

SUPPORTING INFORMATION

The mechanism of ionic Diels-Alder reactions.

A DFT study of the oxa-Povarov reaction.

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Table S1. Total (E, in a.u.) and relative energies (ΔE ,^a in kcal/mol) in gas phase and DCM of the stationary points involved in the I-DA reaction of oxonium cation **6** with cyclopentene **7**.

	B3LYP/6-31G*		B3LYP/6-311G*		B3LYP/6-311G*	
	Gas phase		DCM ^b		DCM ^c	
	E	ΔE	E	ΔE	E	ΔE
6	-592.996399		-593.179745		-593.1799581	
7	-195.327139		-195.369741		-195.3697785	
TS1n	-788.324324	-0.5	-788.541933	4.7	-788.5422446	4.7
TS1x	-788.326419	-1.8	-788.543493	3.8	-788.5438526	3.7
8	-788.365181	-26.1	-788.582968	-21.0	-788.5834792	-21.2
10	-788.370622	-29.5	-788.587722	-24.0	-788.5881072	-24.1

(a) relative to **6** + **7**.

(b) single point energy calculations in DCM

(c) full geometrical optimizations in DCM

Table S2. Total (E, in a.u.) and relative energies (ΔE ,^a in kcal/mol) in gas phase and DCM of the stationary points involved in the I-DA reaction of oxonium cation **6** with styrene **12**.

	B3LYP/6-31G*		B3LYP/6-311G*	
	Gas phase		DCM ^b	
	E	ΔE	E	ΔE
12	-309.648259		-309.716427	
TS21n	-902.655865	-7.0	-902.895169	0.6
TS21x	-902.656939	-7.7	-902.896383	-0.1
IN1	-902.674805	-18.9	-902.911858	-9.8
IN2	-902.674588	-18.8	-902.912694	-10.4
TS22n	-902.673201	-17.9	-902.910214	-8.8
TS22x	-902.672144	-17.3	-902.909612	-8.4
13	-902.685334	-25.5	-902.926711	-19.2
15	-902.687422	-26.8	-902.927814	-19.9
TS3n	-902.629473	9.5	-902.873936	14.0
TS3x	-902.634514	6.4	-902.872043	15.1
17	-902.677141	-20.4	-902.921164	-15.7
18	-902.685576	-25.7	-902.927686	-19.8

(a) relative to **6** + **12**.

(b) single point energy calculations in DCM

Table S3. MPWB1K /6-311G* total (E, in a.u.) and relative energies^a (ΔE , in kcal/mol) in DCM of the stereoisomeric TSs involved in the I-DA reaction of oxonium cation **6** with cyclopentene **7** and styrene **12**.

	E	ΔE
TS1n	-788.119744	
TS1x	-788.119424	0.2
TS21n	-902.407140	
TS21x	-902.406449	0.4

(a) relative to **TS1n** and **TS21n**.

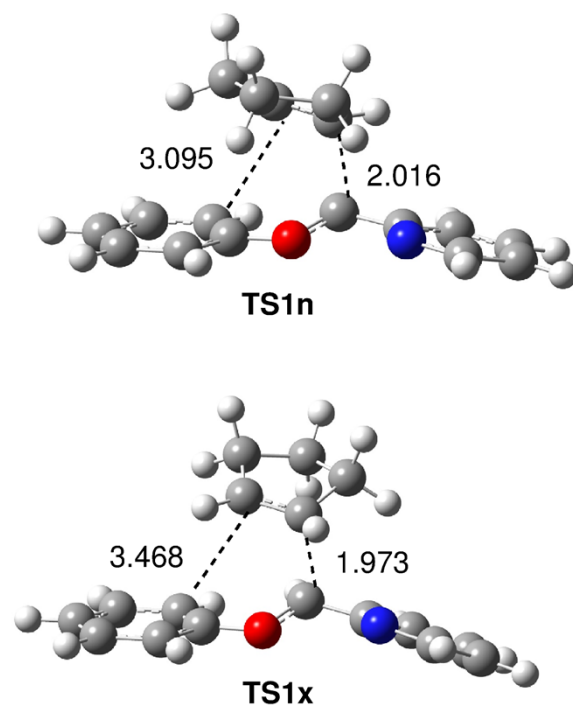


Figure S1. B3LYP(DCM)/6-311G* transition state structures involved in the I-DA reactions between oxonium cation **6** and cyclopentene **7**. Lengths are given in Angstroms.

B3LYP/6-31G* computed total energies, unique frequency imaginary, and cartesian coordinates of the stationary points involved in reaction of cationic aryl oxonium **6** with cyclopentene **7** and styrene **12**.

6

E (RB3LYP) = -592.996399 a.u.

C	2.41920400	-1.17344600	0.01047600
C	1.81647200	0.08324100	0.00076800
C	-0.48622000	-0.61769000	-0.00575100
H	-0.19177800	-1.66658000	-0.01415800
H	1.85361900	-2.09898300	0.02045700
C	2.53476000	1.27604700	-0.00848900
C	3.92672800	1.20665600	-0.00919500
H	4.50871200	2.12228500	-0.01654000
C	4.56332800	-0.03617100	-0.00033900
H	5.64730300	-0.08974800	-0.00059900
C	3.81175200	-1.21763500	0.00968900
H	2.00442600	2.22219200	-0.01532900
H	4.31133700	-2.18090000	0.01769500
C	-1.87075100	-0.26004200	-0.00159200
C	-2.82736600	-1.29458100	-0.00939600
C	-4.17652300	-0.94099500	-0.00706400
H	-2.52172100	-2.33706700	-0.01699300
C	-3.46282900	1.37412300	0.01038300
C	-4.49972600	0.41183700	0.00278900
H	-4.94967200	-1.70217600	-0.01290700
H	-3.70213200	2.43473200	0.01867000
H	-5.53503900	0.73829900	0.00476600
O	0.41659600	0.28341200	0.00033600
N	-2.17868400	1.06037000	0.00836900

7

E (RB3LYP) = -195.327139 a.u.

