

Supporting Information

Mechanistic Insight into the Rh(III)-Catalyzed C-H Activation of 2-Acetyl-1-Arythydrazines in Water

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Cartesian coordinates and electronic energies for all of the calculated structure

R1

SCF done: -495.58993273

C	-0.88956900	0.95061200	-0.05302200
C	-2.16005300	1.49917200	0.12985800
C	-3.29181500	0.68575600	0.18453200
C	-3.14157900	-0.69748800	0.05286400
C	-1.88110200	-1.25825800	-0.13227000
C	-0.74337100	-0.43705900	-0.18350900
H	-0.01694900	1.59335500	-0.09285700
H	-2.25978700	2.57648800	0.22861100
H	-4.27622800	1.12067500	0.32542800
H	-4.01203200	-1.34650500	0.08918200
H	-1.77187000	-2.33572300	-0.23392500
N	0.52556600	-1.04230400	-0.32064000
H	0.49320400	-1.96581500	-0.73799400
N	1.57967200	-0.28351800	-0.80251300
H	1.48819200	0.18502800	-1.70103500
C	2.61327200	0.17172700	-0.00035300
O	3.42454600	0.96301600	-0.45272100
C	2.66708500	-0.38645400	1.40733400
H	1.77580200	-0.09979800	1.97318000
H	2.70368100	-1.47934600	1.39871900
H	3.55775700	0.01254900	1.89209000

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

1

SCF done:-1452.24843684

Rh	0. 69589700	-0. 25818100	-0. 25608100
C	-0. 45023800	-1. 50384200	-1. 68080700
C	0. 84100000	-1. 18642500	-2. 27506300
C	-0. 20775200	-2. 31383500	-0. 52130900
C	1. 85968700	-1. 73251900	-1. 44137100
C	1. 21539800	-2. 39459900	-0. 31977400
C	-1. 77241000	-1. 18598400	-2. 30809900
H	-2. 00044300	-1. 90965800	-3. 10254900
H	-2. 58450300	-1. 20930500	-1. 58054600
H	-1. 75748400	-0. 18934300	-2. 75483800
C	1. 02067100	-0. 37595300	-3. 51717800
H	2. 04904500	-0. 41771000	-3. 88201700
H	0. 35812300	-0. 73589900	-4. 31110300
H	0. 77272900	0. 67018600	-3. 30032700
C	3. 34020200	-1. 62020900	-1. 62003800
H	3. 75518000	-0. 96548700	-0. 84519100
H	3. 81312000	-2. 60454200	-1. 53608600
H	3. 59735900	-1. 19921100	-2. 59385200

C	1. 92080700	-3. 21631000	0. 71655300
H	2. 13462100	-4. 22017200	0. 32790100
H	2. 87334600	-2. 76215500	1. 00073600
H	1. 31592800	-3. 33458100	1. 61772600
C	-1. 22913500	-3. 04068300	0. 29461700
H	-1. 18114200	-4. 10928900	0. 04713000
H	-1. 05484400	-2. 93957300	1. 36832200
H	-2. 23719600	-2. 68450400	0. 08634900
O	2. 54340000	0. 52076200	0. 47808600
C	2. 70490200	1. 53656300	1. 26436900
O	1. 82745800	2. 03050300	1. 99434700
C	4. 10581200	2. 12937700	1. 25222000
H	4. 24021800	2. 70193500	0. 32790500
H	4. 24041900	2. 79554600	2. 10546100
H	4. 86059800	1. 33812800	1. 26206900
O	0. 45013000	1. 61591200	-1. 25963500
C	0. 12606200	2. 83159500	-0. 94973800
O	-0. 40486200	3. 22720700	0. 09721100
C	0. 44774200	3. 83594000	-2. 05660400
H	1. 51564400	3. 80100900	-2. 29402300
H	-0. 09786800	3. 57264900	-2. 96901300
H	0. 17084800	4. 84290400	-1. 74158200
C	-4. 56026800	-0. 78010600	0. 49329700
C	-3. 37944900	-0. 45973300	1. 16514800
C	-2. 68607400	0. 72078200	0. 85008400
C	-3. 22664200	1. 58011900	-0. 12625800
C	-4. 41742500	1. 25907800	-0. 77601700
C	-5. 08863800	0. 07093100	-0. 48090500
H	-5. 08585700	-1. 69477100	0. 75645600
H	-2. 99919200	-1. 09293800	1. 95424400
H	-2. 70847400	2. 50524400	-0. 35724200
H	-4. 81710600	1. 94115700	-1. 52176500
H	-6. 01521100	-0. 18038200	-0. 98879700
N	-1. 55527600	1. 18768300	1. 57248700
N	-0. 31879600	0. 44433900	1. 64260000
C	-0. 22195900	-0. 53872300	2. 68719900
O	-1. 17379300	-1. 18604200	3. 07263300
C	1. 16082700	-0. 69562700	3. 28303700
H	1. 93168900	-0. 79329700	2. 51692100
H	1. 40029100	0. 20207300	3. 86239200
H	1. 15280700	-1. 56572400	3. 93972300
H	-1. 23855900	2. 07631400	1. 15544900
H	0. 44169200	1. 16965400	1. 80686300

TS1-2

SCF done: -1452.24132573

Rh	0.67188900	-0.28410600	-0.22899900
C	-0.36626800	-1.77567200	-1.43309000
C	0.78058000	-1.33800800	-2.21778200
C	0.13464800	-2.44615300	-0.25828000
C	1.95421000	-1.62863300	-1.48163600
C	1.56119200	-2.30181500	-0.24611800
C	-1.77877600	-1.73467400	-1.92665700
H	-1.90194900	-2.44027300	-2.75993000
H	-2.49304100	-1.99465500	-1.14498600
H	-2.04028900	-0.73566900	-2.28684100
C	0.66639800	-0.63112000	-3.52728500
H	1.64492500	-0.40105300	-3.95292100
H	0.11212500	-1.24633300	-4.24485100
H	0.12866400	0.31217100	-3.38149100
C	3.36709900	-1.29349400	-1.84651200
H	3.75783600	-0.52117900	-1.17651200
H	4.00967400	-2.17578500	-1.76098000
H	3.43718200	-0.92013800	-2.86909900
C	2.53600200	-2.91482500	0.71258600
H	2.96210800	-3.83054100	0.28208100
H	3.36508200	-2.23336600	0.92284600
H	2.06655200	-3.18184000	1.65989400
C	-0.69400900	-3.21828200	0.72034200
H	-0.84787000	-4.23706300	0.33955300
H	-0.21031000	-3.30047200	1.69539500
H	-1.67379600	-2.75913600	0.86737300
O	2.40431500	0.91944800	0.36720000
C	2.44418900	1.73704500	1.32505800
O	1.57427200	1.78744000	2.26538600
C	3.56846300	2.74131400	1.38144200
H	3.23757400	3.63443500	0.83817200
H	3.77601500	3.02873300	2.41430500
H	4.46563200	2.34987700	0.89724300
O	0.12566600	1.43605300	-1.37536200
C	0.26601400	2.69008400	-1.07874800
O	0.17432900	3.18836600	0.05255400
C	0.58877100	3.57927700	-2.27897100
H	1.67496600	3.57131000	-2.44279200
H	0.11284200	3.20392900	-3.18907500
H	0.27783800	4.60749500	-2.07921500
C	-4.54976000	-0.67105800	0.31049200
C	-3.38681200	-0.34864300	1.01105500

C	-2.65208100	0.80399500	0.67376200
C	-3.14187200	1.63319800	-0.35418700
C	-4.30914400	1.30389200	-1.04071600
C	-5.01636200	0.14045300	-0.72576900
H	-5.10778800	-1.55995600	0.59602500
H	-3.06735600	-0.94011900	1.85831700
H	-2.59932200	2.53868300	-0.60759700
H	-4.66109800	1.95670200	-1.83514400
H	-5.92079200	-0.12048900	-1.26756000
N	-1.50432900	1.22047600	1.37992100
N	-0.39082900	0.35870200	1.59956900
C	-0.50806700	-0.50101600	2.70897800
O	-1.54184200	-0.72606300	3.31682000
C	0.81397300	-1.05587700	3.22346000
H	1.65192900	-0.92919100	2.53918900
H	1.04240600	-0.52275500	4.15264700
H	0.68807900	-2.11015400	3.47993500
H	-1.09947600	2.07437700	0.98648400
H	0.67850800	1.15109300	1.99675400

2

SCF done: -1452.24431921

Rh	0.72826700	-0.25258200	-0.22180900
C	-0.17133900	-1.82481000	-1.40826600
C	1.03198500	-1.42472800	-2.13409000
C	0.24392600	-2.42961700	-0.16516100
C	2.14220200	-1.65729600	-1.29258200
C	1.66220400	-2.26569200	-0.05372400
C	-1.54753400	-1.80952400	-1.99753100
H	-1.68985800	-2.68400800	-2.64685100
H	-2.32132700	-1.81919100	-1.22933400
H	-1.69496600	-0.91172900	-2.60193500
C	1.01968500	-0.79325800	-3.48781900
H	2.02965600	-0.64101600	-3.87413700
H	0.47161200	-1.41999700	-4.19964200
H	0.52096400	0.18085000	-3.42369400
C	3.57904100	-1.33489100	-1.56340000
H	3.95937900	-0.62834700	-0.81899200
H	4.19331300	-2.24162200	-1.51646200
H	3.71123000	-0.88434700	-2.54846400
C	2.56112200	-2.85389600	0.99174800
H	3.00135500	-3.78940300	0.62192800
H	3.38645000	-2.18063900	1.23926600
H	2.02218000	-3.08400700	1.91129400

C	-0.64344900	-3.17161100	0.78475600
H	-0.63427500	-4.23963900	0.52961300
H	-0.31503300	-3.07638600	1.82137000
H	-1.67251000	-2.81757300	0.72448200
O	2.40322600	1.09922100	0.36132400
C	2.40561400	2.02225300	1.20172800
O	1.47076100	2.20801800	2.08198000
C	3.52773300	3.02327500	1.24157900
H	3.17525600	3.93790000	0.75256200
H	3.77890100	3.27396300	2.27437100
H	4.39999300	2.64492200	0.70888800
O	0.05918000	1.31866800	-1.50671200
C	-0.05700100	2.59355900	-1.30995000
O	-0.12048100	3.16485900	-0.21171000
C	-0.12516800	3.40292800	-2.60482000
H	0.82943100	3.32736200	-3.13694700
H	-0.89881800	2.99723100	-3.26393400
H	-0.33657000	4.44993900	-2.38318100
C	-4.49430900	-1.01420400	0.42896200
C	-3.30913700	-0.58282000	1.02730100
C	-2.73152600	0.64297900	0.64566600
C	-3.39271400	1.42436500	-0.32387800
C	-4.58032400	0.98667100	-0.90326100
C	-5.13730200	-0.24341400	-0.54249300
H	-4.93172700	-1.95759500	0.74722200
H	-2.85947200	-1.14356100	1.83539400
H	-2.96462100	2.38071600	-0.61110400
H	-5.06871200	1.60851000	-1.64916400
H	-6.06210300	-0.58542700	-0.99750300
N	-1.57986800	1.17644000	1.23846500
N	-0.40782000	0.43635900	1.51221800
C	-0.43462700	-0.29663800	2.70449800
O	-1.43231500	-0.49762400	3.38301800
C	0.93034500	-0.73626000	3.22146200
H	1.73324600	-0.65752600	2.48968500
H	1.17266500	-0.09245100	4.07400400
H	0.86509400	-1.75811100	3.60306000
H	-1.26706700	2.04109100	0.79327800
H	0.68862500	1.55733600	1.87398400

3

SCF done: -1223.15559654

C	-3.23598300	0.50484000	-0.84225400
C	-4.46014900	0.03064500	-1.31518300

C	-5.40651500	-0.51795600	-0.44717000
C	-5.10892700	-0.58993800	0.91779400
C	-3.89259300	-0.11998300	1.40397300
C	-2.93983500	0.43595600	0.52888500
H	-2.49631300	0.89766200	-1.52921500
H	-4.66931100	0.08675900	-2.37999200
H	-6.35708600	-0.88272000	-0.82402100
H	-5.82893900	-1.01655500	1.61125800
H	-3.67174400	-0.17627300	2.46740600
N	-1.76055500	0.96668200	1.07307700
H	-1.49284400	0.52354900	1.94287500
N	-0.64531100	1.23452800	0.26899200
C	-0.58022200	2.48713600	-0.26868200
O	0.30642800	2.81716500	-1.06931300
C	-1.64781300	3.50101600	0.13533300
H	-2.62671900	3.22787900	-0.27064000
H	-1.75621700	3.55702400	1.22143300
H	-1.35123000	4.46934400	-0.26934000
Rh	0.84890200	-0.19954500	0.01027200
C	2.71917000	-1.27796700	0.54000000
C	2.77110800	-0.93742700	-0.83295700
C	2.58230400	-0.03686900	1.29983300
C	2.68228200	0.51868900	-0.94917100
C	2.64915300	1.06390000	0.37921800
C	2.74126900	-2.64594300	1.15187200
H	2.72430300	-3.42771700	0.39012800
H	3.64692400	-2.78339100	1.75501900
H	1.87444700	-2.79740300	1.80175400
C	2.85557000	-1.87101200	-2.00148200
H	2.04278400	-1.68150700	-2.70839000
H	3.80506500	-1.73458700	-2.53238600
H	2.78887000	-2.91513000	-1.69042000
C	2.78935000	1.29778500	-2.22287200
H	2.09643300	2.14049900	-2.19837500
H	3.81334600	1.67019000	-2.35876900
H	2.54392600	0.67513200	-3.08676000
C	2.73464900	2.51256400	0.74509600
H	3.79091300	2.81084900	0.79599800
H	2.21874500	3.12952300	0.01002400
H	2.29018200	2.70485400	1.72460400
C	2.55589500	0.04618500	2.79567100
H	3.57530800	0.00007900	3.20075000
H	2.10368900	0.97980600	3.13741800
H	1.99051200	-0.78343300	3.22765700

O	-0.54364400	-1.71463600	0.83487300
C	-0.98197200	-1.97602500	-0.33585100
O	-0.50622800	-1.34008300	-1.32770100
C	-2.06601300	-3.00382300	-0.52865900
H	-1.97930500	-3.79140000	0.22315200
H	-3.03831500	-2.51592100	-0.40730800
H	-2.01377400	-3.42625000	-1.53380700

TS3-4

SCF done: -1223.11953631

N	-0.34040400	1.39092000	-1.09273000
C	0.39830300	2.46070900	-1.47730400
C	-0.34203300	3.67754500	-2.03388100
H	-1.15461000	3.99455700	-1.37322800
H	-0.77889200	3.46653200	-3.01914500
O	1.63857900	2.45519400	-1.43500500
H	0.38353700	4.48245200	-2.15133400
C	-2.44485600	0.49290600	-0.57146300
C	-3.75443100	0.14179700	-0.96486900
C	-4.41168400	-0.88317800	-0.30434300
C	-3.79929500	-1.57585300	0.75938400
C	-2.51860900	-1.21565500	1.14865700
C	-1.79456500	-0.17162600	0.51605200
H	-4.23466500	0.66048200	-1.79143800
H	-5.41816000	-1.15301200	-0.61376500
H	-4.33870400	-2.36191800	1.27928200
H	-2.06561400	-1.71145000	2.00403000
N	-1.75055200	1.48395000	-1.21045000
H	-2.07187200	1.71237100	-2.14561400
C	0.04094100	1.83070200	2.37138300
O	0.88702800	1.25294100	1.62734700
C	0.56119700	2.85931100	3.35788500
H	0.50628400	3.84778900	2.88935700
H	-0.06118500	2.87372100	4.25453900
H	1.60317700	2.65791900	3.61058100
O	-1.21047400	1.62861800	2.33370100
H	-1.42515900	0.68916700	1.40881600
Rh	0.35364800	-0.17930200	0.08811100
C	2.47543900	-0.80750600	-0.33436500
C	1.95743000	-1.60049100	0.76874000
C	1.66840200	-1.08118600	-1.47825700
C	0.84671600	-2.35791600	0.29942500
C	0.61453300	-1.99556200	-1.08991100
C	3.65604700	0.11473400	-0.29353200

