1609.6564902

Rh	1.39784300	0.19510200	0.17700300
C	2.84740800	1.49483800	-0.81829500
C	3.72725300	0.48571300	-0.21650700
C	2.10788200	0.86352900	-1.89289900
C	3.41794600	-0.74224300	-0.80237000
C	2.38350800	-0.52031600	-1.82434100
C	3.02635200	2.96715900	-0.59384600
H	2.19268500	3.55253200	-0.98251300
H	3.13687000	3.20061100	0.46801100
H	3.93677900	3.31066200	-1.10439600
C	4.67860400	0.75890500	0.90851700
H	5.32851900	-0.09796500	1.09827300
H	5.31713800	1.62146200	0.68896600
H	4.13100300	0.96797600	1.83593000
C	4.00409300	-2.08505100	-0.49190100
H	3.21787500	-2.81900900	-0.29152900
H	4.58746700	-2.45790200	-1.34324300
H	4.66118800	-2.04952000	0.37909200

C	1. 90315900	-1. 57283600	-2. 77403900
H	2. 66851200	-1. 76226900	-3. 53949000
H	1. 70212100	-2. 51847900	-2. 26654300
H	0. 98941700	-1. 26747500	-3. 28568200
C	1. 26547400	1. 54136900	-2. 93351500
H	0. 34339300	0. 98747400	-3. 12743700
H	0. 98648600	2. 55374900	-2. 63580400
H	1. 81662900	1. 61751900	-3. 87954500
C	-0. 88156400	-1. 79013200	-0. 64819700
C	-1. 28602400	-2. 64122100	-1. 68619800
C	-0. 79120600	-3. 94228000	-1. 79673500
C	0. 12097200	-4. 42626700	-0. 85649900
C	0. 52131500	-3. 60855500	0. 20210800
C	0. 01881600	-2. 30665700	0. 32434000
H	-1. 99543700	-2. 27153600	-2. 42028700
H	-1. 11483800	-4. 57336400	-2. 61956900
H	0. 50145300	-5. 44104800	-0. 93138200
N	0. 33575500	-1. 56677900	1. 49323100
C	-0. 73873500	-1. 37186300	2. 38153900
C	0. 61033100	0. 43353800	3. 11380600
C	-0. 49949800	-0. 31738000	3. 34405200
H	-1. 14818800	-0. 18899000	4. 19962700
N	1. 45764400	0. 15644800	2. 10456300
O	-1. 74652000	-2. 08538700	2. 34568700
C	1. 08725000	1. 55705600	4. 01516700
H	1. 17921000	2. 48871300	3. 44852700
H	0. 36711600	1. 70870100	4. 82218900
H	2. 06551100	1. 31923800	4. 44342600
H	1. 18455300	-3. 97667600	0. 97842200
C	-0. 61362000	0. 61696100	-0. 04863600
C	-1. 39068500	-0. 40008500	-0. 52221000
C	-1. 16147400	1. 89973900	0. 43553000
C	-2. 20554200	1. 89961300	1. 38668600
C	-0. 65125100	3. 14732900	0. 03121000
C	-2. 71085700	3. 09297200	1. 89982400
H	-2. 61586300	0. 95151600	1. 71425900
C	-1. 16640000	4. 34085600	0. 53208800
H	0. 14785600	3. 17406200	-0. 69866700
C	-2. 19698900	4. 31981400	1. 47538900
H	-3. 51319400	3. 06272800	2. 63203100
H	-0. 76352200	5. 28942900	0. 18658400
H	-2. 59587800	5. 24912900	1. 87222600
C	-2. 82435200	-0. 20070900	-0. 91377400
C	-3. 82468000	-1. 01943500	-0. 35822800

C	-3.20014800	0.77912300	-1.84553700
C	-5.16059600	-0.84817800	-0.71822200
H	-3.54234000	-1.76904500	0.37551700
C	-4.53742500	0.94537200	-2.20821100
H	-2.43612400	1.41434800	-2.28389700
C	-5.52271600	0.13234500	-1.64587400
H	-5.92205900	-1.48094000	-0.27022600
H	-4.80809600	1.70836200	-2.93321500
H	-6.56406100	0.26085600	-1.92800800

III

SCF done: -1609.7132413

Rh	-1.24440800	-0.19472600	-0.03435200
C	-2.17624500	-1.14478600	-2.06556200
C	-3.21732700	-0.57169300	-1.27914900
C	-1.30462800	-0.07150000	-2.49990200
C	-2.96236500	0.84084500	-1.16687700
C	-1.79287900	1.14549600	-1.96550000
C	-2.14139300	-2.58397100	-2.49109400
H	-1.25573100	-2.81569200	-3.08570200
H	-2.15496200	-3.25974300	-1.63049100
H	-3.01734100	-2.82193700	-3.10829900
C	-4.35652700	-1.34460600	-0.68945500
H	-5.05532100	-0.69347800	-0.15944100
H	-4.91527200	-1.86796200	-1.47436100
H	-3.98386800	-2.09014500	0.02235100
C	-3.83825400	1.86438500	-0.50760000
H	-3.24051400	2.64707500	-0.03326400
H	-4.49039800	2.34837400	-1.24679000
H	-4.47585000	1.41910600	0.25928700
C	-1.30835900	2.52145900	-2.30897000
H	-1.89563400	2.93354200	-3.14121100
H	-1.40022800	3.21152200	-1.46742300
H	-0.26022000	2.51541400	-2.61324300
C	-0.14540900	-0.18548700	-3.44448200
H	0.73256300	0.34314400	-3.06125200
H	0.14122500	-1.22477300	-3.61879700
H	-0.39735000	0.25296300	-4.41816900
C	1.14176700	2.00428400	0.02708600
C	1.84055300	3.09166700	-0.52602100
C	1.45042200	4.40569900	-0.28450600
C	0.35347000	4.65995200	0.54415900
C	-0.35821600	3.60507200	1.10866600
C	0.00445600	2.27197300	0.83990600

H	2.71128600	2.89384300	-1.14290600
H	2.00604100	5.22647100	-0.72856400
H	0.05219400	5.68231300	0.75489600
N	-0.70817300	1.18607900	1.36897900
C	-0.94862100	1.14343000	2.72674000
C	-1.72411500	-1.29081900	2.60140200
C	-1.37243100	-0.14460400	3.28246000
H	-1.44093700	-0.13305200	4.36628600
N	-1.86126700	-1.38440200	1.26821000
O	-0.75809300	2.10181800	3.49021600
C	-2.10082300	-2.55133400	3.36688900
H	-1.45455400	-3.37866800	3.05738800
H	-1.99159000	-2.41059100	4.44537500
H	-3.13299400	-2.84019900	3.14630900
H	-1.18932300	3.79069400	1.77583600
C	0.80054600	-0.46170500	-0.07694600
C	1.62673300	0.61368200	-0.13141300
C	1.23703100	-1.86354000	0.09963600
C	1.83053800	-2.23431300	1.32341500
C	1.05348200	-2.86041800	-0.87272400
C	2.22501800	-3.55012900	1.55771400
H	1.97863000	-1.47632600	2.08576600
C	1.45615000	-4.17468400	-0.64088100
H	0.60147700	-2.59645700	-1.82082200
C	2.03959700	-4.52806700	0.57758800
H	2.68333000	-3.81115500	2.50774600
H	1.31495200	-4.92483700	-1.41445400
H	2.34871000	-5.55317000	0.76032300
C	3.10981400	0.43132900	-0.27736100
C	3.99042500	1.01172100	0.65265000
C	3.65574000	-0.31612200	-1.33194800
C	5.36839900	0.83404500	0.53941600
H	3.58632900	1.60013100	1.47095900
C	5.03538300	-0.48849400	-1.44990300
H	2.99154500	-0.76593600	-2.06288300
C	5.89735100	0.08350800	-0.51339700
H	6.03001700	1.28270900	1.27528700
H	5.43584700	-1.06897300	-2.27648900
H	6.97144700	-0.05146300	-0.60367800