C	0.66756300	1.07609400	-0.04571500
C	1.23682800	-0.31767400	0.10073900
C	0.00013800	-1.22755200	-0.13208100
C	-1.23674000	-0.31797000	0.10069500
C	-0.66782300	1.07594500	-0.04557600
H	1.29294100	1.96336400	-0.10188700
H	1.66408900	-0.45624300	1.10599700
H	2.04862700	-0.52651000	-0.60782600

H	0.00029200	-1.57877200	-1.17013700
H	0.00018800	-2.11432700	0.50945300
H	-2.04845100	-0.52679000	-0.60798100
H	-1.66406900	-0.45683300	1.10588300
H	-1.29341500	1.96305300	-0.10188100

TS1n

E(RB3LYP) = -788.324324 a.u.

1 imaginary frequency: -268.66 cm⁻¹

C	-2.12548700	-1.13125900	-1.04989600
C	-1.52776700	-0.98443000	0.20799600
C	0.64044600	-0.40662600	-0.57265900
C	-1.01084000	1.64678700	-1.28953700
C	0.32357900	1.54768500	-0.89499400
H	0.39391800	-0.73519000	-1.57981400
H	-1.53821900	-1.20647900	-1.95852000
H	-1.38208600	1.36303800	-2.27064800
C	-2.28490800	-1.00714900	1.38585000
C	-3.66432900	-1.13953100	1.29705700
H	-4.26133000	-1.15370900	2.20353300
C	-4.28479500	-1.25823700	0.04410000
H	-5.36300900	-1.36626600	-0.01816900
C	-3.51671000	-1.26441600	-1.11823100
H	-1.77661600	-0.91672800	2.34015000
H	-3.99132200	-1.38883700	-2.08651500
C	2.08092300	-0.48011100	-0.22653000
C	3.01255800	-0.74581900	-1.23817000
C	4.35708300	-0.85755500	-0.88310400
H	2.69694300	-0.88323600	-2.26890800
C	3.70026100	-0.41177700	1.38613900
C	4.70910400	-0.69074600	0.45390400
H	5.10879200	-1.07600100	-1.63511900
H	3.94342800	-0.26856600	2.43628100
H	5.74200800	-0.77002800	0.77714300
O	-0.16918900	-0.81452500	0.40430800
N	2.41150900	-0.30201200	1.06247100
C	-1.84749000	2.36167800	-0.28680400
C	-0.93372900	2.48695300	0.95606400
H	-2.06237200	3.35277800	-0.72814800
H	-2.82663700	1.90229800	-0.11068700
C	0.50657600	2.32974300	0.40730600
H	-1.07806000	3.43318100	1.48190200
H	-1.15978200	1.68327600	1.66243900
H	1.09410300	1.55391900	-1.66423900

H	0.94935100	3.30421200	0.16468200
H	1.17698400	1.83148300	1.11193600

TS1x

E(RB3LYP) = -788.326419 a.u.
 1 imaginary frequency : -218.51 cm⁻¹

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39850000
C	2.36076800	0.00000000	1.71956400
C	1.64754500	2.52256200	1.08223800
C	2.66416400	1.99163900	1.86558600
H	2.52875200	-0.11947200	0.65218700
H	0.89064600	-0.23456200	-0.57297800
C	-1.16872200	0.22049400	2.13440300
C	-2.35612600	0.46603900	1.45274200
H	-3.26921700	0.64037700	2.01306699
C	-2.37513600	0.48396600	0.05258600
H	-3.30566000	0.66918300	-0.47458900
C	-1.20309500	0.24766200	-0.66650800
H	-1.12314900	0.19647300	3.21817900
H	-1.22096100	0.23863700	-1.75192300
C	3.42630500	-0.52552100	2.60861700
C	4.49911200	-1.23472200	2.05812500
C	5.44432199	-1.77846900	2.93279300
H	4.58254200	-1.38370500	0.98553200
C	4.18100500	-0.82799400	4.74460600
C	5.28186000	-1.57646600	4.29922099
H	6.28561600	-2.34662500	2.54843300
H	4.03676500	-0.63567300	5.80510000
H	5.99325300	-1.97540600	5.01506000
O	1.13108200	-0.23483400	2.17095600
N	3.27165000	-0.30667100	3.92367900
C	4.00110500	2.30691100	1.19331400
C	2.14977000	3.04616800	-0.22033200
H	1.52288200	2.77389700	-1.07712500
H	2.09907600	4.14787300	-0.15854100
C	3.61686900	2.55496700	-0.28516400
H	2.56246300	1.93408800	2.94799700
H	0.61705400	2.63212400	1.40500300
H	3.67111300	1.62144499	-0.85779501
H	4.27763601	3.27059000	-0.77885801
H	4.41298700	3.21433299	1.65314400
H	4.75186000	1.52197100	1.32143600

TS1n (B3LYP/6-311G* in DCM)

E(RB3LYP) = -788.542245 a.u.

1 imaginary frequency: -289.15 cm⁻¹

C	-2.12857400	-1.15792200	-1.04556300
C	-1.55093600	-0.97349000	0.21106500
C	0.62059700	-0.39844800	-0.55792400
C	-0.94491800	1.68967300	-1.28872700
C	0.37623800	1.57799600	-0.87406100
H	0.36795400	-0.70859900	-1.56479900
H	-1.53357800	-1.24642100	-1.94523200
H	-1.30254600	1.40360400	-2.27157500
C	-2.32167000	-0.96881100	1.37557700
C	-3.69707700	-1.11486100	1.27428300
H	-4.30386800	-1.10556500	2.17231600
C	-4.29877200	-1.27145200	0.02062400
H	-5.37411900	-1.38540100	-0.05356000
C	-3.51519100	-1.30169700	-1.12800100
H	-1.83033300	-0.84549600	2.33318000
H	-3.97377300	-1.44889500	-2.09891900
C	2.05984200	-0.49412300	-0.21552400
C	2.98284200	-0.72244500	-1.23998200
C	4.32607200	-0.85344400	-0.89965100
H	2.66009100	-0.81117200	-2.27158600
C	3.68894100	-0.50369100	1.38518700
C	4.68826900	-0.74292500	0.43769000
H	5.07017200	-1.04180400	-1.66467500
H	3.93971100	-0.40794600	2.43729900
H	5.72155400	-0.83670100	0.74971400
O	-0.19172900	-0.79278900	0.41880400
N	2.39976900	-0.37774700	1.07562900
C	-1.79061200	2.39658200	-0.29536700
C	-0.89670100	2.52038300	0.95959000
H	-1.99941000	3.38583600	-0.73786400
H	-2.77161100	1.94115900	-0.13808400
C	0.54818600	2.34710100	0.43287100
H	-1.03947800	3.47041500	1.47391800
H	-1.14082500	1.72843800	1.66932600
H	1.15744300	1.56844800	-1.62805400
H	1.00628300	3.31470700	0.20311700
H	1.20257200	1.84137400	1.14310500