H	3.98519200	0.28828300	0.73317600
H	4.50185400	-0.30855800	-0.85067000
H	3.38585400	1.07887700	-0.73286900
C	2.53384700	-1.60185000	2.15209300
H	1.91029400	-2.16627200	2.84877300
H	3.53395700	-2.05159900	2.15413300
H	2.62042100	-0.57820500	2.52755700
C	0.10730400	-3.42277600	1.05243600
H	-0.93239400	-3.49603000	0.72888500
H	0.58053800	-4.39841800	0.87986600
H	0.11338900	-3.24085500	2.12987100
C	-0.38878400	-2.63663700	-2.00219300
H	-0.00608000	-3.58336900	-2.40585900
H	-1.32371900	-2.84774900	-1.47739000
H	-0.62475500	-1.98658900	-2.84780800
C	1.88582800	-0.50368800	-2.84314700
H	2.67980400	-1.06005400	-3.35832000
H	0.98331500	-0.56945900	-3.45431200
H	2.17851400	0.54552900	-2.77029100

4

SCF done: -1223.13737064

N	-0.62427600	1.11837600	-1.19502600
C	-0.19343300	2.36235400	-1.51445600
C	-1.13429200	3.25209400	-2.32556100
H	-2.14512900	3.25280800	-1.90924800
H	-1.21161100	2.90308600	-3.36308200
O	0.93094200	2.78040700	-1.18775700
H	-0.71906300	4.26048800	-2.33224200
C	-2.39266500	-0.36122700	-0.87736600
C	-3.68690600	-0.86629100	-1.08287100
C	-4.15002400	-1.91503300	-0.29322400
C	-3.34156900	-2.44492000	0.71821600
C	-2.05190200	-1.94059900	0.91064600
C	-1.53352200	-0.90902600	0.10890600
H	-4.32530700	-0.42282500	-1.84314600
H	-5.15276300	-2.30295800	-0.45039200
H	-3.71332400	-3.24630800	1.35103800
H	-1.43481200	-2.36854400	1.69677800
N	-1.92203900	0.73282100	-1.62377300
H	-1.95358900	0.55611800	-2.62781600
C	-0.95892300	1.92742100	2.15785300
O	0.06557300	1.37257200	1.76640400
C	-0.93842000	3.13565900	3.05455000

H	-1.25499100	4.00929700	2.47546900
H	-1.64481700	3.01077800	3.87898700
H	0.07042700	3.30028000	3.43041400
O	-2.18191200	1.53711600	1.83057900
H	-2.11318300	0.74755400	1.24274400
Rh	0.37851300	-0.17004000	0.05690400
C	2.69995200	-0.01701500	0.18024200
C	2.20294900	-1.04374100	1.09845400
C	2.32456700	-0.38386100	-1.12380700
C	1.55751900	-2.05655500	0.34420100
C	1.52013200	-1.60489700	-1.03962200
C	3.44729300	1.22806700	0.55665900
H	3.41364100	1.40195600	1.63464900
H	4.50312600	1.16066800	0.26388100
H	2.99937100	2.09253900	0.05839100
C	2.43494800	-1.03080100	2.57953800
H	1.82678400	-1.78061000	3.09041100
H	3.48789200	-1.23905100	2.80836100
H	2.19036300	-0.05277200	3.00322500
C	1.07098200	-3.38612300	0.83741300
H	0.16845100	-3.70663900	0.31290600
H	1.84044200	-4.15278600	0.67675000
H	0.84599000	-3.36792900	1.90688000
C	1.05024400	-2.42064000	-2.20792300
H	1.85492400	-3.06622400	-2.58480700
H	0.20802000	-3.05943700	-1.93215400
H	0.72516700	-1.78059300	-3.03169700
C	2.66301200	0.36697900	-2.37590900
H	3.72101200	0.21833600	-2.62814800
H	2.07007800	0.01889800	-3.22487100
H	2.47755900	1.43543200	-2.24182000

I

SCF done: -994.04700978

Rh	-0.17588800	-0.09819300	0.00859700
C	-2.39668400	-0.08730000	-0.67776200
C	-1.67016100	-1.26178300	-1.14101800
C	-2.37101000	-0.08884800	0.73162500
C	-1.26994600	-2.02917100	0.00341800
C	-1.63203100	-1.27002100	1.16721500
C	-3.05945700	0.94072900	-1.54380400
H	-2.79283400	0.81168300	-2.59563800
H	-4.15172200	0.86006900	-1.46890800
H	-2.76614200	1.94719200	-1.23369800

C	-1.51447700	-1.67554200	-2.57264600
H	-0.65484400	-2.33604000	-2.70561900
H	-2.40824400	-2.21221100	-2.91932700
H	-1.37565700	-0.81008600	-3.22533900
C	-0.72762600	-3.42714800	-0.01701200
H	-0.15381200	-3.65413300	0.88461900
H	-1.55048700	-4.15215300	-0.07121300
H	-0.08019300	-3.60220800	-0.87997900
C	-1.44548400	-1.69839500	2.59113000
H	-2.33137300	-2.23885300	2.95168000
H	-0.58231100	-2.35885100	2.69943000
H	-1.29218900	-0.83925200	3.24873200
C	-2.99803800	0.94086400	1.62226000
H	-4.09065400	0.83195400	1.62874300
H	-2.65253800	0.84183900	2.65419700
H	-2.74956500	1.94539800	1.27191600
N	0.67045400	1.73091300	-0.02507500
C	0.02888500	2.94456100	-0.15581700
C	0.87041100	4.18945900	-0.41993200
H	1.56002800	4.04188400	-1.25632200
H	1.46470100	4.46564200	0.46103900
O	-1.19558900	3.03887500	-0.05322100
H	0.18855700	5.01094900	-0.63750900
C	2.64851100	0.51804900	0.02341000
C	4.05010500	0.38381500	0.10045900
C	4.59994800	-0.88202200	0.20907300
C	3.76647800	-2.01485600	0.23353900
C	2.38626500	-1.86649600	0.15784000
C	1.77188400	-0.59949900	0.06237100
H	4.68727400	1.26476200	0.06537700
H	5.67856800	-0.99774100	0.27053000
H	4.20468900	-3.00602000	0.31564800
H	1.77036500	-2.75890200	0.18510600
N	2.06374400	1.76059000	-0.11874500
H	2.51557900	2.53521300	0.35493400

R2

SCF done:-568.58883272

C	-0.81433500	0.11409700	-0.00037100
C	0.43583100	-0.68254800	-0.00067700
C	-2.18845800	-0.46086900	0.00044300
O	-2.36345900	-1.66294600	0.00072600
O	0.49031000	-1.88914200	-0.00108300
O	1.51788600	0.13662700	-0.00029300

C	-3.34749600	0.52498000	0.00105400
H	-4.27729800	-0.04372300	0.00181500
H	-3.31934300	1.17196100	0.88514900
H	-3.32061300	1.17166500	-0.88330300
C	2.80316000	-0.53074300	-0.00064900
H	2.86511300	-1.17309000	-0.88443400
H	2.86410000	-1.17608200	0.88107200
C	3.87316500	0.54380400	0.00190700
H	3.79183100	1.17680000	0.89017000
H	4.86327600	0.07771700	0.00175700
H	3.79287800	1.17998300	-0.88423800
N	-0.68561600	1.42564200	-0.00076500
N	-0.59853200	2.55809100	-0.00109600

5

SCF done:-1562.65428405

Rh	-1.33009200	0.38207000	-0.22207400
C	-2.72045000	-1.34877800	0.48579700
C	-2.46967600	-0.37609900	1.54775600
C	-3.34847000	-0.67839500	-0.58186000
C	-3.01170900	0.88288600	1.14168200
C	-3.48309500	0.72554600	-0.21041500
C	-2.39854500	-2.81033000	0.53862800
H	-1.62673700	-3.03078700	1.27877900
H	-3.29447400	-3.38750900	0.80573800
H	-2.04411200	-3.15444100	-0.43508200
C	-1.89137900	-0.70169900	2.89092000
H	-1.49971500	0.19179800	3.38397400
H	-2.66541800	-1.13021700	3.54225200
H	-1.08277000	-1.43183500	2.81475600
C	-3.20447500	2.09853800	1.99828800
H	-3.09034900	3.02298200	1.42584600
H	-4.21476800	2.10166300	2.43000500
H	-2.49561000	2.12682700	2.82988000
C	-4.18432100	1.77432900	-1.01912100
H	-5.27075300	1.71323300	-0.86539800
H	-3.86236600	2.77872500	-0.73601500
H	-3.99489700	1.64892300	-2.08809900
C	-3.81048300	-1.29451500	-1.86768200
H	-4.76438000	-1.81903100	-1.72161700
H	-3.96871600	-0.53700700	-2.63985700
H	-3.07198800	-2.00811400	-2.23977300
N	0.02702000	-0.11521700	-1.63116300
C	0.09756900	-1.28973500	-2.34837900

C	1. 24337100	-1. 47639300	-3. 33742300
H	2. 20829500	-1. 46124200	-2. 82139000
H	1. 25294700	-0. 69762700	-4. 11088900
O	-0. 73945000	-2. 18449200	-2. 19548800
H	1. 10343400	-2. 43998400	-3. 82561900
C	0. 98142100	1. 92001400	-1. 04299900
C	1. 90142100	2. 97889500	-1. 18683700
C	1. 81092100	4. 07258100	-0. 33996300
C	0. 82076200	4. 11107000	0. 65844600
C	-0. 09155700	3. 06764200	0. 77497700
C	-0. 06535800	1. 94686300	-0. 08358500
H	2. 67587000	2. 93163400	-1. 95059800
H	2. 51282800	4. 89584600	-0. 44541900
H	0. 76449200	4. 96189900	1. 33358000
H	-0. 84640800	3. 12957600	1. 55346500
N	1. 08864100	0. 78095600	-1. 82284300
H	1. 35042600	0. 92452200	-2. 79377400
C	2. 29351800	-1. 63042900	1. 22767300
C	3. 29849300	-1. 22709700	0. 23204300
C	1. 44075000	-2. 84218800	1. 26597800
O	0. 64803100	-2. 99206400	2. 19173900
O	3. 57618800	-1. 86057100	-0. 77010000
O	3. 88878700	-0. 06505300	0. 58274700
C	1. 55779700	-3. 84616200	0. 14575200
H	1. 19447300	-4. 80623100	0. 51790000
H	0. 90795100	-3. 52494500	-0. 67786700
H	2. 57146800	-3. 92449100	-0. 24613000
C	4. 85287500	0. 46978100	-0. 35639500
H	4. 34481800	0. 64071800	-1. 31028700
H	5. 63610000	-0. 27686900	-0. 52117100
C	5. 39526200	1. 75492500	0. 23754700
H	5. 90071600	1. 56632700	1. 18881300
H	6. 11811900	2. 20116400	-0. 45237400
H	4. 58713500	2. 47145600	0. 40588900
N	1. 86334800	-0. 12143300	3. 11456300
N	2. 08416400	-0. 79290300	2. 23482400

TS5-6

SCF done: -1562.61013660

Rh	0. 63291900	0. 25419400	0. 04013000
C	2. 98685600	-0. 04892800	-0. 38282000
C	2. 39928600	0. 86772300	-1. 35187000
C	2. 83549800	0. 51897400	0. 89805000
C	1. 94297600	2. 02349300	-0. 64936500

C	2. 12163600	1. 77922900	0. 75649800
C	3. 75534600	-1. 29605000	-0. 70609600
H	3. 36161700	-1. 79988500	-1. 59225400
H	4. 80877700	-1. 05622600	-0. 90768000
H	3. 73074800	-2. 00063500	0. 12918800
C	2. 50330600	0. 71463000	-2. 84092700
H	1. 81042500	1. 37754200	-3. 36593200
H	3. 51617400	0. 96953800	-3. 17951600
H	2. 29765900	-0. 31168000	-3. 15311900
C	1. 48561400	3. 31388600	-1. 25869700
H	0. 70053200	3. 78962500	-0. 66805500
H	2. 33005200	4. 01221900	-1. 32316300
H	1. 10209000	3. 17479200	-2. 27194400
C	1. 86503100	2. 76468200	1. 85930200
H	2. 75315300	3. 37894900	2. 05623100
H	1. 04325000	3. 43772900	1. 60528100
H	1. 60214200	2. 25679300	2. 79017800
C	3. 38160600	-0. 04428200	2. 17625600
H	4. 47774500	-0. 05739500	2. 14072400
H	3. 08748200	0. 56250900	3. 03515300
H	3. 01266200	-1. 05869500	2. 34077000
N	-0. 21060100	-0. 34128000	1. 84097200
C	0. 12387300	-1. 45178500	2. 52767600
C	-0. 71773400	-1. 81245000	3. 74783000
H	-1. 77850700	-1. 85199300	3. 48798900
H	-0. 60289800	-1. 07475000	4. 55198500
O	1. 10768300	-2. 15419200	2. 21967700
H	-0. 37897500	-2. 78174400	4. 11437900
C	-1. 82389400	1. 25258400	1. 26566600
C	-2. 98642500	2. 01108000	1. 46388600
C	-3. 43944400	2. 86611600	0. 45954100
C	-2. 74857300	2. 94801800	-0. 75015800
C	-1. 58921400	2. 18347500	-0. 93846600
C	-1. 09780900	1. 34052100	0. 05855200
H	-3. 53498500	1. 91831800	2. 39789100
H	-4. 33576200	3. 45802200	0. 62087400
H	-3. 09773700	3. 60728400	-1. 53949900
H	-1. 05946400	2. 27616900	-1. 88284200
N	-1. 37537000	0. 36666800	2. 26089700
H	-1. 21056000	0. 85214600	3. 14384900
C	-0. 32678900	-1. 32623500	-1. 00870100
C	-1. 64271600	-1. 80962900	-0. 43879000
C	0. 62889800	-2. 40023400	-1. 49772900
O	1. 11372500	-2. 30480400	-2. 61978000

O	-1.68749100	-2.67306800	0.41224200
O	-2.70493500	-1.17692100	-0.95208400
C	0.95361300	-3.53246900	-0.56415000
H	1.78043900	-4.09742400	-0.99742700
H	1.18033900	-3.16925400	0.44443600
H	0.07299100	-4.17682900	-0.46883900
C	-3.98657100	-1.47877500	-0.33393500
H	-3.91534400	-1.22291400	0.72620500
H	-4.16699800	-2.55379300	-0.41668500
C	-5.03535100	-0.65604600	-1.05341200
H	-5.07490200	-0.90986200	-2.11774000
H	-6.01843800	-0.85852300	-0.61682300
H	-4.82312600	0.41200500	-0.95160200
N	-1.01870900	0.07731800	-3.23608100
N	-0.72645100	-0.65042700	-2.44395300