TSIII-6

SCF done: -1609.7000621

Rh	-2.52733400	-0.11685700	0.66653000
C	-3.23819500	-0.89475800	-1.38146400

C	-4.38487200	-0.62227700	-0.57344200
C	-2.59117300	0.36969400	-1.70508800
C	-4.37689000	0.78607700	-0.28906600
C	-3.28972300	1.39601000	-1.04203900
C	-2.88124200	-2.21846600	-1.98930700
H	-1.79892100	-2.33970400	-2.08553000
H	-3.26504100	-3.05051800	-1.39464800
H	-3.30729000	-2.30603400	-2.99801200
C	-5.37522300	-1.61666000	-0.05252700
H	-5.41422600	-2.50872700	-0.68324000
H	-5.08889400	-1.91970400	0.96534000
H	-6.38151400	-1.18860600	-0.02012300
C	-5.42201000	1.53393200	0.48338200
H	-4.98880300	2.37577400	1.02973500
H	-6.18730500	1.93996800	-0.19265300
H	-5.92124300	0.88521500	1.20593700
C	-3.04352500	2.87048000	-1.13477000
H	-3.72878100	3.32692200	-1.86145900
H	-3.20443000	3.36783800	-0.17513800
H	-2.02260200	3.09386800	-1.44844000
C	-1.44330400	0.52653400	-2.65613700
H	-0.92907900	1.47866400	-2.51192300
H	-0.70130300	-0.26674400	-2.53352300
H	-1.79431500	0.49015200	-3.69593500
C	0.23790400	1.80765000	0.32795300
C	0.80599300	2.88644700	-0.36781500
C	0.48181200	4.19434600	-0.00764800
C	-0.40448800	4.43699300	1.04829400
C	-0.99931700	3.37503800	1.73212300
C	-0.69260300	2.06675900	1.35645600
H	1.51222400	2.69937800	-1.17047000
H	0.93010300	5.02712400	-0.54175500
H	-0.63249900	5.45757400	1.34169300
N	-1.28243500	0.92102900	1.94069200
C	-1.05572600	0.70920700	3.31858400
C	-2.70319100	-1.23965200	3.33844300
C	-1.75652700	-0.39966600	3.92063200
H	-1.52788000	-0.52370900	4.97434300
N	-3.16499600	-1.19495500	2.08951800
O	-0.27766000	1.43442400	3.95079500
C	-3.31516300	-2.34217400	4.19815400
H	-3.03089200	-2.24448000	5.24940700
H	-4.40575400	-2.32126600	4.11982400
H	-2.97785000	-3.32038900	3.83936600

H	-1.67747100	3.55117400	2.55955500
C	-0.34287300	-0.48585800	0.76580300
C	0.55211800	0.38272000	0.19667700
C	0.00705100	-1.77728100	1.38152500
C	0.97117300	-1.79432100	2.40897000
C	-0.57382500	-2.99751000	0.98910600
C	1.36200600	-2.99692100	3.00017500
H	1.40693900	-0.85630900	2.73737200
C	-0.16934900	-4.19631800	1.56651600
H	-1.34547600	-2.99376500	0.22861100
C	0.80049100	-4.20028000	2.57627800
H	2.10330000	-2.98852300	3.79400200
H	-0.61311900	-5.13117300	1.23547800
H	1.10705600	-5.13724300	3.03275300
C	1.84203600	-0.07008800	-0.38403500
C	3.03750900	0.62871000	-0.12600400
C	1.91042000	-1.21394400	-1.20025500
C	4.24955900	0.19518700	-0.66054100
H	3.01533600	1.50165400	0.51783700
C	3.12284000	-1.64592800	-1.73468500
H	1.00118700	-1.76662400	-1.41300400
C	4.29894100	-0.94212000	-1.46947500
H	5.15994500	0.74461400	-0.43729600
H	3.14754400	-2.53169200	-2.36335900
H	5.24402500	-1.27655900	-1.88750500

6

SCF done: -1609.7457209

Rh	1.64536900	-0.11125900	-0.27603900
C	2.19655000	0.53385900	-2.29424800
C	3.10907100	-0.48948200	-1.88059800
C	0.87803900	-0.07502000	-2.48157800
C	2.32075900	-1.68243900	-1.66808200
C	0.96152000	-1.43401600	-2.11596900
C	2.55987700	1.93755900	-2.67154100
H	1.72629200	2.62440400	-2.50496900
H	3.41524100	2.29196200	-2.09273900
H	2.82514900	1.99105100	-3.73653700
C	4.57264600	-0.30751500	-1.62736000
H	5.03660700	0.28723700	-2.42040500
H	4.70846800	0.20995300	-0.66601400
H	5.09305600	-1.26750500	-1.58213600
C	2.84687000	-3.01220900	-1.22075200
H	2.12368300	-3.53616500	-0.59066700

H	3.05456500	-3.65035900	-2.09038800
H	3.77334100	-2.90399300	-0.65341900
C	-0.12934300	-2.46101100	-2.18782300
H	-0.09680400	-2.99818400	-3.14508900
H	-0.03643700	-3.20294800	-1.39122800
H	-1.11930600	-2.00898600	-2.09365400
C	-0.29776900	0.63895000	-3.07417400
H	-1.17435000	-0.00885500	-3.11657600
H	-0.56209700	1.53619500	-2.50662700
H	-0.07015700	0.95494600	-4.10030600
C	-1.31125200	-1.67931900	1.13843000
C	-1.60457100	-3.04278000	1.28820100
C	-0.68473000	-3.85904900	1.94380700
C	0.51552400	-3.33345400	2.45231500
C	0.83630600	-1.98591200	2.28886700
C	-0.07688100	-1.18718200	1.59971100
H	-2.53673800	-3.45110600	0.91146500
H	-0.90549800	-4.91397100	2.07868400
H	1.20388200	-3.98287100	2.98481600
N	0.02402900	0.21483100	1.28247400
C	0.28827700	1.05043800	2.57141500
C	2.80001500	1.11902100	2.10807900
C	1.63030100	1.36380500	2.85606400
H	1.74225800	1.87107200	3.80909000
N	2.98271700	0.61359300	0.89599700
O	-0.70450100	1.29629100	3.23673100
C	4.09983000	1.56060900	2.78783600
H	4.07468200	1.37252900	3.86570000
H	4.94817200	1.03677900	2.34417100
H	4.25031400	2.63710000	2.64050600
H	1.75727500	-1.56743800	2.67859000
C	-1.24205000	0.55479700	0.67009500
C	-2.03734500	-0.56030200	0.55284300
C	-1.50284100	1.96704200	0.35257900
C	-2.80966700	2.48858000	0.39128800
C	-0.44576800	2.84640200	0.04762000
C	-3.05144300	3.82805100	0.09914700
H	-3.63362600	1.84577900	0.67556800
C	-0.69267500	4.18879300	-0.23964200
H	0.57469300	2.47586800	0.04005200
C	-1.99658100	4.68489900	-0.22508400
H	-4.06826900	4.20794500	0.14128900
H	0.13986100	4.84812500	-0.46915500
H	-2.18841000	5.73030500	-0.44892500

C	-3.38288100	-0.69375100	-0.04939600
C	-4.39721200	-1.36935500	0.65355800
C	-3.68703500	-0.18574800	-1.32442700
C	-5.66690400	-1.53287500	0.09888000
H	-4.19087400	-1.74813400	1.64970000
C	-4.95578800	-0.35029100	-1.87802500
H	-2.92581500	0.35471200	-1.87505900
C	-5.95125500	-1.02774600	-1.17072000
H	-6.43612900	-2.05169400	0.66399300
H	-5.16634000	0.05058700	-2.86568600
H	-6.93906800	-1.15709100	-1.60332800

II'

SCF done: -1609.739691

Rh	1.27866300	0.21197300	-0.06796800
C	2.28674900	-0.65254300	-1.74689200
C	1.90549600	0.68721800	-2.14931400
C	2.60809200	1.58580700	-1.30810100
C	3.57722700	0.81515900	-0.50763500
C	3.39706600	-0.53907700	-0.78461500
C	-0.84858600	-2.40336600	0.07454700
C	-1.49639400	-1.51950400	-0.81365800
C	-0.73916100	-3.76572000	-0.24732600
C	-2.00669300	-2.03858400	-2.01612500
C	-1.24901700	-4.25477700	-1.44632900
H	-0.28451000	-4.43670800	0.47139700
C	-1.87863700	-3.38643400	-2.34215900
H	-2.53073600	-1.36496600	-2.68866300
H	-1.15987400	-5.31244900	-1.67716600
H	-2.28352300	-3.76050500	-3.27831400
C	1.88610600	-1.92042100	-2.43506800
H	0.86160500	-1.87169400	-2.80841500
H	2.55195500	-2.10829400	-3.28935900
H	1.95221600	-2.77903000	-1.76437500
C	4.15002700	-1.71174300	-0.23059400
H	4.78118500	-2.16763900	-1.00363300
H	4.79947900	-1.42240100	0.59858600
H	3.46816300	-2.48500200	0.13454100
C	4.57425400	1.44868100	0.41421800
H	5.31701400	2.01937600	-0.15795800
H	4.09511700	2.14986800	1.10504200
H	5.11301200	0.70657500	1.00695300
C	2.58746000	3.08370400	-1.35751200
H	3.45870000	3.45733600	-1.91217200