TS1x (B3LYP/6-311G* in DCM)

E(RB3LYP) = -788.543936 a.u.
1 imaginary frequency: -246.32 cm⁻¹

C	2.34656100	-0.31802400	1.13824300
C	1.76656300	-1.03662400	0.09422200
C	-0.44359200	-0.17312800	0.30641700
C	0.93370800	1.72649500	-0.98093000
C	-0.39296700	1.33488400	-1.04811000
H	-0.16261800	0.37360300	1.19874500
H	1.75120500	0.20521800	1.87534200
C	2.53881400	-1.76348300	-0.81209900
C	3.92122300	-1.75384100	-0.67918000
H	4.52979300	-2.31233300	-1.38101700
C	4.52353900	-1.02805500	0.35192100
H	5.60264100	-1.02463600	0.45409200
C	3.73683700	-0.31852100	1.25528600
H	2.04512800	-2.31525600	-1.60299800
H	4.19865600	0.23254600	2.06636900
C	-1.86936500	-0.57027700	0.21979300
C	-2.73130500	-0.25267200	1.27048400
C	-4.05244800	-0.69331200	1.19358800
H	-2.37909600	0.30238300	2.13187800
C	-3.51019300	-1.66172200	-0.93229600
C	-4.44986900	-1.41269900	0.07551100
H	-4.75014600	-0.47520600	1.99359500
H	-3.79463800	-2.20844000	-1.82632200
H	-5.46690700	-1.77061300	-0.03061700
O	0.39451500	-1.11161700	-0.12349200
N	-2.24739300	-1.25093100	-0.87126500
C	-1.25967000	2.48213000	-0.53548500
C	1.10678800	3.02057700	-0.27334400
H	1.93712800	3.02386500	0.43808300
H	1.38212300	3.75965200	-1.04366400
C	-0.28664300	3.32024300	0.32437500
H	-0.73168400	0.66128200	-1.82908000
H	1.75278200	1.19922000	-1.45496400
H	-0.32018100	2.99699300	1.36802200
H	-0.52565700	4.38317300	0.31032300
H	-1.61489100	3.05189300	-1.40043800
H	-2.14588800	2.15427600	0.00906300

8

E(RB3LYP) = -788.365181 a.u.

C	0.00000000	0.00000000	0.00000000
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C	0.00000000	0.00000000	1.48810000
C	2.36913200	0.00000000	1.32098300
C	1.02622500	1.06691600	-0.58958700
C	2.28045000	1.18654000	0.33923600
H	2.38536900	-0.93736800	0.74937900
H	0.44106400	-0.97628200	-0.28147200
H	1.29445900	0.68923500	-1.58005100
C	-1.19195300	0.01825600	2.23781900
C	-2.39136600	0.04160400	1.56226900
H	-3.31330100	0.05578300	2.13789700
C	-2.48163200	0.04705700	0.12842300
H	-3.46134600	0.05980800	-0.33727700
C	-1.35193200	0.03334700	-0.61888900
H	-1.13563400	0.01913000	3.32080600
H	-1.39681100	0.03048900	-1.70467200
C	3.53202800	-0.00450000	2.28975100
C	4.61820500	-0.85225500	2.06298800
C	5.69028600	-0.81047200	2.95595100
H	4.62908900	-1.53291100	1.21600000
C	4.48633800	0.85915100	4.18411700
C	5.62371500	0.05992600	4.04073500
H	6.55262700	-1.45391200	2.80996800
H	4.39495100	1.54713400	5.02146100
H	6.42944600	0.12048700	4.76511900
O	1.13295300	-0.03879500	2.12389900
N	3.46000000	0.83905200	3.32766400
C	0.45483800	2.49936300	-0.66960900
C	0.78036700	3.13034600	0.69049600
H	0.99778500	3.03117900	-1.46050300
H	-0.60674500	2.53025000	-0.93410100
C	2.18629500	2.59272300	1.01440100
H	0.74555200	4.22306800	0.66363800
H	0.05334300	2.81243400	1.44957900
H	3.18588600	1.11747700	-0.27227400
H	2.94486800	3.24509700	0.57023600
H	2.38901800	2.54182100	2.08562600

9-endo

E(RB3LYP) = -788.019899 a.u.

C	2.12210600	0.01016200	0.47007400
C	1.43235700	-1.05067100	-0.13987400
C	-0.64655000	-0.20404100	0.60079700
C	1.39438400	1.26264200	0.94098500
C	-0.10776600	1.23442600	0.54331600

H	-0.48043100	-0.57942600	1.62346200
H	1.50542900	1.34749000	2.03056200
C	2.11387600	-2.17277600	-0.62761300
C	3.49468600	-2.25996400	-0.49173000
H	4.01854500	-3.13423300	-0.86905400
C	4.20055600	-1.23272000	0.14266000
H	5.27764000	-1.30060800	0.26708000
C	3.51193000	-0.11680000	0.61151300
H	1.53573300	-2.96120500	-1.09965400
H	4.06290200	0.68577100	1.09757400
C	-2.12727800	-0.33349800	0.29292200
C	-3.04376600	-0.49852500	1.33844500
C	-4.40312300	-0.57933000	1.04186600
H	-2.69413900	-0.56948200	2.36482000
C	-3.81330500	-0.34474500	-1.26352000
C	-4.80202400	-0.50364900	-0.29090600
H	-5.13383700	-0.70872100	1.83586200
H	-4.08333000	-0.28404600	-2.31689800
H	-5.84825500	-0.56849300	-0.57447600
O	0.07029400	-1.05298500	-0.30076400
N	-2.50807700	-0.25603100	-0.99056400
C	1.90238200	2.54519500	0.24187500
C	1.21154600	2.51125400	-1.13116700
H	1.56469800	3.41894800	0.81600500
H	2.99396000	2.59716100	0.17693700
C	-0.19610800	1.92793000	-0.85179900
H	1.17521400	3.49644900	-1.60825200
H	1.76747600	1.84743900	-1.80315000
H	-0.67013700	1.82049600	1.28082800
H	-0.95360600	2.71851800	-0.82540300
H	-0.50708300	1.22069300	-1.62322400

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E(RB3LYP) = -788.370622 a.u.