6

SCF done: -1562.64829228

Rh	-0.71749500	-0.00381600	-0.15049600
C	-2.49640300	1.62271500	-0.34043100
C	-1.59722600	1.71146500	-1.46721100
C	-3.07931600	0.32693500	-0.35104100
C	-1.69259100	0.47571900	-2.20936500
C	-2.57562300	-0.39337100	-1.50457800
C	-2.84234600	2.73609300	0.60251800
H	-1.99563300	3.40852200	0.76085200
H	-3.66811500	3.33794100	0.19889600
H	-3.16145300	2.34829600	1.57378500
C	-0.89291900	2.95681900	-1.92237200
H	-0.07884900	2.72824700	-2.61422700
H	-1.59620000	3.61839600	-2.44649900
H	-0.46898300	3.50155100	-1.07766100
C	-1.06609100	0.20763300	-3.54474700
H	-0.83469500	-0.85052600	-3.68122200
H	-1.74997500	0.51038200	-4.34817000
H	-0.13763900	0.76653200	-3.67676200
C	-3.00807900	-1.76316000	-1.94176100
H	-3.93001000	-1.71901200	-2.53611300
H	-2.24187300	-2.24372500	-2.55580000
H	-3.20378900	-2.41046300	-1.08260200
C	-4.10389100	-0.17314000	0.62352300
H	-5.07416100	0.30545400	0.43476900
H	-4.24380000	-1.25280200	0.53479700
H	-3.79996800	0.03687300	1.65126800

N	-0.95648800	-1.70733400	0.96323100
C	-1.25082900	-1.64039000	2.29212600
C	-1.02286400	-2.89109900	3.12856700
H	0.03225900	-3.17328500	3.09162500
H	-1.60238700	-3.74273300	2.75866800
O	-1.72022100	-0.61376800	2.80045300
H	-1.32039800	-2.66786100	4.15351000
C	0.65464800	-2.54486100	-0.49993200
C	1.51081800	-3.52011700	-1.02843700
C	2.44775200	-3.16582500	-1.99999400
C	2.55368400	-1.83895100	-2.42360300
C	1.70601700	-0.86467500	-1.87992500
C	0.73175600	-1.20945600	-0.94264100
H	1.44861300	-4.54215500	-0.66394000
H	3.10758600	-3.92474000	-2.41135500
H	3.28828200	-1.56001400	-3.17514800
H	1.80482500	0.16766200	-2.20297100
N	-0.30686500	-2.87566800	0.48151200
H	-0.99508700	-3.52522700	0.10418000
C	0.57022300	0.79167500	0.99701400
C	1.80710700	0.10630100	1.48097900
C	0.34455600	2.11622700	1.66430500
O	0.43074000	3.16110800	1.03148500
O	1.79473500	-0.64258400	2.44030100
O	2.89696300	0.45289100	0.78430700
C	0.01214800	2.06413000	3.13840800
H	-0.16594300	3.08004700	3.50127500
H	-0.85559800	1.41334700	3.29182500
H	0.83928400	1.60425500	3.69337100
C	4.13823600	-0.19613700	1.17751700
H	3.96439300	-1.27641700	1.21159100
H	4.39873200	0.13777500	2.18759200
C	5.19390200	0.18152100	0.15361400
H	5.33846400	1.26611500	0.11195000
H	6.14749200	-0.28225500	0.42551600
H	4.90669200	-0.17425500	-0.83989800
N	2.90616400	3.39932900	-1.61261200
N	3.30882600	3.44771600	-0.58475500

II

SCF done: -1453.12204253

Rh	0.60711100	0.11537800	-0.03559000
C	2.97051900	-0.24192300	0.19344700
C	2.70165200	0.07753900	-1.17546200

C	2. 58926300	0. 89479100	0. 99233700
C	2. 12386200	1. 39514000	-1. 21795800
C	2. 08685700	1. 91429000	0. 12961900
C	3. 60470700	-1. 48700900	0. 73658000
H	3. 74755500	-2. 23874300	-0. 04370100
H	4. 59057500	-1. 26752100	1. 16620900
H	2. 96859100	-1. 91268200	1. 51809300
C	3. 13580100	-0. 70140600	-2. 38079900
H	2. 35999300	-0. 73663600	-3. 15022000
H	4. 02972200	-0. 23584600	-2. 81895800
H	3. 39487800	-1. 73261600	-2. 12605700
C	1. 86548900	2. 17819300	-2. 47056800
H	1. 15275800	2. 98802000	-2. 30372100
H	2. 79930800	2. 62978700	-2. 83191200
H	1. 47881900	1. 54129400	-3. 27001900
C	1. 69573200	3. 31188600	0. 51367100
H	2. 51036000	4. 01639400	0. 30167600
H	0. 81198400	3. 64573700	-0. 03599200
H	1. 46971000	3. 38650600	1. 58019600
C	2. 77666300	0. 97666600	2. 47792200
H	3. 82182200	1. 21589400	2. 71452100
H	2. 15226500	1. 75445700	2. 92336100
H	2. 52944400	0. 02266800	2. 94856500
N	-0. 32616200	-0. 10026000	1. 77614600
C	-0. 05798900	-1. 11812700	2. 62894300
C	-0. 95597400	-1. 26660100	3. 85250000
H	-2. 01146100	-1. 17647800	3. 58722300
H	-0. 73529400	-0. 49174500	4. 59666000
O	0. 90805400	-1. 87852900	2. 45629900
H	-0. 75311400	-2. 24035100	4. 29829700
C	-1. 78782400	1. 49157200	0. 89490600
C	-2. 88597600	2. 36209900	0. 91170600
C	-3. 24604200	3. 04702200	-0. 24955500
C	-2. 53607000	2. 84107400	-1. 43419300
C	-1. 44559800	1. 96148700	-1. 44857000
C	-1. 04053100	1. 31329900	-0. 28390500
H	-3. 46064700	2. 48470700	1. 82644800
H	-4. 09352400	3. 72675200	-0. 23068000
H	-2. 82802900	3. 35566500	-2. 34545600
H	-0. 91544500	1. 78754300	-2. 37942000
N	-1. 42550900	0. 76370800	2. 04808400
H	-1. 19861200	1. 39467000	2. 81691500
C	-0. 34668600	-1. 34273500	-0. 78745900
C	-1. 68904700	-1. 82669600	-0. 33450000

C	0.25866100	-2.22450800	-1.83582900
O	0.32885500	-1.82008800	-2.98888300
O	-1.77602000	-2.81513000	0.37821500
O	-2.72168800	-1.11532900	-0.80127600
C	0.74358600	-3.58972500	-1.40003900
H	1.13578800	-4.12566100	-2.26725600
H	1.51309500	-3.48970400	-0.62882700
H	-0.07841000	-4.14304900	-0.93561300
C	-4.03834300	-1.53363800	-0.35268600
H	-4.09020100	-1.38588800	0.72926400
H	-4.15373600	-2.60289700	-0.55408900
C	-5.05319600	-0.68857300	-1.09079500
H	-4.98305700	-0.85085100	-2.17113500
H	-6.06319300	-0.95969800	-0.76599700
H	-4.89097600	0.37203200	-0.88716600

TSII-III

SCF done: -1453.11282876

Rh	0.73005600	0.09128200	0.02039500
C	2.77582500	0.99662000	0.53817200
C	2.85096100	-0.43049700	0.74944800
C	2.53867900	1.22531600	-0.86163400
C	2.63009800	-1.07227200	-0.51005300
C	2.42068300	-0.03842400	-1.51738100
C	3.01837600	2.06969800	1.55535000
H	3.00784500	1.66460200	2.57028100
H	3.98820100	2.54425400	1.38897100
H	2.23007300	2.83164000	1.48727800
C	3.22515800	-1.11819000	2.02651900
H	2.77739000	-2.10841500	2.08686500
H	4.32002900	-1.22354200	2.08827700
H	2.88672500	-0.54106200	2.90036900
C	2.79104600	-2.54218700	-0.77955600
H	2.24675300	-2.85742100	-1.67375300
H	3.85304500	-2.77808400	-0.92747600
H	2.43355200	-3.13771800	0.05943500
C	2.24904200	-0.28442100	-2.98690000
H	3.21092900	-0.50300000	-3.46094000
H	1.57672700	-1.12504900	-3.17071300
H	1.83060300	0.58947800	-3.48982800
C	2.45259800	2.58432900	-1.49017600
H	3.45884100	2.95932400	-1.72997300
H	1.87190100	2.57232800	-2.41711100
H	1.98053000	3.28321300	-0.79597800

N	-0.67108700	1.53031900	-0.48679900
C	-0.69461900	2.81022600	-0.04028800
C	-1.77748000	3.73835400	-0.59318300
H	-2.75453100	3.25636200	-0.60951200
H	-1.53859200	4.04502500	-1.61515300
O	0.15426800	3.24587400	0.75065900
H	-1.79403300	4.62441800	0.03878900
C	-1.62308100	-0.23083600	-1.69424100
C	-2.46186100	-0.78921200	-2.67326600
C	-2.44906900	-2.16189800	-2.89644100
C	-1.60902700	-2.99531900	-2.14738500
C	-0.77366800	-2.44570600	-1.17297200
C	-0.74685100	-1.06426600	-0.95245300
H	-3.12303500	-0.14485800	-3.24712100
H	-3.10460500	-2.58683900	-3.65296400
H	-1.61188100	-4.06821500	-2.31573700
H	-0.13265100	-3.08581700	-0.57746100
N	-1.61924900	1.14296700	-1.46196400
H	-1.53726400	1.68749500	-2.32063000
C	-0.54066300	-0.71731300	1.26060000
C	-1.78029300	-0.00165400	1.70187100
C	-0.17556000	-1.90452600	2.07591300
O	0.54664700	-2.79154700	1.61505400
O	-1.77036200	0.58870200	2.76762800
O	-2.85777800	-0.11678800	0.91694700
C	-0.66468100	-2.00323900	3.51027500
H	-0.43031000	-3.06127200	3.85360300
H	-0.10110900	-1.22080000	4.17175900
H	-1.80014700	-1.75007300	3.60191500
C	-4.03472300	0.62313400	1.31804900
H	-3.78618700	1.69282100	1.32882700
H	-4.30428000	0.33428100	2.34021100
C	-5.10820800	0.29253800	0.29546600
H	-5.30234100	-0.78622600	0.26997300
H	-6.04275100	0.80719300	0.54866500
H	-4.78786900	0.61379400	-0.70398800

III

SCF done: -1453.18338208

Rh	0.84133700	0.15396900	-0.29964600
C	2.72011500	0.93965400	0.55989300
C	2.72418500	-0.48722000	0.79793900
C	2.77460100	1.15437000	-0.87963900
C	2.65650300	-1.13658500	-0.46896000

C	2. 72151600	-0. 11481600	-1. 50992500
C	2. 83445400	2. 01537400	1. 59137200
H	2. 63799300	1. 63062300	2. 59445000
H	3. 84738300	2. 44037400	1. 58549300
H	2. 11819100	2. 81199100	1. 37404000
C	2. 87661900	-1. 16510200	2. 12362300
H	2. 33878200	-2. 11496800	2. 15055300
H	3. 93796600	-1. 37163400	2. 31463400
H	2. 51170600	-0. 53921100	2. 94073300
C	2. 67608700	-2. 61656400	-0. 70500000
H	2. 23423300	-2. 86999500	-1. 67176600
H	3. 70973000	-2. 98740400	-0. 70423200
H	2. 11426100	-3. 14353400	0. 06771900
C	2. 77094700	-0. 39310600	-2. 98150800
H	3. 78816000	-0. 67536000	-3. 28460200
H	2. 10699500	-1. 21685100	-3. 25634500
H	2. 48082900	0. 48295900	-3. 56518300
C	2. 93457800	2. 48567100	-1. 54874000
H	3. 99343300	2. 77733600	-1. 55243500
H	2. 59700700	2. 45383400	-2. 58760200
H	2. 35629000	3. 24667300	-1. 02420300
N	-0. 52792400	1. 64526400	-0. 78862800
C	-0. 55108900	2. 92462600	-0. 31880200
C	-1. 84911000	3. 71876900	-0. 43409600
H	-2. 66620800	3. 20213700	0. 07680100
H	-2. 14940900	3. 87525500	-1. 47834500
O	0. 45735100	3. 46518200	0. 15441100
H	-1. 68169100	4. 69319100	0. 02394500
C	-1. 73065400	-0. 19498700	-1. 65178400
C	-2. 26130300	-0. 60210500	-2. 89205800
C	-2. 19205700	-1. 92423000	-3. 29030800
C	-1. 57202900	-2. 87587200	-2. 45811900
C	-1. 07738500	-2. 50378800	-1. 22328300
C	-1. 17098500	-1. 16189300	-0. 74868600
H	-2. 69784400	0. 14800700	-3. 54772400
H	-2. 59246400	-2. 21851500	-4. 25623200
H	-1. 50264000	-3. 91190600	-2. 77603000
H	-0. 63890900	-3. 23751600	-0. 56172200
N	-1. 75582900	1. 14745600	-1. 30735000
H	-2. 10387700	1. 73183600	-2. 06174900
C	-0. 87938200	-0. 75321100	0. 65808300
C	-1. 91804600	0. 16384900	1. 28509100
C	-0. 36678800	-1. 73901200	1. 65324500
O	0. 18319900	-2. 80031300	1. 34509900

O	-1.70843000	1.11976500	2.00258400
O	-3.16942600	-0.29827100	1.03437200
C	-0.51615400	-1.40415900	3.13236300
H	0.06812800	-2.12311700	3.70783400
H	-0.20781200	-0.38089500	3.35482000
H	-1.56821900	-1.49154400	3.42949300
C	-4.25526200	0.47589700	1.58318600
H	-4.24582300	1.47022200	1.12329100
H	-4.09418300	0.60990500	2.65738100
C	-5.54314800	-0.26952600	1.28531800
H	-5.53661400	-1.26024900	1.74898600
H	-6.39787500	0.28963000	1.67920100
H	-5.68045700	-0.39694700	0.20766400

7

SCF done: -1682.27191523

N	-0.02263300	-1.64384600	1.02285900
C	0.35334700	-2.96172700	0.79083800
C	-0.52825100	-4.07591700	1.34088200
H	-1.49416600	-4.09416000	0.82759100
H	-0.73791500	-3.93804500	2.40439700
O	1.37925700	-3.24139800	0.17270700
H	-0.00870800	-5.02037600	1.17512300
C	-2.42663100	-1.26287300	0.70478800
C	-4.83938200	-1.50670900	0.45228500
C	-4.76603400	-0.86623500	-0.78750900
C	-3.53376800	-0.41892100	-1.24902000
C	-2.33800000	-0.57694600	-0.51741200
H	-5.79007100	-1.86593500	0.83612300
H	-5.65908800	-0.71368700	-1.38644800
H	-3.48466500	0.10018100	-2.20357200
N	-1.32491100	-1.54385600	1.54586100
H	-1.35829100	-1.05204600	2.43010600
Rh	0.84648200	0.01138700	-0.03151600
C	3.09792300	-0.48999600	0.07707000
C	2.57172400	-0.56562100	-1.28282900
C	2.23142100	0.78480500	-1.70110200
C	2.33449100	1.62174200	-0.56385900
C	2.91854300	0.83391900	0.52403200
C	3.81450800	-1.57694900	0.82080700
H	3.48961600	-2.56104100	0.49089900
H	4.89674900	-1.48034000	0.65765600
H	3.64113800	-1.51029800	1.89909400
C	3.36557600	1.39723300	1.83834000