H	1.69031500	3.46242700	-1.84825300
H	2.62326500	3.52025800	-0.35545500
C	0.96334600	1.02319000	-3.26651900
H	0.12742300	0.32147400	-3.31100100
H	0.54924100	2.02771100	-3.15595600
H	1.48713900	0.98413000	-4.23045300
C	-0.68791400	0.72032500	-0.14779800
C	-1.71791600	-0.08535600	-0.46805700
C	-0.78071500	2.06670500	0.46547900
C	-0.84213200	2.17376700	1.87167300
H	-0.86321800	1.26426800	2.46402400
C	-0.89428900	3.42092700	2.49401600
H	-0.92628800	5.56181900	2.21713000
H	-0.95453200	3.47757000	3.57744800
C	-0.88151500	4.59106200	1.73199000
C	-0.82279700	4.50294200	0.33815500
C	-0.76713600	3.25835400	-0.28575800
H	-0.73548400	3.19887400	-1.36952600
H	-0.82929900	5.40761100	-0.26414400
C	-3.15278500	0.34438700	-0.42982200
C	-4.08331000	-0.41551100	0.30229300
C	-5.42327200	-0.03774300	0.36358600
H	-6.12248800	-0.63305300	0.94430400
H	-3.74608400	-1.30212200	0.83147400
C	-3.61490500	1.47647600	-1.11848800
H	-2.91835900	2.05924100	-1.71171000
C	-4.95844000	1.85104300	-1.06239400
C	-5.86732100	1.09794200	-0.31860100
H	-6.91318700	1.38879100	-0.27523500
H	-5.29497100	2.72925900	-1.60700100
N	-0.35066000	-1.96246400	1.33023000
C	-0.45136700	-2.73206400	2.53099700
C	1.25664600	-1.22446600	2.65311000
C	0.57815700	-2.18203600	3.37400500
H	0.76221300	-2.48262000	4.39432300
N	0.72070600	-1.06557000	1.40928000
O	-1.27107000	-3.63712900	2.69436700
C	2.38278400	-0.35600700	3.12460300
H	2.04112100	0.66449500	3.33414600
H	2.80866800	-0.76488700	4.04425000
H	3.17848700	-0.28923600	2.37679300

TSII*-5

SCF done: -1609.7064802

Rh	1. 06317000	-0. 24491400	0. 02126800
C	2. 76328900	-1. 51283900	1. 01086000
C	1. 80438900	-2. 38619900	0. 39468000
C	1. 87346100	-2. 20357400	-1. 04153400
C	2. 81967600	-1. 17939300	-1. 30621800
C	3. 34489500	-0. 73260400	-0. 02366300
C	-0. 73140000	1. 93765600	1. 73089200
C	-0. 96620000	0. 58252300	2. 01732000
C	-0. 75211300	2. 92364600	2. 71051200
C	-1. 09993700	0. 21203900	3. 36799300
C	-0. 95363100	2. 54545000	4. 03910300
H	-0. 59982700	3. 96169500	2. 43627100
C	-1. 09563000	1. 19090700	4. 36092800
H	-1. 21500000	-0. 83166800	3. 63856700
H	-0. 97248000	3. 29874000	4. 82035000
H	-1. 21432500	0. 89378000	5. 39925600
C	3. 10584100	-1. 45673300	2. 47225800
H	2. 23170300	-1. 65160000	3. 10032000
H	3. 87077000	-2. 20075400	2. 73568000
H	3. 49535100	-0. 47468000	2. 75383300
C	4. 47582900	0. 23519700	0. 18239200
H	5. 39339500	-0. 30761100	0. 44347400
H	4. 68705600	0. 81775800	-0. 71517600
H	4. 26686200	0. 93457500	0. 99708600
C	3. 33689300	-0. 81367300	-2. 66730500
H	4. 06754900	-1. 55516300	-3. 02130300
H	2. 53581200	-0. 77412900	-3. 41214800
H	3. 84291400	0. 15443800	-2. 67234800
C	1. 21641700	-3. 06435300	-2. 08391300
H	1. 94939900	-3. 74360000	-2. 53969300
H	0. 42734000	-3. 68717400	-1. 65784900
H	0. 77691400	-2. 47276600	-2. 89326600
C	1. 06733700	-3. 47748700	1. 11437200
H	0. 79920900	-3. 17500400	2. 13020900
H	0. 14655400	-3. 76746200	0. 60620500
H	1. 70072200	-4. 37135100	1. 19423900
C	-0. 77857000	0. 28050400	-0. 44732200
C	-1. 09579700	-0. 28084800	0. 82836900
C	-1. 54519800	0. 44725400	-1. 66889000
C	-2. 90997000	0. 80202400	-1. 61585700
H	-3. 38567300	0. 93530600	-0. 65030400
C	-3. 63225500	0. 99131700	-2. 78932300
H	-3. 57651400	0. 98248400	-4. 94510500
H	-4. 68094800	1. 26827200	-2. 73854300

C	-3.00877600	0.83368700	-4.03092300
C	-1.65429900	0.49301600	-4.09788200
C	-0.92620700	0.30916000	-2.92642500
H	0.12818500	0.05379700	-2.95478600
H	-1.16969900	0.37697500	-5.06310400
C	-2.01094800	-1.46731600	0.84029400
C	-3.04691300	-1.60162900	1.78545200
C	-3.94665500	-2.66625600	1.72615700
H	-4.73555600	-2.73605000	2.47012500
H	-3.17510700	-0.85183800	2.55624700
C	-1.94513000	-2.43361700	-0.18194100
H	-1.17885700	-2.34030600	-0.94132500
C	-2.84789600	-3.49279400	-0.24593400
C	-3.85076400	-3.62359100	0.71623900
H	-4.55181400	-4.45196200	0.67313900
H	-2.76637500	-4.21762500	-1.05154600
N	-0.35604100	2.16793500	0.37881800
C	-0.79800600	3.36992100	-0.35028600
C	1.36234900	2.81784500	-0.82668800
C	0.34121700	3.69955700	-1.13888600
H	0.40110400	4.53960600	-1.81422200
N	1.03610000	1.91510300	0.13847500
O	-1.92002800	3.83215300	-0.19531100
C	2.73392200	2.84666800	-1.42298300
H	2.91492200	1.95542200	-2.02894200
H	2.84825400	3.72513000	-2.06175700
H	3.49663200	2.88190900	-0.64072700

5

SCF done: -1609.7180845

Rh	1.06996700	-0.28326000	0.06550500
C	2.67579300	-1.69521800	0.99623800
C	1.69171100	-2.48069900	0.31271400
C	1.77949500	-2.19539600	-1.11103500
C	2.76547100	-1.19432700	-1.29607300
C	3.28232100	-0.85317500	0.02001500
C	-0.73908400	2.01809500	1.63066000
C	-0.98468000	0.71185700	2.06477200
C	-0.66779400	3.12275200	2.45804700
C	-1.10766100	0.51146400	3.44886000
C	-0.85045700	2.90882700	3.82929900
H	-0.47614400	4.11292800	2.05930400
C	-1.04609400	1.61066100	4.31056700
H	-1.22973900	-0.48378700	3.85920000

H	-0.82280700	3.74865000	4.51593900
H	-1.15595400	1.44864700	5.37924400
C	3.03148400	-1.76775300	2.45341800
H	2.16947700	-2.04576800	3.06611800
H	3.81894700	-2.51186700	2.64062800
H	3.39799400	-0.80616200	2.82402500
C	4.43283700	0.07216200	0.29847200
H	5.35030000	-0.50567500	0.47078000
H	4.62799600	0.74655800	-0.53710400
H	4.25752700	0.67880200	1.19175800
C	3.28918200	-0.70691600	-2.61617500
H	4.09600200	-1.35379800	-2.99041300
H	2.50694700	-0.69435700	-3.38111400
H	3.69921500	0.30414900	-2.54771200
C	1.08774000	-2.94957800	-2.21053200
H	1.78164800	-3.65212700	-2.69153200
H	0.24755200	-3.53570500	-1.83339400
H	0.70722900	-2.28324800	-2.99121000
C	0.92199200	-3.60956100	0.93162800
H	0.71466000	-3.42125700	1.98805200
H	-0.03434000	-3.78315900	0.43687400
H	1.50394800	-4.53935700	0.87075400
C	-0.78244900	0.56972700	-0.31715900
C	-1.03083400	-0.19790900	0.89877100
C	-1.57626800	0.57800200	-1.58349300
C	-2.97152600	0.73344800	-1.55127000
H	-3.47424100	0.83665800	-0.59543500
C	-3.70931100	0.75892000	-2.73335400
H	-3.64154900	0.65723000	-4.88689300
H	-4.78795700	0.87953400	-2.69180900
C	-3.06484400	0.63673300	-3.96635700
C	-1.67758500	0.48885400	-4.01150700
C	-0.94018700	0.45871000	-2.82700500
H	0.13804800	0.33438600	-2.84847200
H	-1.16994800	0.39413300	-4.96751700
C	-1.89483200	-1.41227800	0.86533900
C	-2.78497500	-1.72638200	1.91071500
C	-3.64024900	-2.82734200	1.83557400
H	-4.31209300	-3.03361100	2.66448400
H	-2.84839000	-1.08617300	2.78013000
C	-1.93384200	-2.24446100	-0.27268000
H	-1.28187300	-2.02212800	-1.10695300
C	-2.79528700	-3.33535300	-0.35373500
C	-3.65019800	-3.64444300	0.70684300