C	2.13233000	0.06645600	0.35345300
C	1.40011900	-1.21953800	0.19709500
C	-0.60981700	0.06962900	0.38707400
C	1.51179000	1.13766000	-0.64260300
C	-0.05131800	1.06940300	-0.63710700
H	-0.41468600	0.39590500	1.41558900
H	1.90102200	0.44520700	1.36629000
C	2.06458100	-2.44065800	-0.02763700
C	3.43851300	-2.43719000	-0.10818500
H	3.95315700	-3.37741800	-0.28887900

C	4.22362000	-1.24235700	0.02661200
H	5.30354100	-1.31009800	-0.05071600
C	3.61249100	-0.05428500	0.24851200
H	1.47925700	-3.34582900	-0.14580600
H	4.19221400	0.85702500	0.35836600
C	-2.07584400	-0.24985400	0.20432100
C	-2.96260500	-0.21801600	1.28068200
C	-4.30389000	-0.52835500	1.04302000
H	-2.61936400	0.03959700	2.27874400
C	-3.72339800	-0.87103000	-1.25963400
C	-4.69246800	-0.86420500	-0.25061200
H	-5.02525500	-0.51007800	1.85433400
H	-3.99098400	-1.12788000	-2.28209500
H	-5.72286800	-1.11426400	-0.48193000
O	0.10254600	-1.22675500	0.24021600
N	-2.44093400	-0.56641300	-1.04613400
C	-0.52223900	2.51148000	-0.30535500
C	1.88230300	2.59283400	-0.24924500
H	2.79767900	2.66462300	0.34753600
H	2.05941100	3.16773300	-1.16503300
C	0.64243600	3.13652800	0.47684300
H	-0.42670000	0.73642400	-1.60770700
H	1.89665900	0.88510700	-1.63371900
H	0.62964300	2.80550000	1.52464600
H	0.60912000	4.22950700	0.49042600
H	-0.68307100	3.05844500	-1.24050000
H	-1.47222900	2.52840500	0.23825600

11-exo

E(RB3LYP) = -788.023448 a.u.

C	2.21902800	0.04574900	-0.20389200
C	1.52680800	-1.16548900	-0.05228600
C	-0.53344600	-0.02364800	0.28306600
C	1.47061700	1.33834100	-0.44421100
C	-0.06692700	1.15671600	-0.57601600
H	-0.31442200	0.19080500	1.34138500
C	2.21348600	-2.37692900	0.09573300
C	3.60408300	-2.38846300	0.10640200
H	4.13306900	-3.33074000	0.22277900
C	4.31581800	-1.19164800	-0.02640100
H	5.40213100	-1.19400000	-0.01598500
C	3.62047400	0.00465000	-0.18427100
H	1.63496100	-3.28955000	0.20176100
H	4.17122300	0.93477100	-0.30990900

C	-2.01404000	-0.33437100	0.14466600
C	-2.78233400	-0.65520200	1.26833300
C	-4.13102400	-0.96580800	1.10001900
H	-2.32624200	-0.66570000	2.25420400
C	-3.81781900	-0.61417400	-1.24617400
C	-4.66430700	-0.94808400	-0.18685500
H	-4.75084300	-1.21786400	1.95636000
H	-4.19820500	-0.58595700	-2.26627800
H	-5.70853700	-1.18274100	-0.37072100
O	0.15785800	-1.23596800	-0.06608200
N	-2.52545400	-0.31097500	-1.09531000
C	-0.68966700	2.50243500	-0.09506100
C	1.62926100	2.43445700	0.63514700
H	1.47571200	2.00176700	1.63293400
H	2.62316700	2.89511200	0.63112400
C	0.49898800	3.41469200	0.29082200
H	-0.34992900	0.92814800	-1.60643600
H	1.83470800	1.76686100	-1.38952400
H	0.25725200	4.09983100	1.11055600
H	0.79706800	4.03127400	-0.56708500
H	-1.32761400	2.95121000	-0.86215200
H	-1.33219300	2.33201100	0.77868500

12

E (RB3LYP) = -309.648259 a.u.

C	-1.78074200	-1.04649400	0.00055200
C	-0.40627500	-1.28103600	0.00004900
C	0.51526900	-0.22003000	-0.00055200
C	0.00867400	1.09268900	-0.00074900
C	-1.36253400	1.32947700	-0.00023800
C	-2.26539200	0.26154100	0.00041900
H	-2.47165500	-1.88545800	0.00106200
H	-0.03465600	-2.30345900	0.00012200
H	0.69363700	1.93569200	-0.00143000
H	-1.73079900	2.35216100	-0.00042700
H	-3.33554000	0.45010300	0.00077400
C	1.95467000	-0.52914700	-0.00089400
C	2.97758800	0.33471000	0.00119400
H	2.18560100	-1.59466200	-0.00296600
H	4.00457100	-0.01747600	0.00062400
H	2.84129400	1.41283900	0.00355700

TS21n

E(RB3LYP) = -902.655865 a.u.