H	3.38111100	0.63932900	2.62460700
H	4.38320600	1.79879800	1.74462500
H	2.72480400	2.22161100	2.16033700
C	2.08725800	3.09904900	-0.53297700
H	2.99978100	3.64686900	-0.80491400
H	1.29666800	3.37129100	-1.23388600
H	1.78691600	3.43297000	0.46399000
C	1.95975100	1.25003500	-3.09498800
H	2.82429100	1.83605900	-3.43596600
H	1.81520800	0.42049000	-3.78491100
H	1.06481300	1.87213100	-3.13481100
C	2.72899700	-1.73644700	-2.20156600
H	2.06486600	-1.65575500	-3.06393000
H	3.76047900	-1.77523600	-2.57851200
H	2.51024600	-2.66655500	-1.67783500
C	-1.09836700	0.07399600	-1.12864300
C	-0.81118300	-0.58361000	-2.46877100
O	-0.62794600	0.03490100	-3.50764100
C	-0.81766200	-2.11130000	-2.50890000
H	-1.83463500	-2.48823800	-2.36538300
H	-0.46588800	-2.42523500	-3.49346100
H	-0.18716900	-2.54801300	-1.73246800
C	-1.26886000	1.57398900	-1.17894000
O	-0.73881700	2.36252800	-1.94503200
O	-2.10358800	2.01293100	-0.19602500
C	-2.28256800	3.43656800	-0.11039300
H	-2.60545900	3.82022900	-1.08357300
H	-1.32099200	3.90702300	0.12361900
C	-3.31446700	3.69864900	0.97194300
H	-3.49067300	4.77483500	1.07052300
H	-4.26400700	3.21333800	0.72826700
H	-2.97204600	3.31365600	1.93724400
C	-3.67393600	-1.71343500	1.17730300
H	-3.69823100	-2.24995900	2.12208300
C	0.30813000	0.87810900	2.96665700
O	0.02721800	1.25378300	1.82704500
O	0.74398500	-0.34156500	3.24873200
C	0.17600000	1.76747500	4.17489900
H	-0.12033700	2.77040000	3.87046600
H	-0.57136100	1.35091000	4.85721300
H	1.12616600	1.79925000	4.71594500
H	0.70652800	-0.90566100	2.40102500

TS7-7''

SCF done: -1682.26891663

N	-0.00080400	1.75829500	0.96923300
C	-0.42506400	3.05107800	0.55996100
C	0.51755700	4.22123400	0.77823800
H	1.44411000	4.09619500	0.20961600
H	0.80235900	4.29592300	1.83072100
O	-1.51330700	3.20810900	0.04151600
H	0.00388000	5.12749900	0.45587400
C	2.41273300	1.37452500	0.59244700
C	4.81990000	1.61652500	0.27079500
C	4.73540500	0.83472300	-0.88418400
C	3.50228500	0.32317400	-1.26588200
C	2.31358300	0.54675600	-0.53731500
H	5.77051600	2.02997000	0.59493600
H	5.61923700	0.62372500	-1.47842600
H	3.44385600	-0.30156300	-2.15384300
N	1.33857500	1.76656300	1.42389800
H	1.39939800	1.42264400	2.37550400
Rh	-0.86251000	-0.05526000	-0.00331400
C	-3.14061000	0.40731500	0.06828000
C	-2.63243100	0.41358100	-1.30089900
C	-2.22311300	-0.93217500	-1.62491900
C	-2.28187800	-1.70108400	-0.42345800
C	-2.90963300	-0.87357100	0.60555500
C	-3.88650400	1.51140100	0.75524900
H	-3.70598000	2.47309600	0.28127200
H	-4.96302500	1.29558500	0.72719300
H	-3.59618400	1.59789400	1.80635400
C	-3.31591900	-1.34977000	1.96614200
H	-3.31371900	-0.53644600	2.69589400
H	-4.33238100	-1.76566700	1.93025600
H	-2.65294100	-2.14100000	2.32533300
C	-1.98471900	-3.16271400	-0.28963900
H	-2.89394300	-3.75421600	-0.46076700
H	-1.22370000	-3.47064200	-1.00684400
H	-1.61751500	-3.39868900	0.71305200
C	-1.91818400	-1.47873900	-2.98101800
H	-2.75674900	-2.11573100	-3.29340000
H	-1.79135900	-0.69218300	-3.72349200
H	-1.00318800	-2.07259300	-2.96781900
C	-2.83702900	1.52319000	-2.28605600
H	-2.18927000	1.40681400	-3.15700300
H	-3.87620300	1.52078100	-2.64272200

H	-2.63284900	2.49176600	-1.82868200
C	1.08412300	-0.18596900	-1.07575600
C	0.80333700	0.33959000	-2.47429900
O	0.70062900	-0.37212600	-3.46305600
C	0.72868600	1.85645600	-2.65045500
H	1.72914800	2.28888000	-2.56633400
H	0.34638900	2.06275200	-3.65090600
H	0.09233200	2.33592800	-1.90661600
C	1.29523700	-1.68098600	-1.00538800
O	0.77795600	-2.53513900	-1.71177600
O	2.15066800	-2.01955100	-0.00419900
C	2.36003000	-3.42764600	0.20075900
H	2.70325800	-3.88417500	-0.73479900
H	1.40607700	-3.89911800	0.46403200
C	3.38518600	-3.57151700	1.31125500
H	3.58115200	-4.63123100	1.50685300
H	4.32814400	-3.09018000	1.03456900
H	3.02341500	-3.10859700	2.23475700
C	3.66315000	1.89371700	0.98343300
H	3.69450500	2.53994700	1.85645100
C	-0.28448400	-0.49758400	2.92476100
O	-0.02138200	-1.03062600	1.81652700
O	-0.71805300	0.70693300	3.06454100
C	-0.07541100	-1.29700700	4.19233000
H	0.30238000	-2.29463500	3.96242600
H	0.62805400	-0.77238500	4.84725100
H	-1.02457600	-1.37256400	4.73374100
H	-0.54554000	1.31709900	1.97477000

7'

SCF done: -1682.27415712

N	-0.05405700	1.78205300	1.11349300
C	-0.47803400	3.10676200	0.74088000
C	0.57692000	4.18303500	0.66499600
H	1.40495000	3.89205000	0.01455700
H	1.00440300	4.35152700	1.65737700
O	-1.65011500	3.31613100	0.50090200
H	0.10358000	5.09219700	0.29446300
C	2.34741400	1.39075100	0.72154400
C	4.75347900	1.68954400	0.41929900
C	4.67562900	1.00425200	-0.79553600
C	3.44893800	0.50860500	-1.21472500
C	2.25522900	0.64868600	-0.46949200
H	5.69889100	2.08759600	0.77617400

H	5.56001800	0.85523300	-1.40789100
H	3.39960900	-0.04204600	-2.15067700
N	1.28023500	1.74369300	1.59575700
H	1.27916600	1.24722100	2.48025500
Rh	-0.89187400	-0.07436400	0.02482000
C	-3.17271600	0.29223700	0.25290500
C	-2.75147200	0.48075900	-1.13587100
C	-2.29712300	-0.78445300	-1.63335100
C	-2.25776300	-1.69801600	-0.52260600
C	-2.86962300	-1.03171600	0.62336200
C	-3.91087000	1.28392100	1.09947400
H	-3.66147000	2.30746200	0.82910000
H	-4.99206900	1.13820600	0.97089200
H	-3.68516000	1.14770800	2.16045000
C	-3.16623300	-1.67330600	1.94392800
H	-3.05396400	-0.96549800	2.76773600
H	-4.19591300	-2.05359400	1.95628100
H	-2.50090300	-2.51884900	2.12890500
C	-1.93120600	-3.15744400	-0.58952400
H	-2.83964100	-3.73656400	-0.80439700
H	-1.19136500	-3.35738500	-1.36375800
H	-1.52624300	-3.51212900	0.36183500
C	-2.02453200	-1.15873300	-3.05297900
H	-2.85629300	-1.77929900	-3.41341900
H	-1.94415300	-0.28825400	-3.70365800
H	-1.09601100	-1.72615500	-3.13575500
C	-3.03873100	1.70146000	-1.95644500
H	-2.44384900	1.71574500	-2.87187200
H	-4.09746200	1.71995100	-2.24785300
H	-2.83104200	2.61319100	-1.39333200
C	1.04408700	-0.06716900	-1.07926900
C	0.74289500	0.56510700	-2.43113300
O	0.65316400	-0.06496600	-3.47458000
C	0.61110200	2.08800800	-2.48815100
H	1.56940700	2.56290500	-2.25862700
H	0.31689900	2.36378000	-3.50237700
H	-0.12937600	2.46367800	-1.77968600
C	1.29845700	-1.55699700	-1.16202300
O	0.74078500	-2.35050300	-1.90257400
O	2.23794300	-1.96711200	-0.27528600
C	2.47484200	-3.38470300	-0.21568100
H	2.74261400	-3.74867200	-1.21288300
H	1.54901200	-3.88912300	0.08047800
C	3.58879500	-3.61525300	0.78935000

H	3.81084500	-4.68475900	0.86434100
H	4.50064100	-3.09307200	0.48548100
H	3.30141600	-3.25093100	1.78002500
C	3.59254800	1.89452800	1.14877200
H	3.61353300	2.47495400	2.06690800
C	-0.10642800	-0.82615500	2.82770800
O	0.09548600	-1.15418900	1.60436800
O	-0.62490200	0.24910700	3.22309500
C	0.32224100	-1.85687300	3.86365200
H	1.04298700	-2.56178800	3.44693400
H	0.73742200	-1.35570900	4.74091200
H	-0.56248200	-2.41446000	4.19144900
H	-0.62719200	1.38814700	1.90257700

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SCF done: -1911.37993339

N	-5.02180600	-0.23535100	-0.94679200
C	-5.68298200	-1.35104200	-0.47101800
C	-4.85043700	-2.34044000	0.32412100
H	-5.53522700	-3.02571900	0.82290700
H	-4.20511500	-1.85112200	1.05712900
O	-6.87200100	-1.50610300	-0.70887900
H	-4.20359300	-2.91937700	-0.34475400
C	-3.09169700	0.66242500	0.19756600
C	-3.45190200	1.86102400	2.28898500
C	-2.08766300	2.13823900	2.36910700
C	-1.24149000	1.68407900	1.36237300
C	-1.69342000	0.93917400	0.25919200
H	-4.13718500	2.21167200	3.05609900
H	-1.68507000	2.71516400	3.19674200
H	-0.18739600	1.91387100	1.40129000
N	-3.64459600	-0.02415300	-0.91624200
H	-3.12857200	-0.85556600	-1.18398800
Rh	1.51410600	-0.43828900	0.03254000
C	3.23231600	-1.67171300	0.58984600
C	2.23740400	-2.55482800	-0.00639600
C	2.05646400	-2.18174400	-1.36260300
C	2.87813500	-1.00700500	-1.61858100
C	3.64968600	-0.74806600	-0.42985100
C	3.81005400	-1.78721800	1.96476300
H	3.17328600	-2.39374800	2.61252000
H	4.79788200	-2.26512400	1.92123300
H	3.90264900	-0.79449500	2.40825000
C	4.72565800	0.28336900	-0.29881900

H	4.82941200	0.61024900	0.73568300
H	5.67873300	-0.14230200	-0.64014100
H	4.50898800	1.16018900	-0.91337900
C	3.05747300	-0.33321600	-2.94601400
H	3.23859900	-1.07387700	-3.73212600
H	2.18092300	0.26504000	-3.20851100
H	3.91459600	0.34247200	-2.92406800
C	1.27154900	-2.97412900	-2.36044400
H	1.73743000	-3.96110400	-2.48406600
H	0.23972600	-3.12722000	-2.02858800
H	1.25148800	-2.48984000	-3.33731600
C	1.60032500	-3.73770000	0.65727100
H	2.17414500	-4.64631700	0.43252100
H	1.57697900	-3.62550700	1.74317200
H	0.57721700	-3.89055600	0.30742000
C	-0.73097300	0.61072300	-0.86397200
C	-0.94262000	-0.59239400	-1.62117200
O	-1.38258400	-1.65888400	-1.06378100
C	-0.85084600	-0.64556200	-3.13636800
H	-1.16118600	-1.63657300	-3.46700900
H	-1.52941200	0.10321600	-3.55630700
H	0.13709300	-0.40208900	-3.51702900
C	-0.14239300	1.77266900	-1.59702900
O	0.58860700	1.70073200	-2.57904700
O	-0.50980800	2.96273200	-1.08421600
C	0.09836400	4.12381600	-1.68295900
H	-0.12055600	4.13185200	-2.75552400
H	1.18487200	4.04878000	-1.56887000
C	-0.46549900	5.34485100	-0.97907700
H	-0.02583400	6.25407000	-1.40177300
H	-1.55147800	5.39867000	-1.09942800
H	-0.24096400	5.31741200	0.09102100
C	-3.94245400	1.12932200	1.21380700
H	-5.00281500	0.92215900	1.13670400
C	2.48751900	1.96593500	1.55640600
O	1.76978900	1.57301900	0.53641800
O	3.17761300	1.25676300	2.28913200
C	2.38318100	3.47085400	1.79743000
H	2.47284700	4.02311800	0.85881300
H	1.39981200	3.70287800	2.22075300
H	3.15471700	3.78934900	2.49993000
H	-5.55401500	0.35521700	-1.57388700
O	0.42617800	-0.73008400	1.90898700
C	-0.57657000	-1.39412000	2.22701400

O	-1.37458500	-2.01999400	1.41049100
C	-0.96880100	-1.49431700	3.67816900
H	-0.10388000	-1.32006300	4.31850000
H	-1.71191500	-0.71254800	3.87176800
H	-1.42850300	-2.46197800	3.88943300
H	-1.28456700	-1.79409000	0.38846600

8'

SCF done: -1911.39225151

N	3.53131200	-2.05856000	-0.78007400
C	4.90559600	-2.22547600	-0.89986100
O	5.33828700	-3.14169900	-1.58223500
C	2.67764400	-0.77793600	1.09739600
C	2.67074500	-1.67450000	3.34243000
C	2.17632000	-0.46487800	3.82684700
C	1.92895800	0.57988000	2.93521800
C	2.16490900	0.44853200	1.56268300
H	2.86973600	-2.49904400	4.02159300
H	1.98531500	-0.33279500	4.88797200
H	1.53511900	1.52392500	3.29972900
N	2.88801800	-0.89450900	-0.31921700
H	3.36907100	-0.05001800	-0.64430400
Rh	-1.95338300	0.01675300	0.12080300
C	-3.78050700	1.06742900	-0.56037000
C	-3.99613500	-0.37992100	-0.63886200
C	-3.88047700	-0.91566900	0.67290500
C	-3.49206900	0.16820400	1.56200500
C	-3.52932900	1.40802700	0.79480900
C	-3.85297200	1.99370400	-1.73517800
H	-3.49130200	2.99254500	-1.48471400
H	-3.24795400	1.61498900	-2.56375300
H	-4.88739500	2.08505500	-2.08804500
C	-3.25141100	2.75944100	1.37358100
H	-3.25925600	3.53807600	0.60871300
H	-4.00830300	3.01336200	2.12465500
H	-2.26865900	2.76465500	1.85497600
C	-3.28631500	0.07792800	3.04193800
H	-4.23221500	0.24321300	3.57428200
H	-2.90189000	-0.90284600	3.32893200
H	-2.56812400	0.82805200	3.38010300
C	-4.10887800	-2.33962300	1.06958600
H	-5.17746400	-2.49863800	1.26462000
H	-3.78686300	-3.02068000	0.28123500
H	-3.56361700	-2.59125000	1.98171400