H	-4.31747500	-4.49934000	0.64803300
H	-2.79834600	-3.94633100	-1.25266300
N	-0.38573200	1.99328700	0.21343000
C	-0.83173700	3.29998800	-0.60522300
C	1.44071700	2.91721700	-0.66050100
C	0.40581200	3.75967100	-1.08182100
H	0.52360200	4.65926100	-1.66666700
N	1.07814000	1.90430900	0.13507300
O	-1.99459500	3.62284300	-0.60766400
C	2.88054200	3.09541400	-1.02984000
H	3.12600500	2.47368000	-1.89761700
H	3.08112100	4.13613000	-1.29437100
H	3.53278700	2.80364600	-0.20541600

TS5-6

SCF done: -1609.6919397

Rh	1.09136900	0.29127800	0.04245900
C	2.27349900	0.40873500	-1.97416500
C	1.40608200	1.55397800	-1.89646900
C	1.81874100	2.36233500	-0.77865000
C	2.89798900	1.69143000	-0.12362500
C	3.16307800	0.46929900	-0.86452500
C	-0.93577100	-2.31585000	0.56707500
C	-1.23196000	-1.51873400	-0.55846600
C	-0.94913300	-3.71320000	0.54057100
C	-1.50112200	-2.17104900	-1.77682800
C	-1.27061700	-4.33056300	-0.66178600
H	-0.72469500	-4.28707000	1.43264400
C	-1.52567700	-3.56155000	-1.81340800
H	-1.67631800	-1.60617700	-2.68535900
H	-1.31305200	-5.41388100	-0.71698900
H	-1.74942300	-4.06428700	-2.75006000
C	2.25581900	-0.64903600	-3.03775100
H	1.23685800	-0.89439300	-3.35065000
H	2.80374600	-0.32266700	-3.93268000
H	2.72237000	-1.57246900	-2.68518500
C	4.25901700	-0.52266100	-0.59571100
H	4.94978500	-0.57219700	-1.44568100
H	4.84485000	-0.24833400	0.28427400
H	3.85694000	-1.52754800	-0.43121600
C	3.74190300	2.27197800	0.97299400
H	4.52418500	2.92455900	0.55920500
H	3.14645600	2.87909900	1.66055300
H	4.24105700	1.49867900	1.55994300

C	1. 33692400	3. 74580200	-0. 45054900
H	2. 03363700	4. 49860700	-0. 84429000
H	0. 35746500	3. 94812600	-0. 88652800
H	1. 26277000	3. 90744700	0. 62936700
C	0. 41676600	1. 94173200	-2. 95496200
H	-0. 06499200	1. 06469900	-3. 39524900
H	-0. 37034400	2. 58970000	-2. 56810300
H	0. 92602500	2. 47860300	-3. 76666900
C	-0. 72840700	-0. 07399500	1. 22851600
C	-1. 15976500	-0. 10887400	-0. 15678600
C	-1. 21201400	0. 81503100	2. 33126400
C	-2. 51145900	0. 64879400	2. 83824000
H	-3. 14834400	-0. 12980000	2. 43142200
C	-2. 98022400	1. 46587700	3. 86631900
H	-2. 52746900	3. 09462200	5. 20589100
H	-3. 98757500	1. 32485300	4. 24716600
C	-2. 15943200	2. 45835900	4. 40590900
C	-0. 86312600	2. 62575500	3. 91648400
C	-0. 39321000	1. 80617600	2. 88927800
H	0. 61401700	1. 92413000	2. 49981500
H	-0. 21657800	3. 39199400	4. 33547100
C	-1. 99216300	0. 96654800	-0. 76229100
C	-2. 99629700	0. 66965100	-1. 70403200
C	-3. 81631300	1. 66661000	-2. 23497400
H	-4. 57953700	1. 39546000	-2. 95941000
H	-3. 17141300	-0. 35570900	-2. 00129400
C	-1. 87870500	2. 31107800	-0. 35319600
H	-1. 13610000	2. 57993200	0. 38571400
C	-2. 70460400	3. 30421800	-0. 87465400
C	-3. 67452800	2. 99277500	-1. 83062600
H	-4. 31460700	3. 76807800	-2. 24138400
H	-2. 58962600	4. 32790300	-0. 52810100
N	-0. 49154900	-1. 49559700	1. 59922200
C	-0. 48942000	-1. 98751500	3. 03657500
C	1. 74314200	-1. 34787500	2. 59795400
C	0. 82518600	-1. 84129200	3. 52613000
H	1. 07443400	-2. 07500000	4. 55185600
N	1. 44427000	-1. 23161700	1. 30759500
O	-1. 52417300	-2. 41879900	3. 51284000
C	3. 13353000	-0. 93165100	3. 03878700
H	3. 14107100	0. 14271800	3. 25230400
H	3. 41432300	-1. 46340300	3. 95151300
H	3. 87408600	-1. 13620400	2. 26448600

SCF done: -1609.80025129

Rh	-2.60736000	0.22042700	0.16879700
C	-4.43544200	0.01200900	1.35183400
C	-4.67382500	-0.55885800	0.06645400
C	-3.44553200	-0.81466400	2.05953300
C	-3.70932000	-1.62092600	-0.09423300
C	-3.01420000	-1.82019600	1.18056500
C	-5.18806800	1.16024900	1.95250200
H	-4.55381500	1.75234700	2.61715300
H	-5.57540900	1.82427400	1.17736000
H	-6.03747200	0.79429300	2.54498100
C	-5.63243900	-0.04479400	-0.96502100
H	-6.58497500	0.24145800	-0.50891500
H	-5.20041400	0.83417600	-1.46371500
H	-5.84219900	-0.80352700	-1.72319500
C	-3.57243700	-2.51386400	-1.28871400
H	-2.53739500	-2.83636600	-1.42538000
H	-4.18983200	-3.41403500	-1.16331600
H	-3.89429900	-2.00804300	-2.20140000
C	-2.00374900	-2.89568600	1.44301300
H	-1.29722200	-2.99693300	0.61482800
H	-1.42367500	-2.68790700	2.34466700
H	-2.49717300	-3.86664300	1.58041000
C	-3.00091100	-0.58218000	3.47154500
H	-2.03491100	-1.05009100	3.67266700
H	-2.90407300	0.48535200	3.68813500
H	-3.72872700	-0.99568400	4.18203800
C	3.53317000	1.81746900	0.32112600
C	4.52085700	2.72454400	0.74350100
C	4.19202000	4.06796000	0.87007900
C	2.89138500	4.52524900	0.57889100
C	1.90154000	3.65414700	0.13647100
C	2.24238800	2.30419700	-0.00437100
H	5.52383100	2.37494000	0.96802000
H	4.94575500	4.77770200	1.19881000
H	2.65655500	5.57936200	0.69555700
N	1.47459600	1.22101100	-0.42797500
C	0.05150200	1.25960100	-0.59719700
C	-1.89859800	2.25333800	-1.75046300
C	-0.48433600	2.11015100	-1.53818900
H	0.19878900	2.68644900	-2.15297200
N	-2.87024500	1.57667700	-1.19726100
O	-0.60841700	0.47638700	0.18489500
C	-2.30436400	3.31347700	-2.77116500

H	-1.86712600	3.09578400	-3.75308300
H	-3.39076700	3.34017700	-2.86424000
H	-1.94506900	4.30402100	-2.46808200
H	0.90262400	4.00613000	-0.09570500
C	2.25463100	0.05810900	-0.34702500
C	3.52584800	0.39176000	0.09221200
C	1.73047400	-1.25897000	-0.75301000
C	1.99660300	-2.39838800	0.02598200
C	0.98782700	-1.41479100	-1.93672500
C	1.54005900	-3.65458300	-0.36985100
H	2.56355000	-2.29048400	0.94430500
C	0.52844600	-2.67183600	-2.32888200
H	0.77745300	-0.54736200	-2.55428900
C	0.80372500	-3.79818000	-1.54901900
H	1.75976600	-4.52337500	0.24447800
H	-0.03311700	-2.77265700	-3.25367700
H	0.45478500	-4.77873300	-1.86075600
C	4.70042600	-0.49424200	0.23019700
C	5.47049700	-0.47215700	1.40704300
C	5.10168800	-1.35339400	-0.80820800
C	6.59803900	-1.28277300	1.54234300
H	5.16944200	0.17701500	2.22399700
C	6.22488500	-2.16712800	-0.67002000
H	4.52905200	-1.37258300	-1.73001100
C	6.97954100	-2.13526400	0.50508600
H	7.17571700	-1.25100600	2.46223200
H	6.51710100	-2.82183100	-1.48660100
H	7.85734400	-2.76666200	0.60963200