1 imaginary frequency: -101.32 cm⁻¹

C	1.19815300	-2.34807000	0.70475400
C	0.80608200	-1.62022100	-0.41825400
C	-1.33961500	-0.95113600	0.39057100
C	0.58350000	0.78731400	1.89911100
C	-0.78416200	0.72924300	1.96596200
H	-1.27595600	-1.69282100	1.18033400
H	0.57953800	-2.43107400	1.59115000
H	1.15263400	0.20791300	2.62547800
H	-1.26087400	0.23348500	2.80641800
H	-1.39517100	1.43733900	1.41893400
C	1.60349000	-1.51947100	-1.55745700
C	2.83345100	-2.17005100	-1.57209900
H	3.46304300	-2.10464700	-2.45369500
C	3.25285300	-2.90550900	-0.45886700
H	4.21156800	-3.41417800	-0.47351300
C	2.43752200	-2.99120300	0.67092400
H	1.24941400	-0.94074600	-2.40366300
H	2.75983600	-3.56499400	1.53416700
C	-2.64734800	-0.40554800	0.04084400
C	-3.77612400	-0.85083300	0.74471400
C	-5.02552200	-0.36150200	0.36242800
H	-3.68250000	-1.56990500	1.55355100
C	-3.89507100	0.94840900	-1.31237800
C	-5.08884900	0.55237200	-0.68539400
H	-5.92553600	-0.68965800	0.87270400
H	-3.91540500	1.67016500	-2.12558800
H	-6.03744300	0.96277900	-1.01614200
O	-0.41809300	-0.93951000	-0.52687300
N	-2.69624200	0.48932600	-0.96536300
C	1.37519300	1.54272600	0.95386300
C	2.77250700	1.61682600	1.15387900
C	0.81016600	2.21063600	-0.15866300
C	3.57591200	2.35034400	0.29043600
H	3.21554300	1.10214800	2.00263900
C	1.62042400	2.92995900	-1.02666800
H	-0.25534300	2.14337600	-0.35592300
C	3.00087500	3.00808800	-0.80196700
H	4.64608900	2.41096400	0.46240700
H	1.18121700	3.43617300	-1.88095500
H	3.62715600	3.58023400	-1.48022600

TS21x

E(RB3LYP) = -902.656939 a.u.

1 imaginary frequency: -105.14 cm⁻¹

C	-0.98939300	1.99113000	1.32508300
C	-0.21551400	2.22908600	0.19091800
C	1.23106300	0.35242000	0.29337800
C	-0.92093800	-0.64593800	-1.36643800
C	0.42975900	-0.80280200	-1.54442200
H	0.51535300	-0.14603500	0.94145400
H	-0.65424500	1.32118700	2.11068000
H	-1.36572900	0.28165000	-1.72343300
H	0.92322600	-1.74352800	-1.32118600
H	0.97696200	-0.12030100	-2.18662200
C	-0.58498800	3.14777000	-0.78942600
C	-1.79546900	3.82405200	-0.64296900
H	-2.10214500	4.54110100	-1.39787500
C	-2.60248300	3.58802400	0.47391300
H	-3.53865400	4.12529400	0.58895600
C	-2.19617800	2.68032900	1.45532700
H	0.06873300	3.31915400	-1.63824900
H	-2.80841500	2.51861000	2.33698600
C	2.60725000	-0.13551600	0.24007700
C	2.96203400	-1.25843900	1.00306000
C	4.29127500	-1.68050500	0.97139800
H	2.22626300	-1.77410100	1.61397400
C	4.73043500	0.12752000	-0.55907300
C	5.19283800	-0.97643400	0.17804400
H	4.61232600	-2.53709100	1.55559000
H	5.41190700	0.68981000	-1.19317200
H	6.23637800	-1.26890400	0.12006000
O	1.02533200	1.60308700	-0.01689600
N	3.46900900	0.54631500	-0.53778200
C	-1.84136500	-1.55969600	-0.72055000
C	-3.17481200	-1.13904100	-0.51813300
C	-1.47078300	-2.85740900	-0.29830900
C	-4.10194000	-1.97771600	0.08990800
H	-3.47259700	-0.14577400	-0.84385700
C	-2.39903500	-3.69218000	0.30859100
H	-0.46163200	-3.21980500	-0.46995600
C	-3.71552900	-3.25503100	0.50550100
H	-5.12410400	-1.64262200	0.23626700
H	-2.10730100	-4.69044900	0.62018800
H	-4.43941900	-3.91483900	0.97457700

INI

E(RB3LYP) = -902.674805 a.u.

C	1.16572200	-2.23103200	0.64177400
C	0.67727400	-1.54614500	-0.48790400
C	-1.31111500	-0.84898000	0.63812300
C	0.83147500	0.28513800	1.66152200
C	-0.63440800	0.10135400	1.72660700
H	-1.42211600	-1.84495400	1.07729800
H	0.53259700	-2.43487100	1.49740300
H	1.43931000	-0.21573700	2.41019800
H	-0.91020700	-0.29822400	2.70659600
H	-1.12337200	1.07064900	1.58815200
C	1.47534200	-1.41887100	-1.63846200
C	2.75376000	-1.94851300	-1.64447800
H	3.36975200	-1.84810400	-2.53318800
C	3.26235300	-2.61769500	-0.51261500
H	4.26459300	-3.03365500	-0.53342100
C	2.46606800	-2.76521200	0.61251300
H	1.06955100	-0.89379400	-2.49673800
H	2.83277100	-3.30948700	1.47768500
C	-2.67360100	-0.31385800	0.23323000
C	-3.76121300	-1.17366100	0.08242200
C	-4.97993000	-0.63600400	-0.33646400
H	-3.66046500	-2.23621900	0.28277200
C	-3.91312900	1.50952600	-0.40629000
C	-5.05882500	0.73124400	-0.58849700
H	-5.84874100	-1.27528300	-0.46079000
H	-3.93641700	2.58177600	-0.58598500
H	-5.98607500	1.19264600	-0.91221300
O	-0.54169000	-0.94178600	-0.54982800
N	-2.74386100	1.00347100	-0.00108000
C	1.49360200	1.22220900	0.84274600
C	2.90183200	1.39293600	0.99671500
C	0.79783200	2.01414800	-0.12033800
C	3.58382400	2.31882700	0.22876500
H	3.43056100	0.78845000	1.72836800
C	1.49582900	2.93167400	-0.88556100
H	-0.27399200	1.89539500	-0.25076900
C	2.88077200	3.08659800	-0.71226500
H	4.65334300	2.45408200	0.35220000
H	0.97262300	3.53915900	-1.61702500
H	3.41605900	3.81607500	-1.31360200

IN2

E (RB3LYP) = -902.674588 a.u.