C	-4.33462100	-1.15538300	-1.87373700
H	-3.75605500	-2.08150000	-1.89558800
H	-5.40428200	-1.39918000	-1.89612800
H	-4.10392600	-0.58353000	-2.77501900
C	0.48978600	1.84927700	0.38074700
O	-0.43535100	1.18171700	1.01848500
C	0.00021200	2.89746500	-0.60002100
H	-0.39474300	3.75683200	-0.04416900
H	0.77357900	3.26353000	-1.27140200
H	-0.81606500	2.46843600	-1.18516200
C	2.95496400	2.27709900	0.02009700
O	4.03173300	1.73896100	-0.25585500
O	2.76807700	3.60006100	-0.21875600
C	3.86622100	4.28724400	-0.85659500
H	4.07896300	3.81339000	-1.82068200
H	4.76101600	4.17705600	-0.23656500
C	3.46217900	5.74169300	-1.01426000
H	4.27645400	6.30538500	-1.48060700
H	2.57322100	5.83856500	-1.64466100
C	2.92491300	-1.83172900	1.97909100
H	3.31088400	-2.76851900	1.59320400
C	-0.92307000	-2.73822400	-0.05480300
O	-1.72569200	-2.93596700	-0.97954400
O	-0.73312200	-1.60826400	0.56203000
C	-0.02716200	-3.86014300	0.45783100
H	1.02205000	-3.60808400	0.27728900
H	-0.14258600	-3.96972200	1.54017800
H	-0.27346900	-4.79653400	-0.04515100
H	2.98798800	-2.60382300	-1.43905900
C	1.82637200	1.57837300	0.63450300
O	-0.87918400	0.04941000	-1.91711800
C	-0.24469900	-0.81723300	-2.52832700
O	0.92070400	-1.30237700	-2.15624200
C	-0.75100300	-1.43585800	-3.80277600
H	-1.46576800	-0.76917400	-4.28555600
H	0.06991100	-1.68246000	-4.47813400
H	-1.26061600	-2.36231800	-3.51717700
H	1.31200600	-0.93157100	-1.31066000
H	3.24404700	6.19310100	-0.04208400
C	5.78524200	-1.26456800	-0.12566000
H	5.58604400	-0.22023800	-0.38338000
H	5.60598000	-1.36484500	0.94942100
H	6.82293900	-1.51178400	-0.34832600

TS8'-IV

SCF done: -1911.37094764

N	4.01612600	-2.44075100	-0.53157500
C	5.38968600	-2.31149100	-0.62946500
O	6.07112900	-3.26388500	-0.97667000
C	2.80658200	-0.97968300	0.96443300
C	2.88403600	-1.35452100	3.36734500
C	2.14974600	-0.18926900	3.58284400
C	1.74674600	0.56915400	2.48596800
C	2.04098000	0.20043800	1.16601200
H	3.21555900	-1.96050700	4.20585400
H	1.90040900	0.13348900	4.58864400
H	1.17344000	1.47499500	2.64651700
N	3.11992800	-1.40202900	-0.33703800
H	3.16220500	-0.67513600	-1.04580900
Rh	-2.21899900	0.04483600	0.05390500
C	-4.14988200	0.93408900	-0.55961600
C	-4.21444500	-0.52714500	-0.51411800
C	-3.99601800	-0.93918700	0.84765900
C	-3.67930500	0.23681100	1.61516300
C	-3.83196500	1.40045300	0.74019500
C	-4.32480100	1.73788600	-1.81193700
H	-4.16525400	2.80296600	-1.63595900
H	-3.60879700	1.40705300	-2.57110000
H	-5.33517200	1.60753200	-2.21498000
C	-3.61223900	2.81370500	1.18198600
H	-3.72727800	3.51644600	0.35423000
H	-4.33310300	3.08696400	1.96148300
H	-2.60383700	2.93000100	1.58897300
C	-3.38850800	0.30508000	3.08198400
H	-4.30521900	0.52097100	3.64718700
H	-2.97793800	-0.63633000	3.45131300
H	-2.66339800	1.09343900	3.29757400
C	-4.06250000	-2.34572900	1.35300000
H	-5.10564100	-2.60622500	1.56882000
H	-3.67068500	-3.04185300	0.60987200
H	-3.48657600	-2.46677100	2.27241900
C	-4.57061900	-1.42366000	-1.65763000
H	-3.93039600	-2.30750400	-1.64663500
H	-5.62195600	-1.73291700	-1.58878300
H	-4.42823800	-0.91198300	-2.61155900
C	0.33675400	1.78590100	0.10940600
O	-0.61795200	1.38427200	0.84461600

C	0.04157700	2.94633500	-0.82140100
H	0.22863600	3.88533000	-0.28267500
H	0.66814500	2.95369400	-1.71858000
H	-1.01585100	2.88433800	-1.10820500
C	2.76399800	1.83927500	-0.57743500
O	3.56794300	1.30439600	-1.32965600
O	2.88623900	3.11381100	-0.16565800
C	4.03865200	3.83231900	-0.65787300
H	3.98456300	3.87573300	-1.75206400
H	4.94008600	3.27017300	-0.39094200
C	4.01207700	5.21063300	-0.01909800
H	4.85643600	5.80227500	-0.38341800
H	3.08697700	5.74150800	-0.27028100
C	3.20758400	-1.74647200	2.07321600
H	3.77360600	-2.65600200	1.90441000
C	-0.95221200	-2.62200200	-0.17104800
O	-1.84207200	-2.98386900	-0.95378100
O	-0.86936600	-1.45927000	0.41746200
C	0.22603700	-3.52703700	0.16470300
H	1.10227000	-3.15582900	-0.37896600
H	0.46520300	-3.47930900	1.23106600
H	0.00764500	-4.55138100	-0.14160800
H	3.63403200	-3.32371800	-0.84837800
C	1.59104000	1.11031200	0.03189300
O	-1.37650400	0.26403300	-1.95849200
C	-0.38574600	-0.31734900	-2.48811100
O	0.81817700	-0.31728700	-2.04965400
C	-0.62891500	-1.11403500	-3.74831400
H	-1.36022600	-0.60562100	-4.38176700
H	0.29628100	-1.29119900	-4.29650200
H	-1.05699300	-2.07152000	-3.43043900
H	1.05106900	0.29530700	-1.08958000
H	4.08364300	5.13842600	1.07190500
C	5.94768100	-0.95002900	-0.27915800
H	5.53711400	-0.17389600	-0.92800000
H	5.68512300	-0.68522000	0.74891500
H	7.02982600	-0.99216100	-0.38733300

IV

SCF done: -954.73095574

C	-3.63955200	-1.84077800	0.36129800
C	-3.21379000	-1.81910400	1.81556900
H	-3.04078800	-0.79344700	2.15508400
H	-2.28002300	-2.36847000	1.96278800

O	-4.72314600	-2.25072000	-0.02514400
H	-4.01122300	-2.27179500	2.40438300
C	-1.35860600	0.60216900	-0.32658300
C	-0.10726600	1.18827900	-0.00908300
C	0.01944700	2.57626200	-0.12659200
C	-1.04559900	3.38357500	-0.52960700
C	-2.27638500	2.79753700	-0.80874300
C	-2.43196100	1.41619700	-0.70819400
H	0.95996500	3.05467700	0.12074700
H	-0.91204400	4.45797800	-0.60519900
H	-3.12196600	3.40950600	-1.10901800
H	-3.39249300	0.96095900	-0.92007700
N	-1.50140900	-0.80333600	-0.20260300
H	-0.72735700	-1.29506600	-0.64225700
C	3.14983200	1.90369800	0.73293100
H	4.09084200	1.36847900	0.88980500
H	3.00218500	2.02595100	-0.34222200
H	3.24022500	2.88123600	1.21377000
C	1.68363800	-0.59845100	-0.46656600
O	1.11753200	-1.08529800	-1.42812000
O	2.95087600	-0.89088800	-0.13686100
C	3.63607600	-1.85039200	-0.98808700
H	3.67262000	-1.44692800	-2.00417000
H	3.04397200	-2.76955400	-1.01615100
C	5.01737500	-2.07212200	-0.40475600
H	5.56106800	-2.79864100	-1.01626500
H	5.59232000	-1.14187000	-0.38721500
H	4.95440200	-2.46013900	0.61563800
N	-2.71943000	-1.36891600	-0.55473500
H	-3.03780000	-1.32759900	-1.51911800
C	1.02157000	0.32303400	0.56175200
O	1.93337700	1.11087500	2.62314200
H	0.55438000	-0.36851100	1.27828600
C	2.03673200	1.11989500	1.41441100

TSIV-V

SCF done: -954.64781606

C	-3.61284900	-1.88326400	0.39251500
C	-3.20728700	-1.78589600	1.85058200
H	-3.10655700	-0.74026300	2.15665200
H	-2.24055300	-2.26615400	2.02442700
O	-4.65654100	-2.39237300	0.01110200
H	-3.97986100	-2.27208800	2.44598500
C	-1.40678000	0.63959000	-0.38166800

C	-0.13943100	1.25180600	-0.18339700
C	-0.04753800	2.64048400	-0.35654200
C	-1.15394600	3.42594500	-0.68336000
C	-2.39050600	2.81196100	-0.86044200
C	-2.51244400	1.42967400	-0.71930400
H	0.91715400	3.12500000	-0.23581700
H	-1.04326800	4.49930100	-0.80219800
H	-3.26626400	3.40132200	-1.11636800
H	-3.47630700	0.95254200	-0.85509600
N	-1.52530200	-0.75339800	-0.17825200
H	-0.72680800	-1.25953000	-0.56127900
C	3.19167600	1.90117700	1.11738500
H	3.93677100	1.21655000	0.70015100
H	3.07005300	2.71160700	0.39230900
H	3.53223300	2.29084200	2.07753000
C	1.62920500	-0.58080800	-0.57246600
O	1.01328500	-1.25379800	-1.39337600
O	2.94457100	-0.82181600	-0.29407000
C	3.54543400	-1.93225400	-0.99911100
H	3.47478100	-1.75021600	-2.07577800
H	2.97310400	-2.83936800	-0.78200500
C	4.98542800	-2.04528200	-0.53495700
H	5.47313200	-2.88336900	-1.04230900
H	5.54716400	-1.13498500	-0.76617300
H	5.03842400	-2.22088400	0.54357100
N	-2.72834700	-1.35487300	-0.52286400
H	-3.01236100	-1.40354500	-1.49755200
C	1.05596700	0.45715200	0.27899100
O	1.41419100	0.94159900	2.41322700
H	0.67247400	0.22335000	1.75181600
C	1.92497500	1.13844400	1.26338900

V

SCF done: -954.73435436

C	-3.42278800	-1.90307400	0.68559500
C	-2.98157500	-1.65924100	2.11567800
H	-2.90203900	-0.58824800	2.32346400
H	-1.99650400	-2.09571000	2.30296600
O	-4.43826900	-2.51061800	0.38174900
H	-3.72111000	-2.11192200	2.77583900
C	-1.33489000	0.63669900	-0.39928900
C	-0.07392400	1.28712000	-0.33731500
C	-0.01013100	2.64378200	-0.69904400
C	-1.14309700	3.36718800	-1.07597800

C	-2.37701800	2.72027800	-1.09879900
C	-2.47200900	1.36915800	-0.77018400
H	0.96093600	3.13250700	-0.68352800
H	-1.05747400	4.41427100	-1.34831700
H	-3.27470700	3.26202700	-1.38296000
H	-3.43318900	0.86878000	-0.79535300
N	-1.41450700	-0.72506200	-0.04799600
H	-0.60584400	-1.24275700	-0.39092100
C	2.92384800	0.53468500	2.07160700
H	3.25644500	-0.42987400	1.70009400
H	3.74784100	1.24854600	1.95815800
H	2.69095500	0.47242200	3.13834100
C	1.74885100	-0.46294400	-0.65684800
O	1.07538400	-1.17843400	-1.39272500
O	3.08983400	-0.60441100	-0.57011100
C	3.66237500	-1.68086500	-1.35321200
H	3.39114100	-1.53193300	-2.40229000
H	3.21981200	-2.62882900	-1.03141100
C	5.16399500	-1.64872100	-1.14185500
H	5.63612600	-2.44038700	-1.73182500
H	5.58286500	-0.68896300	-1.45740800
H	5.41977400	-1.80773300	-0.09014100
N	-2.60723100	-1.38834700	-0.30056800
H	-2.89878200	-1.56226800	-1.25857600
C	1.17935000	0.62219000	0.16267700
O	1.12353000	2.01787300	2.07889700
H	0.34275800	2.34098500	1.59502800
C	1.71063600	1.04280000	1.35112900

IV'

SCF done: -1031.16398241

C	-3.47521600	-1.88688100	0.38804700
C	-2.84104900	-2.05749600	1.75225900
H	-2.33219100	-1.15975800	2.10918700
H	-2.08395000	-2.84855500	1.70504400
O	-4.59946600	-2.27180900	0.10382600
H	-3.62436100	-2.36150300	2.44687200
C	-1.34443000	0.68281500	-0.40208600
C	-0.09809400	1.27525300	-0.07838300
C	0.01290600	2.66754600	-0.15324900
C	-1.06798600	3.47517700	-0.51015100
C	-2.29818800	2.88350100	-0.78125700
C	-2.43549800	1.49777700	-0.72856900
H	0.95104000	3.15031500	0.09872800

H	-0.94877400	4.55312500	-0.55147400
H	-3.15768700	3.49561400	-1.03871600
H	-3.39707400	1.04065100	-0.93095800
N	-1.45569200	-0.72661900	-0.34894700
H	-0.71153800	-1.18658300	-0.86559800
C	3.20202000	1.91946300	0.59458900
H	4.08493400	1.27656600	0.66193300
H	3.00220500	2.10477700	-0.46358500
H	3.42320600	2.85581200	1.11139800
C	1.69357700	-0.51590500	-0.54690300
O	1.18392300	-0.89567600	-1.58373600
O	2.89345200	-0.94725300	-0.11714300
C	3.56766900	-1.92194100	-0.95871300
H	3.71869500	-1.48151300	-1.94853300
H	2.91005300	-2.78793100	-1.07755300
C	4.87532200	-2.28265800	-0.28195500
H	5.40674000	-3.02644600	-0.88338300
H	5.52047600	-1.40574600	-0.17572800
H	4.69965100	-2.70581700	0.71096400
N	-2.69318900	-1.30028800	-0.59202800
H	-3.14055300	-1.18348200	-1.49712100
C	1.03316600	0.40531800	0.47736900
O	1.92341400	1.32063100	2.50578700
H	0.56461000	-0.27556200	1.20730200
C	2.05097900	1.22365000	1.29600600
O	-0.21397400	-0.37327200	3.38366800
H	0.44663300	0.33501000	3.28001700
H	0.25504800	-1.06599600	3.86419400

TSIV'-V'

SCF done:-1031.11794729

C	-3.27955400	-2.20771300	0.12841400
C	-2.70797100	-2.49228600	1.49272700
H	-2.47038600	-1.57351300	2.03241500
H	-1.77880700	-3.05709200	1.38831400
O	-4.26504100	-2.75976300	-0.32929000
H	-3.43299600	-3.10107300	2.03317000
C	-1.37278500	0.77170700	-0.25416900
C	-0.13148600	1.42189400	-0.01704300
C	-0.10321000	2.82277100	-0.10614500
C	-1.24318300	3.57941400	-0.35617100
C	-2.46369600	2.92844700	-0.52492600
C	-2.52349000	1.53765200	-0.48371500
H	0.84697800	3.33368200	0.02699900