TS7-IV

SCF done: -1838.9108163

Rh	2.33550000	-0.09960900	-0.32996400
C	4.13437300	-1.00304600	-1.25429900
C	3.95804200	-1.57549200	0.03704300
C	3.00417700	-1.40687100	-2.10273600
C	2.64923900	-2.19162200	0.05820800
C	2.11355400	-2.14858600	-1.30694200
C	5.33743100	-0.25211600	-1.74209800
H	5.06059400	0.48192400	-2.50296600
H	5.83529000	0.27992500	-0.92912100
H	6.06259600	-0.93942300	-2.19681600
C	4.89733500	-1.48589700	1.20212300
H	4.97827900	-2.45370600	1.70717300
H	5.89907400	-1.18910600	0.88291600

H	4.53915500	-0.74654600	1.92832200
C	2.08578700	-2.99438700	1.19097500
H	0.99546000	-3.02580000	1.15549200
H	2.45282200	-4.02932600	1.15136800
H	2.37994000	-2.57141400	2.15484600
C	0.79502000	-2.73447400	-1.70564600
H	0.80149600	-3.82257600	-1.57270600
H	-0.01284100	-2.32840100	-1.09019600
H	0.55912000	-2.52216000	-2.75029700
C	2.86445300	-1.03883900	-3.54938700
H	1.86690400	-1.27056400	-3.92754100
H	3.03302300	0.03208300	-3.69885900
H	3.59362300	-1.58025800	-4.16529500
C	-3.57851000	1.99131700	0.10911000
C	-4.38657600	3.10716300	-0.17246500
C	-3.83975000	4.37889500	-0.06268700
C	-2.49813100	4.55836800	0.33005000
C	-1.68420200	3.47377300	0.63797800
C	-2.24379600	2.19520300	0.53812700
H	-5.42110800	2.97143800	-0.47255300
H	-4.45235300	5.24881000	-0.28181400
H	-2.09235300	5.56353000	0.40162200
N	-1.68084500	0.94615900	0.79882200
C	-0.24908500	0.76388100	0.88752800
C	1.79295800	1.35355700	2.17919900
C	0.36690200	1.23168500	2.02832700
H	-0.26812900	1.61271000	2.81968300
N	2.71146600	0.92146200	1.36849400
O	0.28706100	0.23591600	-0.15149600
C	2.25986000	2.11715400	3.41337300
H	1.91404200	1.61437500	4.32419900
H	3.34913300	2.17933600	3.43940800
H	1.83990300	3.12944000	3.42341700
H	-0.65576500	3.60827500	0.95368700
C	-2.63315200	-0.03873800	0.50499300
C	-3.81273400	0.56700100	0.10065800
C	-2.36607500	-1.46944100	0.72959500
C	-2.79042400	-2.43083600	-0.20534800
C	-1.74102100	-1.91169200	1.90943200
C	-2.60869300	-3.79114200	0.03914600
H	-3.26724000	-2.10171700	-1.12224700
C	-1.56148800	-3.27411700	2.15100400
H	-1.41032900	-1.18309700	2.64245700
C	-1.99601600	-4.21990600	1.21928900

H	-2.94750700	-4.51779500	-0.69401500
H	-1.09111300	-3.59698200	3.07582500
H	-1.86177400	-5.28041800	1.41265300
C	-5.11180400	-0.07365300	-0.19270300
C	-5.81705100	0.25918000	-1.36333600
C	-5.69605500	-0.99735200	0.69220600
C	-7.05834500	-0.31420300	-1.64122300
H	-5.37680000	0.96299800	-2.06356700
C	-6.93313500	-1.57469000	0.41076500
H	-5.17508800	-1.25397300	1.60914400
C	-7.62136700	-1.23543800	-0.75652700
H	-7.58311500	-0.04383700	-2.55362100
H	-7.36563400	-2.28481300	1.11046600
H	-8.58767400	-1.68244800	-0.97240600
C	3.48015100	2.71269200	-0.87621200
O	2.61848400	1.91240000	-1.30482900
O	4.13982200	2.57289800	0.23083700
H	3.64136000	1.78664300	0.86213600
C	3.80492300	3.95686300	-1.67148500
H	3.34734200	3.91116500	-2.65962000
H	3.42469000	4.83225100	-1.13506200
H	4.88903200	4.07267900	-1.75423400

IV

SCF done: -1838.9347698

Rh	2.43937800	-0.17805900	-0.20073600
C	3.99694900	-0.96517400	-1.56884000
C	4.19863600	-1.47423800	-0.24073400
C	2.70567900	-1.40158000	-2.03167200
C	3.04269800	-2.29047200	0.10428100
C	2.13973000	-2.24632600	-1.00372900
C	4.97533500	-0.12355300	-2.32713200
H	4.48494700	0.43712900	-3.12531400
H	5.46763800	0.58727000	-1.66147900
H	5.73854300	-0.76514800	-2.78628900
C	5.43230600	-1.27219000	0.58602200
H	6.25563600	-1.89668300	0.21721200
H	5.74100800	-0.22441600	0.54859600
H	5.25857200	-1.54303600	1.63073900
C	2.87640500	-3.07882300	1.36896300
H	1.82486000	-3.29748600	1.56642500
H	3.41499700	-4.03294500	1.30790000
H	3.26772200	-2.53115300	2.23037100
C	0.80632000	-2.91564200	-1.10779300

H	0.49299500	-3.36119300	-0.16352800
H	0.03464400	-2.20124200	-1.40513900
H	0.84450800	-3.70875400	-1.86464900
C	2.09650800	-1.13607700	-3.37606000
H	1.00553900	-1.12220700	-3.31670900
H	2.41653000	-0.17028700	-3.77374700
H	2.38300300	-1.91009900	-4.10015200
C	-3.50531300	2.05251000	-0.14356100
C	-4.27806300	3.16998000	-0.50687500
C	-3.70290900	4.43258800	-0.44970700
C	-2.36756900	4.60313600	-0.03093500
C	-1.58786600	3.51920500	0.35667000
C	-2.17791400	2.25119300	0.31022200
H	-5.30708900	3.04229400	-0.82861200
H	-4.28766500	5.30315400	-0.73276700
H	-1.93929200	5.60105200	-0.00546500
N	-1.65387000	1.00753800	0.65208900
C	-0.23574600	0.79118500	0.84234600
C	1.65872000	1.18497100	2.41850600
C	0.28808200	1.25286300	2.04240000
H	-0.40484600	1.70290100	2.74209900
N	2.58437300	0.59997100	1.70551700
O	0.35320600	0.22446800	-0.13061900
C	2.04426200	1.84443000	3.72774100
H	1.41228900	1.47785100	4.54287700
H	3.08973900	1.65545200	3.98381200
H	1.89335000	2.92714800	3.66035200
H	-0.56213300	3.64624700	0.68504600
C	-2.61702300	0.02507100	0.38506300
C	-3.77163000	0.63509500	-0.08301200
C	-2.37324800	-1.39904200	0.67360700
C	-2.82388400	-2.39298600	-0.21421400
C	-1.72964500	-1.80320500	1.85766800
C	-2.64997800	-3.74425700	0.07969000
H	-3.31466300	-2.09699100	-1.13498200
C	-1.55036700	-3.15654800	2.14541100
H	-1.38126300	-1.05252600	2.55923600
C	-2.01354700	-4.13388600	1.26118900
H	-3.01163000	-4.49514700	-0.61725600
H	-1.06393300	-3.44703300	3.07284300
H	-1.88422700	-5.18753400	1.49208200
C	-5.07680000	0.00794400	-0.37929100
C	-5.73917800	0.28716700	-1.58826200
C	-5.70779400	-0.84947700	0.53944900

C	-6.98482400	-0.27480600	-1.87033700
H	-5.26221400	0.93928000	-2.31402600
C	-6.94922000	-1.41546200	0.25429700
H	-5.21935200	-1.06302900	1.48489200
C	-7.59464300	-1.13033600	-0.95135700
H	-7.47630800	-0.04718800	-2.81241900
H	-7.41862500	-2.07384500	0.98027100
H	-8.56430200	-1.56834400	-1.17054300
C	3.72499700	2.45856300	-0.43833000
O	2.64829200	1.81799300	-0.78536700
O	4.68995700	1.99382200	0.18579500
H	3.53704400	0.75639200	2.01809900
C	3.71805500	3.91699800	-0.89269600
H	2.84579600	4.43240400	-0.47971000
H	4.63276300	4.41622100	-0.56997400
H	3.63311400	3.96840200	-1.98263000

IV'

SCF done: -1838.9071509

Rh	2.32633300	-0.31567900	-0.18377800
C	2.81758000	0.14256700	-2.30585700
C	3.70136000	-0.87839100	-1.84559800
C	1.45620500	-0.34993200	-2.21612600
C	2.89261300	-2.02774700	-1.47181700
C	1.51882200	-1.70848300	-1.74091000
C	3.22787700	1.49576300	-2.79881600
H	2.43243800	2.22836100	-2.64672100
H	4.11686100	1.84818100	-2.27288700
H	3.44776500	1.45712700	-3.87360100
C	5.19437700	-0.76250600	-1.76298300
H	5.64536300	-0.79690400	-2.76257200
H	5.47451500	0.18023000	-1.28463900
H	5.62502200	-1.57936700	-1.17908400
C	3.42045800	-3.35956600	-1.02573300
H	2.67524100	-3.91514900	-0.45164500
H	3.69673400	-3.97494400	-1.89161600
H	4.30999600	-3.25004700	-0.40064900
C	0.35187000	-2.63971600	-1.61292200
H	0.50240400	-3.38836900	-0.83230600
H	-0.57129400	-2.10502900	-1.38245200
H	0.19880900	-3.17503400	-2.55927300
C	0.23092900	0.35886500	-2.71267000
H	-0.67253100	-0.00770200	-2.21958000
H	0.28871600	1.43455600	-2.53172500