C	-0.83322700	1.70337000	1.03138500
C	0.09255300	1.94859600	0.00191100
C	1.39640800	-0.01566800	0.48327900
C	-0.88518600	-0.72442600	-0.51098900
C	0.40475900	-1.14626500	0.02228700
H	1.24396300	0.16588700	1.55287300
H	-0.66432700	0.93317600	1.77487200
H	-0.84632900	0.01409700	-1.30748200
H	0.32983600	-1.89554600	0.81391500
H	0.96584300	-1.61023700	-0.82141300
C	-0.10878500	3.01260000	-0.89486800
C	-1.23017900	3.81691300	-0.76225200
H	-1.38119700	4.64067700	-1.45349700
C	-2.16739000	3.57593500	0.25761400
H	-3.03865700	4.21549200	0.35734000
C	-1.96173400	2.52840700	1.14665400
H	0.62633500	3.18128700	-1.67506600
H	-2.66778300	2.34693800	1.95152700
C	2.83535800	-0.44995300	0.23860300
C	3.87972200	0.10792800	0.97865900
C	5.18447700	-0.28500600	0.68208700
H	3.67781900	0.83480400	1.75976500
C	4.28503900	-1.71914400	-1.01582500
C	5.39397800	-1.21545200	-0.33524800
H	6.02172500	0.12730600	1.23711300
H	4.40121500	-2.44947100	-1.81275700
H	6.39260200	-1.55067900	-0.59572600
O	1.20727900	1.19248500	-0.23682500
N	3.03230700	-1.34406000	-0.73395600
C	-2.15590600	-1.28839700	-0.25995900
C	-3.26205200	-0.81226300	-1.02315700
C	-2.37841200	-2.31804200	0.69958000
C	-4.52646900	-1.34515700	-0.84107300
H	-3.09887100	-0.02278600	-1.75130900
C	-3.64574900	-2.84282500	0.87523400
H	-1.55372600	-2.69909700	1.29191500
C	-4.71814100	-2.35974900	0.10687600
H	-5.36401600	-0.98199900	-1.42755900
H	-3.81359700	-3.62979300	1.60329700
H	-5.70960800	-2.77993100	0.24970900

TS22n

E(RB3LYP) = -902.673201 a.u.

1 imaginary frequency: -170.32 cm⁻¹

C	-1.08216800	-2.01945800	-0.62918400
C	-0.51905800	-1.53602100	0.58612300
C	1.43819800	-0.87406500	-0.58664800
C	-0.87686000	-0.01962300	-1.51511600
C	0.62706900	0.02038100	-1.58953200
H	1.59361900	-1.86645900	-1.02281700
H	-0.43410100	-2.38822800	-1.41654700
H	-1.38098900	-0.41105600	-2.39401600
H	0.94036200	-0.27480100	-2.59594300
H	0.96150200	1.04589000	-1.41557700
C	-1.30585900	-1.44132900	1.74774900
C	-2.63247700	-1.81960800	1.69256400
H	-3.24588700	-1.73249000	2.58473500
C	-3.21430300	-2.32035500	0.49710600
H	-4.25455900	-2.62871700	0.49509400
C	-2.44143000	-2.45252500	-0.63046900
H	-0.85779100	-1.04405300	2.65193200
H	-2.85140500	-2.88575100	-1.53801100
C	2.77424600	-0.25322600	-0.23130000
C	3.94575200	-1.00892200	-0.23488900
C	5.13979100	-0.38336500	0.13154900
H	3.92935400	-2.05868200	-0.51300700
C	3.88192300	1.63190500	0.46047900
C	5.10845000	0.96167800	0.48907100
H	6.07268500	-0.93891900	0.13704400
H	3.81915900	2.68396300	0.72860700
H	6.01142700	1.48884000	0.77957300
O	0.71929000	-1.03499800	0.65023200
N	2.73615500	1.04426100	0.10440800
C	-1.64102600	0.95730800	-0.77566100
C	-3.02098200	1.10039500	-1.05803900
C	-1.04657000	1.80593200	0.19183500
C	-3.77867200	2.06889300	-0.41231300
H	-3.48353700	0.45397600	-1.79919900
C	-1.81266700	2.76812500	0.83426300
H	0.01112100	1.71652400	0.42279900
C	-3.17501600	2.90347500	0.53396000
H	-4.83247300	2.18145800	-0.64667300
H	-1.35153300	3.42522800	1.56508200
H	-3.76441400	3.66587600	1.03492600

TS22x

E(RB3LYP) = -902.672144 a.u.

1 imaginary frequency: -165.08 cm⁻¹

C	0.94983500	1.35145300	-0.89583600
C	-0.11817800	1.94781300	-0.16798300
C	-1.44051700	-0.00207000	-0.48493300
C	0.94303500	-0.38697500	0.53004000
C	-0.41619900	-0.93375800	0.23148800
H	-1.25284300	-0.01453900	-1.56457200
H	0.73976100	0.61902400	-1.66685600
H	0.98907800	0.28616200	1.38140000
H	-0.36018900	-1.85612000	-0.35113500
H	-0.88711300	-1.17534400	1.19601700
C	0.07755800	3.15634700	0.52742900
C	1.31641200	3.76627300	0.48215300
H	1.46962600	4.69702300	1.02052400
C	2.39389100	3.19582500	-0.24294700
H	3.35331700	3.70216600	-0.26664800
C	2.20512200	2.02165200	-0.93429300
H	-0.74920100	3.57267200	1.09267200
H	3.00907900	1.58951300	-1.52184700
C	-2.87077700	-0.42654800	-0.21133300
C	-3.84292500	-0.34741300	-1.20895400
C	-5.15182000	-0.71261500	-0.88920700
H	-3.58799900	-0.00527700	-2.20795500
C	-4.38556500	-1.18498900	1.33384500
C	-5.43084200	-1.13729200	0.40748500
H	-5.93509100	-0.66568300	-1.63970400
H	-4.56245900	-1.51668100	2.35430800
H	-6.43328600	-1.43247900	0.70011200
O	-1.30806400	1.35096300	-0.01719500
N	-3.12951600	-0.84030300	1.03546900
C	2.17127100	-1.10242600	0.27681300
C	3.30894700	-0.77807600	1.05516400
C	2.28347900	-2.12319800	-0.69739100
C	4.50457300	-1.46184000	0.88263000
H	3.23518500	0.00744800	1.80244400
C	3.48416000	-2.79605800	-0.87362600
H	1.43231000	-2.38708800	-1.31704100
C	4.59434500	-2.47045700	-0.08326500
H	5.36555500	-1.21558900	1.49595200
H	3.56127000	-3.57910600	-1.62127800
H	5.52929500	-3.00557400	-0.22079200

13

E(RB3LYP) = -902.685334 a.u.