H	-1.16766700	4.66000500	-0.42638800
H	-3.36984100	3.49695700	-0.70681500
H	-3.47025700	1.02881400	-0.62169500
N	-1.42486900	-0.64660100	-0.22953200
H	-0.63901800	-1.03308700	-0.75678600
C	3.53127500	1.68785000	0.73325500
H	4.21302400	1.02363500	1.27824600
H	3.66940000	1.54357100	-0.33738400
H	3.76803500	2.71658600	1.02227400
C	1.61799800	-0.38926100	-0.50633400
O	1.03089200	-0.86730500	-1.47507300
O	2.79275900	-0.92079000	-0.05862900
C	3.29356500	-2.05487400	-0.79498800
H	3.37252300	-1.79093200	-1.85006600
H	2.56618500	-2.86692200	-0.71664100
C	4.63193000	-2.44562800	-0.19418800
H	5.02409200	-3.32569900	-0.71138800
H	5.36157300	-1.63016500	-0.28944900
H	4.53341700	-2.69688200	0.86525100
N	-2.62643200	-1.23716100	-0.61864700
H	-2.96166400	-1.11087300	-1.57147800
C	1.13542000	0.69149800	0.35368900
O	1.76990600	1.92768000	2.27252700
H	0.38811300	0.04866300	1.72564900
C	2.10805800	1.42676900	1.14942800
O	0.07135400	0.29744700	2.75103300
H	0.80202200	1.23997600	2.69383000
H	0.44986000	-0.37829400	3.32949400

V'

SCF done: -1031.16911396

C	-3.14918300	-2.32429100	0.61431400
C	-2.64448500	-2.30952000	2.04462300
H	-2.57496600	-1.28892800	2.43127500
H	-1.64246400	-2.74363300	2.10870200
O	-4.11989300	-2.96770000	0.24611100
H	-3.33802800	-2.89197400	2.65070500
C	-1.21815500	0.49595100	-0.17340100
C	0.03577500	1.15656200	-0.08174900
C	0.06900100	2.53947600	-0.30499800
C	-1.08830000	3.28354800	-0.55588300
C	-2.31856700	2.62429800	-0.59532300
C	-2.38263000	1.24233100	-0.41099500
H	1.03161600	3.04118900	-0.26099200

H	-1.02499900	4.35359000	-0.72757400
H	-3.23292300	3.17886600	-0.78732300
H	-3.33587000	0.72830900	-0.45919500
N	-1.26115800	-0.89983800	0.01678500
H	-0.45863500	-1.34396900	-0.43116300
C	3.27831700	0.21298400	1.92986100
H	3.37723000	-0.85676500	1.74493500
H	4.09347000	0.70409900	1.39099600
H	3.38067200	0.41727600	2.99649800
C	1.84291300	-0.49177500	-0.70912500
O	1.13344900	-1.06647100	-1.53393200
O	3.17785100	-0.70349000	-0.66752100
C	3.69354000	-1.66695900	-1.61610300
H	3.46119800	-1.32228400	-2.62821800
H	3.17944200	-2.62202000	-1.47030000
C	5.18832500	-1.78031700	-1.38309000
H	5.62025400	-2.49117600	-2.09438800
H	5.68102700	-0.81367000	-1.52200100
H	5.40438300	-2.13505300	-0.37105100
N	-2.45366800	-1.54649000	-0.28841400
H	-2.74876900	-1.62412000	-1.25826200
C	1.31951400	0.46456200	0.27665900
O	1.41993700	1.52712200	2.41676500
H	-1.39125700	2.89468400	1.83058000
C	1.94186400	0.74149400	1.47125900
O	-1.12864700	2.44203900	2.64795900
H	0.48795700	1.82848800	2.27127400
H	-1.72512800	1.68388200	2.69592100

TSIV''-V''

SCF done:=-1183.8013286

C	3.42265600	2.12456800	0.09519700
C	2.74855000	2.29147000	1.44441600
H	2.40622400	1.33852400	1.85396400
H	1.86058900	2.92654900	1.34265800
O	4.46871900	2.67975700	-0.20920700
H	3.45783400	2.77558900	2.11640400
C	1.32325200	-0.57358100	-0.99535100
C	0.01404600	-1.13556800	-0.97246600
C	-0.12645500	-2.45232600	-1.44033200
C	0.95365100	-3.22359600	-1.86148200
C	2.23387400	-2.67795200	-1.82160300
C	2.41105400	-1.36354000	-1.39967100
H	-1.11213700	-2.90351900	-1.45472400

H	0.78880100	-4.23836300	-2.21018900
H	3.09526200	-3.26345800	-2.13007600
H	3.40485300	-0.93248000	-1.37514800
N	1.51260600	0.77711600	-0.61110100
H	0.79521200	1.36361700	-1.03728000
C	-3.74582400	-1.00486400	-0.64402200
H	-4.42505300	-0.66358900	0.14353900
H	-3.76338400	-0.28632400	-1.46264800
H	-4.11314300	-1.97637100	-0.99280000
C	-1.50272500	0.95135800	-0.92990200
O	-0.87562100	1.56063300	-1.78930600
O	-2.53329200	1.52972900	-0.25870100
C	-2.86858500	2.88614700	-0.63369000
H	-3.43692300	2.86132100	-1.57060100
H	-1.94404900	3.43618500	-0.82385200
C	-3.67498800	3.49419500	0.49888400
H	-3.95018500	4.52269400	0.24479900
H	-4.59345500	2.92906000	0.68220400
H	-3.09122400	3.51305500	1.42372400
N	2.78043900	1.31737800	-0.82076300
H	3.16369700	1.33872200	-1.76300100
C	-1.19531400	-0.40121300	-0.40389800
O	-2.25366100	-2.24450500	0.66634000
H	-0.73456100	-0.19655500	0.90469800
C	-2.36015700	-1.23694800	-0.08221800
H	-1.18893500	-2.34330800	1.44628200
O	-0.39468700	-2.39146000	2.21944000
C	0.10593600	-1.25885300	2.54116700
O	-0.20163300	-0.15133500	1.99975200
C	1.15475700	-1.25214400	3.61651400
H	2.14009400	-1.22617900	3.13162300
H	1.05905900	-0.34974700	4.22645200
H	1.08914600	-2.15236000	4.23121600

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SCF done: -954.72986924

C	2.92750100	-1.87287200	-1.98582400
C	2.01388100	-1.32989800	-3.06474600
H	1.98714100	-0.23637600	-3.02947900
H	0.98370600	-1.66894300	-2.93066300
O	3.97405100	-2.46181600	-2.20143200
H	2.40049400	-1.65757300	-4.02949000
C	1.55852500	0.39018800	0.13366200
C	0.43846900	1.02936000	0.72416400

C	0.58600800	2.34732600	1.17980600
C	1.79681400	3.03408300	1.06891800
C	2.88472100	2.39159400	0.47951600
C	2.77273100	1.08190100	0.01529200
H	-0.27939800	2.83934500	1.61660400
H	1.88187100	4.05504100	1.42671900
H	3.83467700	2.90878400	0.37818800
H	3.62472200	0.58992500	-0.44060700
N	1.41315300	-0.91425900	-0.34391300
C	-1.25437500	-0.11161600	2.11301900
C	-2.51016300	-0.82814500	2.52185800
H	-2.76342900	-1.62478600	1.82367700
H	-2.37164600	-1.23390000	3.52556500
H	-3.35798400	-0.13623500	2.53499500
C	-1.67027500	0.18270300	-0.36782000
O	-1.25865600	0.49980600	-1.47019200
O	-2.92075200	-0.32087700	-0.18019600
C	-3.71942900	-0.45258300	-1.37684400
H	-3.20475100	-1.11696800	-2.07842600
H	-3.80074700	0.52685200	-1.85813500
C	-5.07403600	-0.99877800	-0.96580800
H	-5.71381600	-1.10485100	-1.84744000
H	-4.97703700	-1.98119500	-0.49398100
H	-5.57065800	-0.32551100	-0.26096300
N	2.51021300	-1.67659500	-0.67731600
H	3.17373700	-1.95114500	0.04284000
C	-0.87453200	0.31720100	0.86988100
O	-0.45620500	0.09017100	3.18524100
H	0.62448100	-1.43148700	0.02248600
H	0.32583500	0.59377700	2.89428200

TS9-10

SCF done: -954.66985047

C	2.01338700	-2.08512000	-1.05545700
C	1.53028400	-1.03162000	-2.01995100
H	2.25882600	-0.21839600	-2.08694600
H	0.58000200	-0.59025900	-1.70765700
O	2.37796700	-3.19843200	-1.38647600
H	1.42256000	-1.50693500	-2.99479800
C	1.65259300	0.62517700	0.59827900
C	0.46472100	1.32129700	0.28224100
C	0.61507800	2.66177400	-0.14852600
C	1.88374900	3.22111300	-0.23560300
C	3.04429500	2.49705500	0.09241600

C	2. 92766000	1. 17258700	0. 50952100
H	-0. 27040600	3. 21702300	-0. 43038200
H	1. 98100600	4. 25078800	-0. 56984800
H	4. 02184800	2. 96255200	0. 02213000
H	3. 80216000	0. 57445600	0. 74930900
N	1. 37459200	-0. 75228100	0. 98471700
C	-0. 47588700	-0. 70478400	1. 14452800
C	-0. 98035600	-2. 07909000	0. 79334800
H	-0. 79476500	-2. 32441100	-0. 25284200
H	-0. 52113900	-2. 83103600	1. 44171400
H	-2. 05871200	-2. 09302200	0. 95705200
C	-1. 94692000	0. 84194800	-0. 30262600
O	-2. 17178900	1. 88214900	-0. 91623100
O	-2. 92072200	-0. 12933000	-0. 17392200
C	-4. 16844000	0. 16519800	-0. 82294800
H	-3. 99632500	0. 31929100	-1. 89376200
H	-4. 57305500	1. 10228400	-0. 42596000
C	-5. 10509500	-1. 00312400	-0. 56884000
H	-6. 07315500	-0. 81831100	-1. 04551500
H	-4. 69496400	-1. 93174500	-0. 97787600
H	-5. 27333400	-1. 14494400	0. 50328400
N	2. 13807400	-1. 75666100	0. 30893200
H	2. 26688800	-2. 59022500	0. 87340600
C	-0. 72244100	0. 50746300	0. 36862900
O	-0. 47091400	-0. 55867300	2. 53350100
H	1. 54191800	-0. 90230100	1. 98219200
H	-0. 60994700	0. 38699300	2. 70120500

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SCF done: -954.67089103

C	2. 10653500	-2. 06621200	-0. 98611700
C	1. 80382100	-0. 99102700	-1. 99615800
H	2. 53486300	-0. 18103600	-1. 92610300
H	0. 81456900	-0. 55213300	-1. 83576900
O	2. 45560200	-3. 19509000	-1. 27237800
H	1. 85503500	-1. 45164300	-2. 98259200
C	1. 61455700	0. 64331400	0. 59384400
C	0. 45944100	1. 29363900	0. 11872600
C	0. 63956500	2. 61923000	-0. 34941300
C	1. 90464100	3. 19297100	-0. 30711900
C	3. 03064800	2. 50701500	0. 18728500
C	2. 88447600	1. 19768600	0. 64705400
H	-0. 21778300	3. 15120500	-0. 74194100
H	2. 02849900	4. 21016300	-0. 66999600

H	4.00283100	2.98746800	0.20941800
H	3.73100900	0.62580900	1.01642900
N	1.27462200	-0.72685400	1.00432000
C	-0.40970500	-0.76444900	0.97206100
C	-0.86068900	-2.14169600	0.53370700
H	-0.52713200	-2.38531200	-0.47566000
H	-0.52077500	-2.91031800	1.23467600
H	-1.95020100	-2.12673100	0.53463600
C	-1.97194100	0.82415500	-0.36843900
O	-2.22902400	1.87140300	-0.95950000
O	-2.95526100	-0.12580100	-0.15026600
C	-4.25037800	0.20180100	-0.67777400
H	-4.17962900	0.34151700	-1.76212100
H	-4.58640300	1.15438900	-0.25449500
C	-5.19326400	-0.93396100	-0.31963500
H	-6.19828900	-0.72114900	-0.69812400
H	-4.85650100	-1.87840400	-0.75860400
H	-5.25607700	-1.06327800	0.76529800
N	2.06529900	-1.76257100	0.39615500
H	2.05369600	-2.61524000	0.94744500
C	-0.69944700	0.45356800	0.16964700
O	-0.66424800	-0.64114600	2.35791000
H	1.41854300	-0.84392400	2.01230700
H	-0.94066600	0.27878900	2.49172400

TS10-P

SCF done: -954.64717848

C	2.23286100	-2.17711900	-0.86649400
C	1.82150800	-1.24540700	-1.98156400
H	2.54375400	-0.42748900	-2.06528500
H	0.83919600	-0.79531400	-1.81628200
O	2.73610100	-3.27067400	-1.03766300
H	1.82149000	-1.82050300	-2.90734900
C	1.63569300	0.68266000	0.48830800
C	0.47485500	1.37421500	0.11337300
C	0.61867200	2.72091200	-0.26144000
C	1.89218700	3.29293700	-0.25102700
C	3.03027300	2.56707900	0.12729200
C	2.90704400	1.22728900	0.51272100
H	-0.25624000	3.28098400	-0.56633800
H	2.00344900	4.33216800	-0.54823100
H	4.00687600	3.04004300	0.12550800
H	3.76727200	0.63485500	0.80819900
N	1.26588600	-0.67287600	0.89248100

C	-0.29435600	-0.74916800	0.74344700
C	-0.86706100	-2.10909800	0.47769300
H	-0.75745300	-2.37972400	-0.57692700
H	-0.38880700	-2.86782000	1.09952100
H	-1.93004300	-2.08150100	0.71065100
C	-1.99476300	0.88132700	-0.27775400
O	-2.27722100	1.97939200	-0.74283900
O	-2.94270500	-0.09842100	-0.12753100
C	-4.26982900	0.25707900	-0.55946600
H	-4.24157500	0.54319300	-1.61605700
H	-4.60922200	1.13338400	0.00262700
C	-5.16614400	-0.94541900	-0.32422400
H	-6.18915100	-0.71557100	-0.63870200
H	-4.81923700	-1.81155700	-0.89598500
H	-5.18694000	-1.21832700	0.73530800
N	2.09518300	-1.72799500	0.45762300
H	2.24148800	-2.45039400	1.15259700
C	-0.67648000	0.48365600	0.16239200
O	-0.27826700	-0.78530700	2.53434900
H	1.00967600	-0.70990100	2.01511400
H	-0.63946000	0.07031300	2.81379700

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SCF done: -1031.11163537

C	1.97682200	-1.96774800	-1.21097100
C	1.63456500	-0.91028600	-2.22695400
H	2.34729400	-0.08282600	-2.17169200
H	0.63792100	-0.49285600	-2.05508800
O	2.34339000	-3.09400600	-1.49227100
H	1.68409400	-1.37669000	-3.21065100
C	1.55459300	0.76139400	0.38760900
C	0.40837600	1.39497400	-0.12518100
C	0.58614400	2.70839600	-0.61975200
C	1.84791900	3.29255500	-0.56243300
C	2.96537800	2.62496400	-0.02975700
C	2.81884300	1.32280000	0.45474900
H	-0.26619900	3.22613100	-1.04138100
H	1.97317500	4.30275200	-0.94399700
H	3.93392500	3.11227400	0.00332100
H	3.66066600	0.76519600	0.85473900
N	1.21082600	-0.60543300	0.81245700
C	-0.43150800	-0.63954700	0.78618500
C	-0.90817900	-2.03546200	0.43719600
H	-0.60019000	-2.34316700	-0.56240200