H	0.10597400	0.20792500	-3.79317400
C	-2.98775600	-1.85899300	0.64403300
C	-3.63685300	-3.09018400	0.44998100
C	-3.07584300	-4.24325900	0.98426600
C	-1.88119100	-4.18275700	1.72500300
C	-1.20703100	-2.97901100	1.91281500
C	-1.74736800	-1.82296700	1.33121800
H	-4.57026100	-3.13261600	-0.10227200
H	-3.57240900	-5.19920500	0.84583500
H	-1.47836000	-5.08856400	2.16888700
N	-1.31243300	-0.49539500	1.35082300
C	-0.11909800	-0.00154800	2.00383300
C	2.35037900	-0.43519100	2.43773400
C	1.10830200	-0.73796300	1.70392200
H	1.00573300	-1.77508500	1.40449000
N	3.35205900	-0.57448600	1.62827400
O	-0.18471700	1.00922100	2.68396900
C	2.44324600	0.07222900	3.84399800
H	1.97036300	-0.63127200	4.53770000
H	3.48379700	0.23173300	4.13942100
H	1.88439600	1.00921400	3.91182700
H	-0.30684100	-2.94862800	2.51511500
C	-2.29187400	0.30943300	0.73510500
C	-3.31159800	-0.50352600	0.26700200
C	-2.19097000	1.78017700	0.62140900
C	-3.32041400	2.56322400	0.91584800
C	-1.01798900	2.42550600	0.19464500
C	-3.28464800	3.94921800	0.77412800
H	-4.22633400	2.07906200	1.26421300
C	-0.98718400	3.81214300	0.05544700
H	-0.11402800	1.86194300	-0.00499100
C	-2.11820600	4.58020600	0.33880600
H	-4.16798200	4.53552200	1.01124200
H	-0.06722200	4.29088300	-0.26776400
H	-2.08822400	5.66090600	0.23062600
C	-4.49637600	-0.11056900	-0.52599200
C	-5.77709300	-0.56490900	-0.16369600
C	-4.37919800	0.69406200	-1.67308200
C	-6.89956800	-0.22622800	-0.92051300
H	-5.89146000	-1.17244200	0.72912800
C	-5.50104800	1.03589700	-2.42580100
H	-3.39877000	1.05295300	-1.96964200
C	-6.76678900	0.57585500	-2.05471900
H	-7.87972500	-0.58475600	-0.61803700

H	-5.38591100	1.65965600	-3.30803600
H	-7.64023700	0.84079400	-2.64370600
C	3.31846400	2.34855400	0.54719100
O	2.19699600	1.69935700	0.40955300
O	4.45201600	1.88579800	0.36831000
H	4.28024000	-0.28044800	1.92156800
C	3.12554400	3.81224600	0.93738400
H	2.21007500	3.95106500	1.51565700
H	3.99360700	4.16495300	1.49802200
H	3.04721600	4.41520500	0.02510800

TSIV'-P'

SCF done: -2068.0229296

Rh	2.69604000	0.93006100	-1.56960500
C	4.47272500	-0.34254600	-1.83519000
C	4.13317200	-0.26033700	-0.43758500
C	3.36213400	-0.92047700	-2.53834400
C	2.82900000	-0.88507100	-0.26132000
C	2.35615200	-1.27175200	-1.54948700
C	5.75891900	0.11985200	-2.44435500
H	5.61988000	0.42158000	-3.48425300
H	6.17531600	0.96533200	-1.89438800
H	6.49058100	-0.69806000	-2.42457600
C	5.03675900	0.25012700	0.64372400
H	5.82386500	-0.48095900	0.86768600
H	5.50129100	1.18966800	0.33475700
H	4.48520300	0.43728400	1.56724700
C	2.16002000	-1.14622600	1.05236100
H	1.07828400	-1.24871800	0.95105500
H	2.54703200	-2.07599600	1.48841500
H	2.34696300	-0.34462300	1.76857600
C	1.05383400	-1.93372800	-1.88091100
H	0.42523900	-2.06044300	-0.99813700
H	0.49729700	-1.34483500	-2.61654800
H	1.23434100	-2.92569500	-2.31180500
C	3.27715900	-1.21985100	-4.00411100
H	2.25065300	-1.11916500	-4.36487500
H	3.90278000	-0.54010100	-4.58686300
H	3.60844000	-2.24519200	-4.21384300
C	-3.88756100	0.28276900	1.52479000
C	-4.65752400	-0.66336200	0.82929800
C	-4.05580500	-1.43126200	-0.15999800
C	-2.69361300	-1.26407600	-0.46575900
C	-1.91163200	-0.32095000	0.19710400

C	-2.52273700	0.46569700	1.18212100
H	-5.70956000	-0.78832900	1.06544700
H	-4.64142000	-2.16688400	-0.70372100
H	-2.24074000	-1.87520100	-1.24161300
N	-2.01243600	1.47878500	2.00191500
C	-0.61022500	1.78495200	2.21594000
C	1.48619600	2.34018100	0.99389500
C	0.16462000	1.95921800	1.00786100
H	-0.34388400	1.85919900	0.05778300
N	2.11806500	2.55339100	-0.21826600
O	-0.20589700	1.91883300	3.36438900
C	2.27808800	2.61340900	2.25164200
H	1.82135600	3.42713100	2.82216700
H	2.25838900	1.75494700	2.92893800
H	3.31212500	2.87264000	2.01036100
H	-0.86864500	-0.19460000	-0.06325600
C	-3.04028200	1.91952200	2.85496500
C	-4.20008300	1.22163200	2.57779100
C	-2.85399600	3.04708700	3.79043400
C	-3.27956900	2.94137000	5.12314400
C	-2.29910000	4.26194800	3.35389700
C	-3.15176300	4.02076100	5.99617500
H	-3.70334300	2.00562700	5.47215300
C	-2.17130000	5.33903100	4.22826600
H	-1.97380900	4.36136100	2.32226200
C	-2.59770800	5.22308300	5.55321300
H	-3.48203500	3.91980800	7.02619800
H	-1.74183000	6.27169500	3.87309300
H	-2.49800100	6.06323000	6.23464400
C	-5.54502300	1.43253200	3.15399400
C	-6.29750900	0.34027700	3.62129800
C	-6.12119400	2.71314800	3.22206000
C	-7.58044900	0.52195200	4.13904800
H	-5.86282900	-0.65459400	3.59122200
C	-7.40098800	2.89418700	3.74356600
H	-5.55864400	3.56665200	2.85796600
C	-8.13785400	1.79990400	4.20266300
H	-8.14193400	-0.33636700	4.49802300
H	-7.82702800	3.89293600	3.78493900
H	-9.13661700	1.94251300	4.60549000
C	4.40339500	3.28194000	-2.17807200
O	3.48647700	2.51170900	-2.68635000
O	4.87019900	3.19155000	-1.03294500
H	3.03992400	2.97541900	-0.09824500

C	4.88400200	4.36092800	-3.14174900
H	4.03436800	4.96116100	-3.47992400
H	5.62048500	4.99941400	-2.65282200
H	5.32648500	3.89839200	-4.02970200
C	0.41074700	2.52824200	-2.79986900
O	0.91813100	1.37656100	-2.72850000
O	0.64322600	3.47769100	-1.97084700
H	1.34088500	3.11183500	-1.14694000
C	-0.54054500	2.83782800	-3.93020100
H	-0.82962300	1.92558500	-4.45191600
H	-1.42143000	3.35719400	-3.54580500
H	-0.03874000	3.51178000	-4.63248000

P'

SCF done: -2068.0229296

C	-4.67924700	3.19726600	1.24773400
C	-5.88980700	2.48582900	1.22609900
C	-5.89597700	1.15094300	1.61157900
C	-4.70995800	0.51797400	2.02550400
C	-3.49339600	1.19486300	2.03718600
C	-3.48326700	2.53072900	1.61608800
H	-6.80614600	2.97835300	0.91627700
H	-6.82667900	0.59108000	1.60215600
H	-4.73962600	-0.52005500	2.34429100
N	-2.43703100	3.45661100	1.52160100
C	-1.10397600	3.27764600	2.05095200
C	0.74165200	1.61704100	2.14396800
C	-0.46798200	2.03979800	1.65399400
H	-0.97027900	1.43167000	0.90857200
N	1.29335800	0.44608900	1.71644100
O	-0.60536300	4.16485200	2.73171500
C	1.55264300	2.36224600	3.17117800
H	2.30156700	1.70608800	3.62578000
H	2.06037900	3.21274500	2.70561600
H	0.90989600	2.78378400	3.94356800
H	-2.58984200	0.69951400	2.37122300
C	-2.97271700	4.69629300	1.12672500
C	-4.33431000	4.56522000	0.93210400
C	-2.12228500	5.87755600	0.87737500
C	-2.47109000	7.12516100	1.41702600
C	-0.98258700	5.79230200	0.06033200
C	-1.70142200	8.25561500	1.14687600
H	-3.34533600	7.20054000	2.05492800
C	-0.21375800	6.92292200	-0.20743500