C	0.98753800	1.34548800	-0.92870400
C	0.14859300	1.71916100	0.23958200
C	-1.56165700	0.36841400	-0.75374700
C	0.90970100	-0.22846800	-1.22096600
C	-0.52131800	-0.74084300	-0.91486400
H	-1.65867400	0.97890000	-1.65957900
H	0.48424500	1.80269500	-1.80181000
H	1.10068900	-0.31183400	-2.29472600
H	-0.85702300	-1.40754800	-1.71524300
H	-0.54026300	-1.32225400	0.01001700
C	0.63509100	2.53322700	1.27913000
C	1.93093400	2.99432500	1.19956200
H	2.30933500	3.62276000	2.00176000
C	2.80773200	2.68101800	0.10738000
H	3.81675400	3.07900300	0.11039800
C	2.37063900	1.89055000	-0.90183900
H	-0.01540100	2.77357600	2.11281400
H	3.01887400	1.63327200	-1.73428000
C	-2.91481800	-0.12256400	-0.29730900
C	-4.08281900	0.26337900	-0.95448100
C	-5.30097800	-0.23200800	-0.48322700
H	-4.04700000	0.93178300	-1.81013300
C	-4.06826400	-1.39932300	1.21254900
C	-5.29520600	-1.07732200	0.62259200
H	-6.23197300	0.04174000	-0.97028100
H	-4.02602700	-2.05787500	2.07713800
H	-6.21739000	-1.48450300	1.02452400
O	-1.07915200	1.29427500	0.30516000
N	-2.89688600	-0.94015700	0.76511800
C	1.99571800	-1.00383000	-0.49223100
C	3.03793000	-1.58257600	-1.22641300
C	1.98465100	-1.15761000	0.90252600
C	4.05161700	-2.29765900	-0.58467100
H	3.05481700	-1.48589800	-2.30996900
C	2.99900400	-1.86634700	1.54421800
H	1.17713800	-0.73715600	1.49831400
C	4.03570500	-2.43823100	0.80228600
H	4.84742900	-2.74656000	-1.17171400
H	2.97569800	-1.98017700	2.62420800
H	4.82143600	-2.99571100	1.30321800

14-endo

E(RB3LYP) = -902.341689 a.u.

C	1.09634100	1.29750800	-0.34137800
C	-0.07039700	1.98077800	0.04214000
C	-1.46931100	0.16222200	-0.65265100
C	1.02818500	-0.16069700	-0.78900200
C	-0.31148600	-0.78183700	-0.34102000
H	-1.48269100	0.38683600	-1.73071700
H	1.04213900	-0.17386400	-1.88948800
H	-0.46771300	-1.74209000	-0.84545800
H	-0.31341200	-0.97727700	0.73555500
C	-0.01656100	3.31746400	0.45796100
C	1.19843700	3.99263300	0.47817700
H	1.23112200	5.03019900	0.80017400
C	2.36838100	3.33888400	0.07995800
H	3.32116500	3.86052600	0.08779200
C	2.30562400	2.00651500	-0.32004300
H	-0.94222000	3.80081800	0.75498400
H	3.21539000	1.48880100	-0.61234200
C	-2.82314300	-0.39322100	-0.25160700
C	-3.90930900	-0.33469000	-1.12959500
C	-5.13906600	-0.84802700	-0.71816000
H	-3.79178200	0.10982200	-2.11382100
C	-4.09724600	-1.41203500	1.36129000
C	-5.23945500	-1.39887800	0.55702800
H	-6.00022000	-0.81532800	-1.38023300
H	-4.13529200	-1.83618300	2.36363600
H	-6.17475300	-1.81086900	0.92407100
O	-1.31526800	1.40631500	0.05340800
N	-2.91413900	-0.92662400	0.97626800
C	2.20375400	-1.01033400	-0.32339800
C	2.94866200	-1.75567300	-1.24439600
C	2.54166200	-1.10001300	1.03555400
C	4.00106000	-2.57365700	-0.82551500
H	2.70241300	-1.69564200	-2.30265000
C	3.59030300	-1.91507500	1.45787900
H	1.98400200	-0.51782000	1.76474400
C	4.32445800	-2.65670100	0.52817200
H	4.56723600	-3.14227800	-1.55884400
H	3.83707300	-1.97022100	2.51508100
H	5.14331600	-3.29057300	0.85800800

15

E(RB3LYP) = -902.687422 a.u

C	1.08302800	1.20719300	-0.42171700
C	-0.15802900	2.00430900	-0.23521800
C	-1.33078300	-0.07336600	-0.38673500
C	1.07209300	-0.02620200	0.60340800
C	-0.34063300	-0.67734600	0.61186800
H	-1.03098800	-0.26365700	-1.42363400
H	1.02439300	0.73605400	-1.41882500
H	1.25213800	0.41610800	1.58703500
H	-0.26403100	-1.74491600	0.38686900
H	-0.79622400	-0.58655300	1.60120700
C	-0.12856600	3.39522400	-0.02339000
C	1.09264400	4.03187600	0.00096900
H	1.11714500	5.10563500	0.16848000
C	2.33667000	3.33842600	-0.17526300
H	3.26323900	3.90170000	-0.14286200
C	2.34031500	1.99821800	-0.37538600
H	-1.06210300	3.92725600	0.12274700
H	3.26669500	1.44755600	-0.50578300
C	-2.76190000	-0.50367500	-0.16690800
C	-3.55001900	-0.95467400	-1.22573300
C	-4.86436700	-1.34159800	-0.95411300
H	-3.15284200	-1.00395800	-2.23570200
C	-4.46009800	-0.78091500	1.34367000
C	-5.33023300	-1.25140100	0.35446000
H	-5.50780800	-1.70257000	-1.75073400
H	-4.78994400	-0.69706500	2.37667400
H	-6.34428700	-1.53977500	0.61194600
O	-1.31278600	1.40540200	-0.23922200
N	-3.19896800	-0.41752000	1.09749900
C	2.20947900	-0.98455900	0.30000000
C	3.26622000	-1.12014900	1.20905200
C	2.22772900	-1.74958900	-0.87613100
C	4.31507800	-2.00634700	0.95452000
H	3.26446900	-0.53927100	2.12867700
C	3.27603600	-2.63156800	-1.13409300
H	1.41586400	-1.67173600	-1.59781000
C	4.32290300	-2.76193600	-0.21774800
H	5.12191400	-2.10621100	1.67447700
H	3.27422800	-3.21951800	-2.04715600
H	5.13782100	-3.45117900	-0.41739100

16-exo

E (RB3LYP) = -902.345104 a.u.