H	-0.55060500	-2.76578100	1.17037400
H	-1.99657800	-2.01163200	0.46471000
C	-2.01919900	0.88513900	-0.60650000
O	-2.28554800	1.91348200	-1.22649400
O	-2.99659400	-0.06698700	-0.36300700
C	-4.29113600	0.23558300	-0.90534000
H	-4.21391200	0.35970000	-1.99106400
H	-4.64372600	1.19012900	-0.49987700
C	-5.22243800	-0.90672000	-0.53739400
H	-6.22708700	-0.71298000	-0.92703700
H	-4.86960700	-1.85312800	-0.95918400
H	-5.29274100	-1.02048900	0.54892600
N	1.95520500	-1.64625500	0.16005600
H	2.03996700	-2.46881900	0.74690800
C	-0.74291700	0.53931200	-0.06447700
O	-0.74902100	-0.42625300	2.17396500
H	1.44337500	-0.76995600	1.81394400
H	-1.02536500	0.50189000	2.22914200
O	1.42594400	-1.41835700	3.47162600
H	1.48284700	-2.32776600	3.78863900
H	0.47819600	-1.18638700	3.45414100

TS10'-P

SCF done: -1031.09202310

C	2.06424900	-2.11114700	-1.02365000
C	1.63253700	-1.10114900	-2.05672900
H	2.34042000	-0.26701800	-2.07987400
H	0.64584400	-0.68212700	-1.84202600
O	2.54596800	-3.19761800	-1.29058800
H	1.63129200	-1.60204200	-3.02502200
C	1.63924100	0.63266600	0.54705700
C	0.50407000	1.32803100	0.10843900
C	0.67805700	2.66071900	-0.30385700
C	1.95643100	3.21996100	-0.25695100
C	3.06918100	2.49457700	0.19154500
C	2.91365000	1.16735300	0.60956100
H	-0.17786100	3.22029800	-0.65995600
H	2.09162500	4.24921400	-0.57880000
H	4.05034700	2.95728900	0.21763900
H	3.75741800	0.57672000	0.95333500
N	1.24827500	-0.72061400	0.95348500
C	-0.28899800	-0.75789600	0.83985600
C	-0.85367200	-2.12647700	0.55306800
H	-0.62844100	-2.44190000	-0.46868400

H	-0.45995800	-2.87226100	1.24887300
H	-1.93384000	-2.07207900	0.66426700
C	-1.95518800	0.84345500	-0.31624100
O	-2.22592500	1.92469000	-0.82944100
O	-2.92080900	-0.12381100	-0.14286600
C	-4.23550000	0.22860300	-0.60831200
H	-4.17191000	0.59430500	-1.63884600
H	-4.62655500	1.05235100	0.00198300
C	-5.10815400	-1.00920300	-0.49905900
H	-6.12643300	-0.77995000	-0.82971200
H	-4.71862500	-1.81775100	-1.12502500
H	-5.15679300	-1.36743500	0.53400200
N	1.97395500	-1.77353600	0.33346900
H	2.20282600	-2.54343200	0.95044400
C	-0.65297500	0.45253100	0.15689400
O	-0.73275000	-0.63906600	2.50587600
H	1.52415500	-0.84731900	2.19148900
H	-1.11866900	0.24892300	2.54186000
O	1.44819600	-0.87665100	3.41460600
H	1.62499200	-1.74179400	3.80767000
H	0.34098100	-0.75261200	3.22693900

TS8-V

SCF done: -1911.37799758

N	-5.04887800	-0.24394600	-0.93547100
C	-5.70471500	-1.33149900	-0.38836600
C	-4.86258900	-2.28952500	0.43518000
H	-5.54290700	-2.91768300	1.01056400
H	-4.16165500	-1.78112200	1.10078400
O	-6.89891200	-1.49064200	-0.59826100
H	-4.27299200	-2.93656100	-0.22447600
C	-3.10934600	0.70210200	0.15500200
C	-3.45263100	1.97513500	2.20317000
C	-2.08550800	2.24197200	2.27282400
C	-1.24557200	1.74848800	1.28081100
C	-1.71095600	0.97738900	0.20212800
H	-4.13285100	2.35713500	2.95948500
H	-1.67536000	2.83798200	3.08273400
H	-0.18860200	1.96504900	1.31190800
N	-3.67156100	-0.02511800	-0.93006300
H	-3.16453000	-0.87015700	-1.16911700
Rh	1.51045500	-0.46159200	0.04797200
C	3.13296000	-1.75882200	0.66617300
C	2.16553200	-2.59265100	-0.03817000

C	2. 10313900	-2. 15061700	-1. 38415700
C	2. 97275300	-0. 99290100	-1. 52999500
C	3. 66497100	-0. 81388300	-0. 28436800
C	3. 57767800	-1. 92264900	2. 08371600
H	2. 87184600	-2. 53257400	2. 65039300
H	4. 55782800	-2. 41558400	2. 11893000
H	3. 64361900	-0. 94236300	2. 56013400
C	4. 76678300	0. 16461600	-0. 03170800
H	4. 83413900	0. 41834700	1. 02513700
H	5. 71813700	-0. 27335600	-0. 36141800
H	4. 61094800	1. 08797100	-0. 59376300
C	3. 25474700	-0. 27047300	-2. 81162700
H	3. 80099800	-0. 92051200	-3. 50691300
H	2. 33288200	0. 06725000	-3. 28794000
H	3. 86268500	0. 61824400	-2. 63363900
C	1. 38358800	-2. 85774000	-2. 48659300
H	1. 93289600	-3. 77457700	-2. 73722500
H	0. 37212600	-3. 14596400	-2. 19111900
H	1. 32683100	-2. 24923400	-3. 38883800
C	1. 45020200	-3. 78389600	0. 52191000
H	2. 02854100	-4. 69607400	0. 32543600
H	1. 31865100	-3. 70082700	1. 60177700
H	0. 46191300	-3. 90343000	0. 07427600
C	-0. 76163300	0. 61829700	-0. 91847900
C	-0. 96183500	-0. 58147600	-1. 64595700
O	-1. 41225400	-1. 66831200	-1. 07666700
C	-0. 92156400	-0. 67629600	-3. 15418700
H	-1. 04330300	-1. 71305000	-3. 46375700
H	-1. 77434700	-0. 10173600	-3. 53516300
H	-0. 02942500	-0. 22975200	-3. 58111200
C	-0. 10816800	1. 75174700	-1. 65272400
O	0. 66535000	1. 63833700	-2. 59663400
O	-0. 45378900	2. 95786400	-1. 17150600
C	0. 23291100	4. 08566900	-1. 75381600
H	-0. 00584500	4. 13603300	-2. 82136400
H	1. 31152400	3. 92259400	-1. 66296600
C	-0. 22225800	5. 32744500	-1. 00986500
H	0. 26812700	6. 21241700	-1. 42879200
H	-1. 30493700	5. 45969200	-1. 09431300
H	0. 03383900	5. 26037600	0. 05125200
C	-3. 95319000	1. 21061400	1. 15602700
H	-5. 01494300	1. 00640400	1. 09139500
C	2. 45521200	1. 91948800	1. 60823900
O	1. 79812400	1. 54701400	0. 53921400

O	3.05103800	1.18758800	2.39749000
C	2.41902500	3.43194100	1.81912900
H	2.62282500	3.96006800	0.88435300
H	1.41962300	3.73013500	2.15286200
H	3.14601800	3.71743400	2.58050100
H	-5.59330200	0.32326400	-1.57386200
O	0.42542100	-0.68965700	1.88463300
C	-0.61932500	-1.34929500	2.14168200
O	-1.35373400	-1.96116800	1.29673200
C	-1.05982400	-1.38832200	3.59114500
H	-0.20491000	-1.27380400	4.25948100
H	-1.73649600	-0.54213400	3.75496400
H	-1.60382900	-2.30990400	3.80576500
H	-1.32543200	-1.73222500	0.07086700

TSV-11

SCF done: -1911.34413810

O	1.72843600	0.54872300	3.98205400
C	1.48470200	-0.12047500	2.98281500
O	1.31559000	0.46048200	1.81337200
C	1.34022600	-1.63438700	3.07006400
H	1.86920000	-2.14767800	2.26116300
H	1.71056000	-1.97834900	4.03963500
H	0.28039700	-1.89837500	2.98152500
O	-0.26634300	-1.94170300	0.15282500
C	-0.12883000	-3.25020000	0.35838500
O	0.94741300	-3.82383700	0.32258200
C	-1.42439000	-3.98872000	0.66284500
H	-1.92585000	-3.53367800	1.52298300
H	-2.11828800	-3.93736800	-0.18240700
H	-1.20017000	-5.03352600	0.87477200
C	-4.71369800	-1.11184800	-1.23346800
C	-5.40102100	0.03621900	-0.52714300
H	-5.62358300	0.81375100	-1.26838000
H	-4.82909800	0.47038200	0.29233800
O	-5.28986300	-1.80785900	-2.05051400
H	-6.35975900	-0.34067500	-0.15494000
C	-2.43658500	-0.13169900	0.96289600
C	-1.44914500	0.85764200	1.06712200
C	-1.28336600	1.46478300	2.31972900
C	-2.07729200	1.05692500	3.39556800
C	-3.02595900	0.03977200	3.25916200
C	-3.20939000	-0.58482200	2.02097900
H	-0.51834600	2.21219700	2.46178400

H	-1.93127700	1.52721400	4.36313100
H	-3.61684400	-0.27632900	4.11331300
H	-3.92492300	-1.38920100	1.88642300
N	-2.34151700	-0.71927900	-0.35722300
C	-2.71522700	1.27718200	-1.88489300
H	-3.29784800	1.78048800	-1.11036600
H	-2.18971200	2.02512400	-2.47622500
H	-3.37951500	0.72237400	-2.55142200
C	-0.26470700	2.36442700	-0.64614800
O	-0.12109800	2.72972500	-1.80976800
O	-0.02935900	3.19484000	0.39395300
C	0.25815100	4.57979400	0.09239100
H	0.85825100	4.63782500	-0.81755200
H	0.85144300	4.92553500	0.94210200
C	-1.02845400	5.38061300	-0.05137400
H	-0.79527300	6.44195100	-0.18743200
H	-1.59645400	5.04263100	-0.92203300
H	-1.65315200	5.27680200	0.84060600
N	-3.40160200	-1.48451000	-0.89221800
H	-3.04762100	-2.17180300	-1.55003700
C	-0.71118500	1.00530600	-0.23483600
O	-1.07952800	-0.35494400	-2.32629500
H	-0.14447900	-0.49532300	-2.06241900
C	-1.67196700	0.34473300	-1.27786300
H	-1.36768500	-1.50445100	-0.12472600
Rh	1.25486300	-0.25369100	-0.13178000
C	3.49656300	0.03903500	-0.14265600
C	3.26098900	-1.30074400	-0.54541100
C	2.82379000	0.92326500	-1.07330500
C	2.46900000	-1.25534400	-1.77101300
C	2.26119600	0.10692200	-2.13753800
C	4.27145700	0.51891700	1.04177700
H	4.58876300	-0.30344100	1.68514900
H	5.16754200	1.05625300	0.70707500
H	3.66187800	1.19796000	1.64411800
C	3.83347600	-2.54311100	0.06541600
H	3.07517400	-3.32253700	0.14470900
H	4.65939300	-2.91770200	-0.55335600
H	4.22959500	-2.34940100	1.06467300
C	2.07218200	-2.46519300	-2.56351400
H	1.22766600	-2.26012300	-3.22660000
H	2.91148400	-2.79253500	-3.19070900
H	1.80134000	-3.28967200	-1.90136200
C	1.73592800	0.63528400	-3.44000900

H	2.57733300	1.00044600	-4.04341000
H	1.22601000	-0.13658700	-4.02069900
H	1.04241300	1.46443100	-3.28221200
C	3.00974600	2.40811700	-1.10420000
H	3.99146100	2.64675100	-1.53594200
H	2.24460800	2.89261200	-1.71123900
H	2.97924600	2.82886600	-0.09621700

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SCF done: -1911.35118155

O	2.00592000	0.59532100	3.93728500
C	1.56526300	0.02103000	2.94900500
O	1.45077800	0.64649200	1.79342600
C	1.09553200	-1.42703200	3.02574600
H	1.56622500	-2.04451100	2.25533900
H	1.32643600	-1.83371000	4.01158200
H	0.01213000	-1.46221400	2.86900400
O	-0.17116200	-2.22205500	-0.00121900
C	-0.15965000	-3.50034400	0.45243500
O	0.87202900	-4.13400600	0.46292900
C	-1.48911000	-4.02873800	0.94445800
H	-1.79120200	-3.47286100	1.83845200
H	-2.27653300	-3.89019200	0.19727800
H	-1.38959500	-5.08637800	1.18551800
C	-4.73987200	-1.06893100	-1.23106300
C	-5.35925000	0.08205600	-0.46680800
H	-5.89598800	0.71004000	-1.18212100
H	-4.65855400	0.67839800	0.10963800
O	-5.38653400	-1.74666900	-2.01214500
H	-6.10217700	-0.33713600	0.21998800
C	-2.40228300	-0.23591600	0.89942700
C	-1.42531200	0.76335700	1.05284700
C	-1.28370300	1.34519400	2.31931200
C	-2.09196800	0.91600700	3.37710700
C	-3.03460300	-0.09891300	3.19808500
C	-3.19776300	-0.69619700	1.94318000
H	-0.53641900	2.10661300	2.48052400
H	-1.97098100	1.37431500	4.35370400
H	-3.64969700	-0.42664800	4.03105000
H	-3.93196700	-1.47760500	1.77775700
N	-2.34671600	-0.73730800	-0.42980500
C	-2.62128500	1.23759500	-1.98652500
H	-3.18725600	1.81323700	-1.25088100
H	-2.06370800	1.92589900	-2.61848600

H	-3.31065600	0.67146800	-2.61767500
C	-0.27227600	2.34745800	-0.60972500
O	-0.08250700	2.74740500	-1.75531400
O	-0.11849500	3.16348200	0.45639700
C	0.19944500	4.54941300	0.19758900
H	0.91165100	4.61079600	-0.62741100
H	0.68038300	4.89044700	1.11699000
C	-1.05522800	5.35507300	-0.10725100
H	-0.79986600	6.41402100	-0.22026100
H	-1.51293600	5.01183400	-1.03820000
H	-1.78408500	5.26193000	0.70319600
N	-3.42015500	-1.46081600	-0.96870000
H	-3.11561800	-2.16976100	-1.62639600
C	-0.69020000	0.96392400	-0.24253100
O	-1.00396400	-0.41195400	-2.35047400
H	-0.17672800	-0.76904200	-1.99000400
C	-1.63138600	0.28872100	-1.31008900
H	-1.08964900	-1.81725500	-0.11347800
Rh	1.35128700	-0.12038800	-0.11758800
C	3.60532400	0.05352900	-0.18883300
C	3.29886100	-1.25544900	-0.60648800
C	2.90252000	0.98133400	-1.07536600
C	2.46987800	-1.16189700	-1.81639000
C	2.30687200	0.20371300	-2.15838300
C	4.43361700	0.48372500	0.97932100
H	4.83798200	-0.37036800	1.52565100
H	5.27503700	1.09802200	0.63665700
H	3.83186600	1.07682500	1.67522300
C	3.77432200	-2.54123000	-0.00325200
H	2.95616500	-3.25819300	0.09635600
H	4.54627700	-2.99285200	-0.63998500
H	4.21023500	-2.38159400	0.98498300
C	2.03875600	-2.35805800	-2.61042600
H	1.25793900	-2.11326600	-3.33389900
H	2.89387200	-2.75758400	-3.17083300
H	1.67384700	-3.15183200	-1.95447300
C	1.73905100	0.77584700	-3.41991000
H	2.55574300	1.19156900	-4.02464700
H	1.23028500	0.01820000	-4.01761200
H	1.02816600	1.57527600	-3.20100200
C	3.09271800	2.46452000	-1.05754200
H	4.06191000	2.71918200	-1.50778200
H	2.30842100	2.96805300	-1.62361200
H	3.08975800	2.84316400	-0.03247600