H	-0.70454100	4.83494900	-0.37107700
C	-0.57031100	8.15980500	0.33440800
H	-1.98399900	9.21237900	1.57690700
H	0.66313000	6.83893000	-0.84351000
H	0.02936600	9.04122500	0.12559800
C	-5.27853800	5.58160600	0.42182600
C	-6.49664500	5.81385400	1.08516200
C	-5.00686900	6.31859600	-0.74413900
C	-7.40965100	6.75127600	0.60111400
H	-6.71730900	5.26480800	1.99581000
C	-5.91739700	7.25844300	-1.22421400
H	-4.07675700	6.14506400	-1.27553700
C	-7.12370000	7.47849500	-0.55537600
H	-8.34280900	6.91699700	1.13268900
H	-5.68679400	7.81590900	-2.12798200
H	-7.83384700	8.20882600	-0.93278300
H	2.24124400	0.21380300	1.96249000
H	0.88372800	-0.05719800	0.94480000

R2

SCF done: -539.46467768

C	-0.00028600	0.60790700	-0.00011400
C	0.00028600	-0.60790700	-0.00011400
C	-0.00098100	2.03704000	-0.00006000
C	-0.86032400	2.75297600	0.85638100
C	0.85768100	2.75388300	-0.85643500
C	-0.85768100	4.14572600	0.85317700
H	-1.52355500	2.20489800	1.51784800
C	0.85372300	4.14662800	-0.85307700
H	1.52142800	2.20649800	-1.51795800
C	-0.00231000	4.84722300	0.00009300
H	-1.52541600	4.68534300	1.51868400
H	1.52094800	4.68695100	-1.51852100
H	-0.00282200	5.93332400	0.00015400
C	0.00098100	-2.03704000	-0.00006000
C	0.86032400	-2.75297600	0.85638100
C	-0.85768100	-2.75388300	-0.85643500
C	0.85768100	-4.14572600	0.85317700
H	1.52355500	-2.20489800	1.51784800
C	-0.85372300	-4.14662800	-0.85307700
H	-1.52142800	-2.20649800	-1.51795800
C	0.00231000	-4.84722300	0.00009300
H	1.52541600	-4.68534300	1.51868400
H	-1.52094800	-4.68695100	-1.51852100

H	0.00282200	-5.93332400	0.00015400
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P

SCF done: -1111.36263339

C	-4.10832000	2.80496800	-0.71242800
C	-4.64591600	3.95650900	-1.30983900
C	-3.85402700	5.09292800	-1.41896900
C	-2.52950700	5.09333200	-0.94556200
C	-1.97947600	3.97184900	-0.33077800
C	-2.79055300	2.83892600	-0.19164600
H	-5.66483600	3.95157900	-1.68378200
H	-4.25742600	5.98891000	-1.88177900
H	-1.91985800	5.98504700	-1.05972400
N	-2.52517100	1.58160800	0.36671900
C	-1.23401100	1.10665400	0.78044200
C	0.77732400	1.65236000	2.09399100
C	-0.48703400	1.97999200	1.64648300
H	-0.93958900	2.89762900	1.99487700
N	1.39393900	0.50625700	1.74659100
O	-0.86069200	-0.01143600	0.40855200
C	1.54120100	2.57028700	3.01213200
H	1.78540000	2.06059200	3.95136100
H	2.48620300	2.87642500	2.54833600
H	0.96588900	3.46697100	3.24507800
H	-0.95434100	3.98045100	0.01836400
C	-3.65221600	0.75981600	0.17412000
C	-4.64069000	1.48388300	-0.46354700
C	-3.72121400	-0.61861500	0.69937900
C	-4.16599900	-1.66519300	-0.12305200
C	-3.39257400	-0.90461900	2.03509700
C	-4.27788800	-2.96183600	0.37642400
H	-4.41669100	-1.45602200	-1.15763600
C	-3.50364000	-2.20156600	2.53201000
H	-3.05524600	-0.10323200	2.68616000
C	-3.94728000	-3.23578700	1.70473900
H	-4.61964700	-3.76046600	-0.27593300
H	-3.24740800	-2.40414900	3.56828100
H	-4.03406700	-4.24678600	2.09263100
C	-6.01938200	1.05318400	-0.77803600
C	-6.55210300	1.26656700	-2.06195000
C	-6.84203100	0.45207300	0.19057500
C	-7.86052600	0.89056600	-2.36731200
H	-5.92647800	1.71604700	-2.82743300
C	-8.14754700	0.07251300	-0.11685300

H	-6.45169700	0.28941400	1.18992600
C	-8.66390600	0.29103300	-1.39612900
H	-8.24957300	1.06160300	-3.36739000
H	-8.76610500	-0.38931400	0.64787500
H	-9.68271400	-0.00244100	-1.63278600
H	2.31782600	0.28990700	2.08145300
H	0.87078300	-0.13787300	1.15644900

C6H5NHNHAc

SCF done: -495.590247

N	-1.58106300	0.16860200	-0.73591200
C	0.75361800	-0.27003700	-0.39854500
C	1.74903900	-1.23370900	-0.17682700
H	1.52182500	-2.28528500	-0.33433500
C	3.01946100	-0.84575100	0.23948800
H	3.77718200	-1.60486400	0.41277100
C	3.32098200	0.50439200	0.43759800
H	4.31247300	0.80449400	0.76219100
C	2.32963000	1.46000700	0.21470500
H	2.54636300	2.51365900	0.36862900
C	1.05167100	1.08306500	-0.20097100
H	0.28255500	1.83033600	-0.36094400
N	-0.50243600	-0.70855500	-0.89398700
H	-0.76503000	-1.60889200	-0.49852000
H	-1.88591700	0.61799000	-1.58954000
C	-2.51434200	-0.09302600	0.24690200
O	-2.33776400	-0.96644100	1.08296400
C	-3.75576300	0.77739800	0.19752400
H	-3.88125300	1.25529900	1.17225700
H	-3.71639000	1.55080800	-0.57434200
H	-4.63097000	0.14361800	0.02816200

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SCF done: -1533.5271077

Rh	1.12329400	-0.02841900	-0.07221900
N	0.56610900	-0.45640300	1.92557200
C	2.54870500	-0.07586100	-1.79508000
C	2.13995300	1.27003200	-1.58779000
C	2.52423300	1.62034000	-0.23717700
C	3.34039700	0.52014000	0.30107000
C	3.34925500	-0.51413000	-0.64155100
N	-0.10548200	-1.72560500	2.08064400
C	-0.10165300	-2.44736300	0.88093100
C	-0.66465700	-1.87853200	-0.29696000

C	0.47686400	-3.73098100	0.82496900
C	-0.52639200	-2.60019300	-1.50554100
C	0.53755000	-4.43734900	-0.36888300
H	0.89399500	-4.15931200	1.73374100
C	0.05896300	-3.85983600	-1.55420400
H	-0.93340300	-2.15539400	-2.40950800
H	0.98455400	-5.42746000	-0.38497800
H	0.12690900	-4.39787500	-2.49478800
H	0.36679900	-2.26165500	2.80585700
C	0.44256300	0.41959400	2.94301100
O	0.95709800	1.55580000	2.89675900
C	-0.29640000	-0.02981000	4.20124700
H	0.26153500	-0.80706200	4.73909900
H	-0.39906800	0.83420500	4.85802000
H	-1.27857800	-0.44455000	3.95714700
C	2.37657700	-0.88501100	-3.04542100
H	1.56708400	-0.49797200	-3.66792600
H	3.29834300	-0.86321100	-3.64182200
H	2.15574500	-1.93138300	-2.81725100
C	4.01474900	-1.85384800	-0.53945400
H	4.85072100	-1.93267100	-1.24645500
H	4.41126500	-2.02637900	0.46343000
H	3.31722700	-2.66700100	-0.76675800
C	3.98541300	0.55603500	1.65218000
H	4.85715200	1.22318600	1.63916000
H	3.27769400	0.93583600	2.39369400
H	4.32640700	-0.43303900	1.96647200
C	2.41044400	2.97143300	0.39462000
H	3.35637300	3.51901800	0.27876500
H	1.61888100	3.56174900	-0.07037300
H	2.18021600	2.87137300	1.45669800
C	1.48422800	2.18303900	-2.57895300
H	1.00662500	1.62318500	-3.38654800
H	0.71824600	2.80408100	-2.11064000
H	2.22981500	2.84953800	-3.03152400
C	-0.84221300	0.50572500	-0.27814200
C	-1.54382600	-0.64520200	-0.26719100
C	-1.33553400	1.88317200	-0.42237500
C	-1.07411500	2.86714700	0.55219600
H	-0.49626600	2.60115400	1.43296200
C	-1.55444300	4.16741100	0.38963800
H	-2.64961200	5.53692000	-0.87175900
H	-1.35426900	4.90901900	1.15857100
C	-2.28341400	4.52149800	-0.74863700

C	-2.53490100	3.55878200	-1.72904800
C	-2.06832600	2.25475500	-1.56816000
H	-2.27580600	1.50538300	-2.32644300
H	-3.09895100	3.82189400	-2.62005000
C	-3.01898600	-0.83682400	-0.18829300
C	-3.84038700	0.12369000	0.43641200
C	-5.21684400	-0.06060100	0.53587300
H	-5.82174200	0.69671100	1.02736300
H	-3.39058500	1.01345300	0.86020000
C	-3.63987100	-1.99978700	-0.68142300
H	-3.04067000	-2.77308800	-1.15003100
C	-5.01915600	-2.18337400	-0.58039600
C	-5.81813100	-1.21329500	0.02410200
H	-6.89202400	-1.35610000	0.10448200
H	-5.46787400	-3.09082500	-0.97595200

↳TSII-III

SCF done: -1533.4768123

Rh	-1.33341500	0.12061800	0.05426200
N	-1.19459700	0.56707400	1.93510400
C	-2.16236700	-1.12435200	-1.75727500
C	-2.65810100	-1.70795400	-0.54292000
C	-3.54451500	-0.74229600	0.08469900
C	-3.53088400	0.43777300	-0.68894300
C	-2.62542500	0.22367200	-1.81571400
N	-0.84829600	2.09386000	0.28471000
C	0.30663900	2.74863800	0.04283000
C	1.52169100	2.05862700	-0.29274800
C	0.30963700	4.17206100	0.13366100
C	2.65260800	2.86793700	-0.55977400
C	1.43494700	4.91370100	-0.15660100
H	-0.61656200	4.66725600	0.41740300
C	2.62250400	4.25279900	-0.51187000
H	3.58706200	2.38013500	-0.80501200
H	1.40015900	5.99802700	-0.10174700
H	3.52177900	4.81971700	-0.73194500
H	-1.61674700	2.68127400	0.58416200
C	-0.22691800	0.84402900	2.84678100
O	0.28224200	-0.13486000	3.41585300
C	0.07373500	2.25827200	3.29748700
H	-0.82142100	2.88498400	3.27567300
H	0.47596500	2.21696400	4.31223800
H	0.82280700	2.71317200	2.64345600
C	-1.40362500	-1.83385900	-2.83683500

H	-0.82933900	-2.67383400	-2.44491700
H	-2.10285000	-2.22545000	-3.58748800
H	-0.70912000	-1.16446900	-3.35092600
C	-2.41357800	1.19356300	-2.94173900
H	-1.52054100	0.94714600	-3.52036400
H	-3.26887000	1.18630500	-3.63051000
H	-2.29522400	2.21583100	-2.57274900
C	-4.31918700	1.69355800	-0.45213000
H	-5.22107200	1.71590400	-1.07763400
H	-4.63765700	1.78366400	0.58918800
H	-3.73859900	2.58659500	-0.70424700
C	-4.29368000	-0.98599300	1.36119000
H	-4.91099700	-1.88821000	1.28513800
H	-3.60251000	-1.11914800	2.20022200
H	-4.95348200	-0.15093800	1.60610900
C	-2.51973400	-3.14050400	-0.12145300
H	-2.57183800	-3.24264500	0.96522800
H	-3.32892100	-3.74725000	-0.55145100
H	-1.57020300	-3.56864800	-0.44595300
C	0.63273900	-0.31676900	-0.13816800
C	1.64643400	0.59328300	-0.28441200
C	0.90910900	-1.77759900	-0.06672700
C	1.40870500	-2.49348800	-1.17159000
H	1.60633700	-1.96607500	-2.09871400
C	1.66629100	-3.86230400	-1.08744300
H	1.65659200	-5.61027800	0.17945000
H	2.05065100	-4.39110800	-1.95577700
C	1.44760600	-4.54628800	0.11031200
C	0.97018000	-3.84552000	1.22064900
C	0.69313600	-2.48090700	1.13549500
H	0.34071500	-1.93676900	2.00646400
H	0.81332300	-4.36307200	2.16345700
C	3.06272700	0.06673100	-0.32859700
C	3.70247900	-0.29801800	0.86472000
C	5.00875800	-0.78882400	0.85105100
H	5.48604700	-1.07305600	1.78488200
H	3.16143800	-0.20809500	1.80247800
C	3.76685000	-0.06439500	-1.53447600
H	3.28457100	0.22082700	-2.46609700
C	5.07467300	-0.55286900	-1.54941400
C	5.69958800	-0.91761600	-0.35542400
H	6.71629500	-1.30036700	-0.36557700
H	5.60358600	-0.65034000	-2.49378500

SCF done: -1533.4964685

Rh	-1.31920600	0.22245500	0.21548400
N	-1.19021900	0.25185400	2.03986000
C	-2.38528700	-0.91550800	-1.69711600
C	-2.61053800	-1.61805000	-0.44105400
C	-3.52998600	-0.82920200	0.34564100
C	-3.78762400	0.36530900	-0.36620400
C	-3.11017900	0.28942500	-1.64670600
N	-0.88806200	2.02567300	-0.44749200
C	0.28850500	2.73004200	-0.39950600
C	1.55198600	2.08117200	-0.30090700
C	0.23635200	4.14381800	-0.45981200
C	2.70001000	2.90107000	-0.25824700
C	1.38737800	4.91389400	-0.43127600
H	-0.73780100	4.62276000	-0.53688000
C	2.63402100	4.28786300	-0.32439600
H	3.66976400	2.42870000	-0.16431300
H	1.31408500	5.99656200	-0.48330600
H	3.54601700	4.87538800	-0.28691300
H	-1.68520200	2.64360300	-0.31945100
C	-0.12993500	0.42208900	2.89882000
O	0.40339200	-0.50811600	3.50388300
C	0.24022100	1.87723500	3.15711200
H	-0.61706900	2.54673600	3.05288200
H	0.65872600	1.95332700	4.16323800
H	0.99753000	2.18193500	2.42663300
C	-1.66905800	-1.46749000	-2.89414800
H	-0.86712000	-2.14707300	-2.60299500
H	-2.36268600	-2.03182800	-3.53223500
H	-1.23092600	-0.67301700	-3.50380300
C	-3.12636800	1.36021400	-2.68826500
H	-2.96543700	0.95227200	-3.68936300
H	-4.07533400	1.90463500	-2.69333000
H	-2.32010700	2.08619500	-2.49721100
C	-4.68427500	1.49150300	0.06088100
H	-5.64890200	1.44900800	-0.46199300
H	-4.88602600	1.46094800	1.13359100
H	-4.24763700	2.47008400	-0.16818100
C	-4.06600600	-1.20467700	1.69417300
H	-4.22474500	-2.28435700	1.76843900
H	-3.36229000	-0.91052900	2.48402700
H	-5.02244500	-0.71363800	1.89270000
C	-2.28698300	-3.05915100	-0.18877200
H	-2.17833800	-3.27149200	0.87632300

H	-3.09942200	-3.69101200	-0.57594900
H	-1.36478700	-3.36521700	-0.68323100
C	0.65812100	-0.27779400	-0.04918100
C	1.67208900	0.61195700	-0.22534900
C	0.90033200	-1.74609300	-0.06436500
C	1.32128200	-2.36732700	-1.25798200
H	1.46522100	-1.75942000	-2.14532000
C	1.58412700	-3.73644300	-1.30619600
H	1.65306400	-5.58424800	-0.19125900
H	1.91225300	-4.18797200	-2.23871300
C	1.44112500	-4.51921400	-0.15837900
C	1.03359200	-3.91545600	1.03291200
C	0.75559500	-2.54875000	1.08309000
H	0.45996000	-2.09032000	2.02138400
H	0.93386200	-4.51069500	1.93676500
C	3.08069700	0.07435700	-0.29768600
C	3.69621600	-0.44993700	0.84764400
C	5.00341000	-0.93660300	0.79267000
H	5.46384600	-1.34136400	1.68967200
H	3.13995200	-0.48203700	1.78005200
C	3.80909600	0.10997900	-1.49647700
H	3.34708300	0.52676800	-2.38757300
C	5.11408300	-0.38012100	-1.55304600
C	5.71582100	-0.90557400	-0.40726000
H	6.73225100	-1.28676800	-0.44999600
H	5.66083300	-0.35141100	-2.49176300