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SCF done: -1911.36785078

O	3.40978600	1.86422700	2.59010500
C	2.57768000	1.00457300	2.30557300
O	1.81547800	1.11690300	1.24106900
C	2.37539200	-0.20770700	3.21002600
H	2.65165100	-1.12939800	2.68866300
H	2.98920800	-0.09949300	4.10542800
H	1.32160200	-0.30945400	3.47986300
O	-1.39302300	-2.86729300	0.39989100
C	-0.58056100	-2.59454000	1.40282900
O	0.33516500	-1.76799800	1.36471300
C	-0.88061700	-3.37831600	2.65158500
H	-1.71695100	-2.88703400	3.16031600
H	-1.18697900	-4.39708400	2.40572700
H	-0.01536800	-3.37751900	3.31360100
C	-5.23288800	-0.63058500	-0.99855200
C	-5.57526500	0.84586000	-1.00188900
H	-5.03072400	1.37536900	-1.78823700
H	-5.30779300	1.31395600	-0.05030600
O	-6.04833800	-1.51763300	-1.19147800
H	-6.64757600	0.93785400	-1.17292200
C	-2.63724300	0.12144300	0.98712700
C	-1.37659500	0.72548900	1.11401000
C	-0.97512000	1.14699700	2.38465000
C	-1.79458300	0.89957400	3.49106800
C	-3.01750900	0.23826900	3.34274700
C	-3.46202000	-0.15409100	2.07552000
H	-0.02997700	1.65577900	2.49711300
H	-1.47350400	1.22685000	4.47557900
H	-3.64087000	0.04420500	4.21125900
H	-4.42198300	-0.64112100	1.93741200
N	-2.94782100	-0.05425200	-0.36970000
C	-2.15490800	0.87450700	-2.48832600
H	-2.50271900	1.88478600	-2.26379600
H	-1.32280200	0.95142300	-3.18397700
H	-2.96388700	0.30987400	-2.95990200
C	-0.20125500	2.14582000	-0.66826700
O	0.15867200	2.42391600	-1.80895200
O	-0.17138700	3.04072100	0.33171200
C	0.47852200	4.30595500	0.07781200
H	1.31457000	4.14436000	-0.60522300
H	0.86666400	4.60985300	1.05230300

C	-0.50165500	5.32620100	-0.48186200
H	-0.00837800	6.29859800	-0.58644300
H	-0.85985000	5.01397600	-1.46597700
H	-1.35988600	5.44792700	0.18568400
N	-3.90628100	-0.96231200	-0.76742200
H	-3.72001800	-1.95440600	-0.64200000
C	-0.71073600	0.80523200	-0.23149200
O	-1.31655100	-1.19884200	-1.60780000
H	-0.36008100	-1.09804100	-1.75496000
C	-1.75996600	0.14360900	-1.20926900
H	-1.28117100	-2.22053800	-0.36910500
Rh	1.29474000	-0.36168700	-0.15037800
C	3.52738200	-0.67921900	-0.58982000
C	2.89223500	-1.92805700	-0.72595500
C	2.86931000	0.25440700	-1.50225800
C	1.89764900	-1.83067600	-1.79618600
C	1.95986300	-0.50814500	-2.33128000
C	4.69213300	-0.33607200	0.28442000
H	4.86944200	-1.09778700	1.04679600
H	5.59780900	-0.26856200	-0.33262700
H	4.56367500	0.62379500	0.78973200
C	3.19256100	-3.18714200	0.02833200
H	2.27453600	-3.70518600	0.31799100
H	3.77699100	-3.87728000	-0.59332900
H	3.76602600	-2.98816000	0.93545600
C	1.19050200	-3.02379800	-2.37899100
H	0.39601600	-2.74211700	-3.07321200
H	1.90300500	-3.64846300	-2.93279600
H	0.74586600	-3.64947800	-1.59989700
C	1.31606000	0.00823200	-3.58058900
H	2.06813100	0.05317100	-4.37900500
H	0.50565100	-0.63574800	-3.93040600
H	0.92575400	1.01475100	-3.41862200
C	3.30180800	1.67173900	-1.71222500
H	4.22117800	1.70652000	-2.31183900
H	2.52760100	2.24884100	-2.21935900
H	3.50110500	2.14748700	-0.74863100

TS12-P

SCF done: -1911.35184850

O	2.83946500	1.94737400	2.97803200
C	2.23382100	0.97642200	2.52859700
O	1.71355300	1.02066200	1.31946000
C	2.02104800	-0.26832000	3.37817800

H	2. 28197100	-1. 18009000	2. 83647000
H	2. 61132100	-0. 18338200	4. 29185200
H	0. 96021700	-0. 35655200	3. 62841000
O	-1. 37021400	-2. 78984600	0. 22645900
C	-0. 70901200	-2. 48459600	1. 27093000
O	0. 23875100	-1. 65030400	1. 34498400
C	-1. 11985500	-3. 16295200	2. 56362600
H	-1. 88458900	-2. 54083300	3. 04113400
H	-1. 55235600	-4. 14417100	2. 36006500
H	-0. 27225400	-3. 24339600	3. 24556900
C	-5. 20826700	-0. 65893900	-0. 92059100
C	-5. 54425800	0. 81853400	-0. 94405100
H	-5. 03793900	1. 32454600	-1. 77090700
H	-5. 23171200	1. 30885700	-0. 01751900
O	-6. 03420000	-1. 54753700	-1. 03092400
H	-6. 62301900	0. 91208000	-1. 06484400
C	-2. 62492700	0. 22072400	0. 94584900
C	-1. 42184500	0. 93774400	1. 00131900
C	-1. 05769000	1. 50940900	2. 22395200
C	-1. 86337600	1. 29233100	3. 34774800
C	-3. 02456800	0. 51752900	3. 27151100
C	-3. 43216900	-0. 02837500	2. 04785400
H	-0. 16597000	2. 11366200	2. 29368200
H	-1. 57721300	1. 73817900	4. 29587800
H	-3. 62902700	0. 35306300	4. 15860800
H	-4. 34557900	-0. 60773900	1. 95880700
N	-2. 89066600	-0. 09249300	-0. 40493200
C	-2. 18660100	0. 69898600	-2. 62549600
H	-2. 56438000	1. 72487600	-2. 56951400
H	-1. 32892500	0. 70394500	-3. 29084900
H	-2. 96266900	0. 04580000	-3. 02618700
C	-0. 14880400	2. 12853700	-0. 91524800
O	0. 17121600	2. 28180600	-2. 09414100
O	0. 05060700	3. 07433000	0. 01855000
C	0. 80588200	4. 24804400	-0. 35078600
H	1. 53291300	3. 97955600	-1. 11822100
H	1. 33337900	4. 52804000	0. 56306500
C	-0. 11449400	5. 35766600	-0. 83599000
H	0. 46798300	6. 26388300	-1. 03604400
H	-0. 62042300	5. 06207800	-1. 76002500
H	-0. 86894900	5. 59522900	-0. 07908300
N	-3. 86358400	-0. 98992100	-0. 78859600
H	-3. 65392600	-1. 97068800	-0. 61446700
C	-0. 80057500	0. 92141300	-0. 35518700

O	-1.19920300	-1.40416400	-1.75841800
H	-0.26119300	-1.18960400	-1.87110900
C	-1.81929500	0.24076200	-1.23563800
H	-1.22005700	-2.03957700	-0.84714900
Rh	1.31766900	-0.43307300	-0.09383700
C	3.51378900	-0.65498400	-0.38607200
C	2.90338800	-1.94291300	-0.45461500
C	2.94677600	0.15886800	-1.43990000
C	2.03588300	-1.97658400	-1.62620400
C	2.10606600	-0.69676500	-2.25229200
C	4.56428700	-0.19819600	0.57558900
H	4.66210900	-0.87563700	1.42605600
H	5.53430200	-0.16534300	0.06292900
H	4.35245100	0.80099400	0.96197900
C	3.17003800	-3.11923500	0.43230100
H	2.25028600	-3.67242400	0.63523300
H	3.87664700	-3.80729800	-0.04897600
H	3.59717900	-2.81511300	1.38943000
C	1.38298200	-3.22517100	-2.14893500
H	0.67409300	-3.01746400	-2.95281200
H	2.14724300	-3.90564500	-2.54576700
H	0.84062500	-3.75501900	-1.36139500
C	1.50292300	-0.27630500	-3.55676900
H	2.29658100	-0.19578600	-4.31065900
H	0.76763000	-0.99329600	-3.92956600
H	1.03103900	0.70514900	-3.45762000
C	3.36502800	1.55811700	-1.76898200
H	4.27002100	1.55347100	-2.39127800
H	2.57545400	2.08460900	-2.30809400
H	3.58453900	2.11715300	-0.85592700

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SCF done: -1911.41836413

O	1.00432100	3.29952800	1.87840000
C	1.50319200	2.18505400	1.97545000
O	1.86928100	1.50282200	0.89689100
C	1.82275700	1.56407200	3.32565300
H	2.91081600	1.51847600	3.45511400
H	1.39993500	2.17934000	4.12089300
H	1.43049900	0.54654700	3.37947700
O	-0.76697500	-2.00232700	0.44314800
C	-0.40209500	-1.64085000	1.58237300
O	0.67126700	-0.97112800	1.83028500
C	-1.25858200	-1.93940200	2.80199700

H	-2.02640700	-1.16234200	2.88370300
H	-1.76201300	-2.90119900	2.68134000
H	-0.66403300	-1.93319200	3.71688400
C	-4.50856000	-2.29384800	-1.12994000
C	-5.62052500	-1.41121200	-1.69437000
H	-5.26485500	-0.80576600	-2.53311500
H	-6.00215600	-0.72092700	-0.93794800
O	-4.50607900	-3.48731400	-1.17754100
H	-6.41820600	-2.06921200	-2.03904300
C	-3.38958100	0.56535300	0.55152000
C	-2.56907800	1.69745300	0.35240900
C	-2.53994900	2.68714500	1.34774200
C	-3.31639400	2.50995000	2.49007900
C	-4.11940900	1.36827300	2.66502500
C	-4.16665100	0.37144500	1.69214900
H	-1.89864500	3.55095800	1.23319700
H	-3.29298400	3.26637300	3.26897500
H	-4.70801300	1.25819800	3.57103900
H	-4.77080400	-0.52206400	1.81538000
N	-3.24806000	-0.25927100	-0.56903600
C	-1.95017700	-0.43317600	-2.68954500
H	-2.83912600	-0.57691600	-3.31562700
H	-1.21705500	0.14688700	-3.24725200
H	-1.54636200	-1.42608000	-2.46641000
C	-0.84106000	2.33828100	-1.52253100
O	-0.11296200	1.99625800	-2.44826300
O	-0.77337000	3.54015100	-0.92293100
C	0.35151700	4.40629000	-1.21258100
H	0.94776200	3.95192600	-2.00544100
H	0.92847600	4.43606200	-0.28512300
C	-0.17066100	5.77536300	-1.61555200
H	0.66924400	6.46181200	-1.76825200
H	-0.74428900	5.72164500	-2.54611900
H	-0.81416000	6.19503800	-0.83682000
N	-3.47273500	-1.62034600	-0.50599300
H	-2.68486400	-2.15321800	-0.12870900
C	-1.88087900	1.49596800	-0.91530900
O	-0.98688900	-4.09905400	-1.39000600
H	-1.91637200	-4.16268800	-1.65243900
C	-2.30159600	0.28630900	-1.43302400
H	-0.98302100	-3.49727100	-0.62556600
Rh	2.03558600	-0.41630200	0.36421000
C	4.06632400	-0.38939400	-0.40874000
C	3.78141200	-1.61328300	0.33991200

C	3.16899000	-0.34911100	-1.50692200
C	2.78131400	-2.37430000	-0.38512600
C	2.38014200	-1.58863300	-1.49932800
C	5.07622100	0.65598700	-0.04859800
H	5.37565900	0.57995100	0.99851200
H	5.97678400	0.54102400	-0.66403400
H	4.67534400	1.65916300	-0.20934800
C	4.51013200	-2.08001900	1.55880400
H	3.89675900	-2.76213000	2.15047000
H	5.42111500	-2.61659900	1.26228500
H	4.80791500	-1.24453900	2.19635100
C	2.28054900	-3.73399300	-0.00200100
H	1.38728100	-4.01323600	-0.56212600
H	3.05603300	-4.48532400	-0.19612800
H	2.03847600	-3.77780000	1.06341300
C	1.38404800	-1.94190700	-2.55037100
H	1.92077000	-2.31960400	-3.43226300
H	0.67352600	-2.70557100	-2.22662300
H	0.83073800	-1.05526500	-2.86479400
C	3.04588400	0.73036300	-2.53473400
H	3.41604300	0.36757900	-3.50194500
H	2.00546300	1.04624100	-2.66075500
H	3.62929800	1.60884400	-2.25412600

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SCF done: -878.32607834

C	2.51028600	-1.98588300	-0.05729000
C	2.29628700	-1.78555300	-1.54216200
H	2.45489600	-0.73887500	-1.81962900
H	1.27686000	-2.05126500	-1.83681400
O	3.37845200	-2.68703600	0.42691400
H	3.00953800	-2.41639500	-2.07132800
C	1.13278600	1.00353300	0.20581300
C	-0.03257300	1.70889300	-0.16461600
C	0.05957100	3.08869500	-0.40704800
C	1.29831500	3.70671100	-0.26736800
C	2.44497700	2.98022400	0.10705900
C	2.38061300	1.61059900	0.35056200
H	-0.82636600	3.64263500	-0.69301100
H	1.38499900	4.77382800	-0.44987000
H	3.39577800	3.49469600	0.20918200
H	3.25782300	1.04212600	0.64331300
N	0.76269800	-0.33317800	0.37616700
C	-0.59998700	-0.49187200	0.14525100

C	-1.24808000	-1.83030400	0.28228500
H	-1.57057800	-2.21147700	-0.69239900
H	-0.55690700	-2.54859300	0.72712800
H	-2.14541600	-1.75764200	0.89977200
C	-2.49489700	1.08868200	-0.55267200
O	-2.87762000	2.21249800	-0.83213200
O	-3.32966300	0.01390900	-0.54284900
C	-4.70478500	0.29417000	-0.88346200
H	-4.73871400	0.74877900	-1.87861300
H	-5.10404700	1.02869500	-0.17674100
C	-5.46632700	-1.01708600	-0.83145500
H	-6.51661700	-0.84692300	-1.08801700
H	-5.05291200	-1.73940500	-1.54155500
H	-5.42572000	-1.45609300	0.16988400
N	1.61452400	-1.33167500	0.79159000
H	1.85072900	-1.35645100	1.77844700
C	-1.11590900	0.74762200	-0.20110100