C	-1.39220300	1.31347800	-0.54574700
C	-0.38995500	1.99669000	0.16167200
C	1.05765900	0.08410000	0.12312600
C	-1.13678600	-0.06929000	-1.12115700
C	0.38968000	-0.31237900	-1.19531700
H	0.60783800	-0.50024000	0.93832900
H	-1.51314300	-0.07453700	-2.15287700
H	0.61327900	-1.36220900	-1.40229600
H	0.82349500	0.29387400	-2.00084500
C	-0.61456700	3.28826600	0.65749600
C	-1.84369800	3.90558300	0.45826700
H	-2.01059900	4.90663900	0.84699200
C	-2.85967600	3.23969100	-0.23607800
H	-3.82261600	3.71664000	-0.39410100
C	-2.62312900	1.95973900	-0.72835600
H	0.18886400	3.78160800	1.19602800
H	-3.40594600	1.43580000	-1.27294500
C	2.54974400	-0.18765400	0.11819300
C	3.50273600	0.83509700	0.11169000
C	4.85234800	0.48525500	0.08929300
H	3.18393400	1.87006900	0.13143600
C	4.17416300	-1.80793400	0.07874800
C	5.20202400	-0.86363100	0.07212200
H	5.61827000	1.25653900	0.08655100
H	4.40278400	-2.87270400	0.06752400
H	6.24052800	-1.18054500	0.05614500
O	0.85718500	1.47738100	0.39459000
N	2.87641700	-1.48944000	0.10243700
C	-1.85742000	-1.20170900	-0.38642900
C	-2.13960800	-2.38815700	-1.08046200
C	-2.22196300	-1.12135100	0.96335700
C	-2.75720100	-3.46472100	-0.44640200
H	-1.87191600	-2.46641600	-2.13267000
C	-2.83948100	-2.19918600	1.60309000
H	-2.03639900	-0.20532400	1.51643200
C	-3.10859100	-3.37432800	0.90250300
H	-2.96882500	-4.37219800	-1.00618300
H	-3.11388400	-2.11447900	2.65147700
H	-3.59252400	-4.21083100	1.39956400

TS3n

E(RB3LYP) = -902.629473 a.u.

1 imaginary frequency : -361.77 cm⁻¹

C	2.87436600	-1.21953700	0.62234200
C	2.16912900	-0.75260000	-0.50585200
C	0.03510900	-1.25878000	0.35685300
C	1.41685400	0.40237800	1.89256600
C	0.06413100	0.27520300	1.50877300
H	0.43222100	-1.99558100	1.05369900
H	2.43828700	-1.95364700	1.29032800
H	1.80852600	-0.16636500	2.72851000
H	-0.54411100	-0.21066800	2.27488000
C	2.81245500	-0.00281500	-1.50714900
C	4.15792400	0.28582700	-1.36671300
H	4.66392400	0.86650500	-2.13168300
C	4.87791500	-0.16392900	-0.23855300
H	5.93527400	0.06440400	-0.15016200
C	4.24650900	-0.91622800	0.73718700
H	2.23254500	0.33626600	-2.35890700
H	4.80409600	-1.29772400	1.58664300
C	-1.37249500	-1.50845500	-0.04534300
C	-2.17173600	-2.34283200	0.74627800
C	-3.48569500	-2.57554900	0.33983300
H	-1.77673800	-2.81305700	1.64323200
C	-3.05693600	-1.14696800	-1.54496300
C	-3.93857100	-1.96781600	-0.82863900
H	-4.13532500	-3.22366300	0.91990200
H	-3.37942800	-0.65849200	-2.46150200
H	-4.95193100	-2.12186800	-1.18530500
O	0.83782400	-0.95234800	-0.68696700
N	-1.80162400	-0.90972900	-1.16535100
C	-0.63169800	1.40576000	0.81813200
C	-1.96524000	1.67077300	1.15880600
C	0.00448700	2.21742500	-0.13103600
C	-2.64916800	2.73237300	0.56784300
H	-2.46801400	1.05131700	1.89807400
C	-0.68225600	3.27454500	-0.72503300
H	1.03660400	2.03155400	-0.41473800
C	-2.00928500	3.53552600	-0.37685100
H	-3.67853700	2.93315300	0.84947900
H	-0.17967700	3.89734800	-1.45909100
H	-2.53983400	4.36346000	-0.83748000
H	2.03611000	1.21814800	1.53642700

TS3x

E(RB3LYP) = -902.634514 a.u.
1 imaginary frequency: -318.51 cm⁻¹

C	-2.74849500	-0.70727600	0.82325900
C	-2.58575500	0.56096600	0.23305900
C	-0.22590600	0.57984700	0.40435400
C	-1.19519200	-1.34027200	-1.20265300
C	0.04261700	-0.70832700	-1.01679800
H	-0.22023300	-0.12088600	1.23757400
H	-1.96296900	-1.16237800	1.41568200
H	-1.95884100	-0.90265300	-1.83509000
H	0.25110900	0.07752300	-1.74603800
C	-3.65939200	1.22217700	-0.38660200
C	-4.89778600	0.60407000	-0.41850000
H	-5.73410600	1.10375800	-0.89714100
C	-5.07893300	-0.66707100	0.16178600
H	-6.05748300	-1.13588000	0.13594700
C	-4.01747800	-1.31052100	0.78158800
H	-3.48773300	2.19574200	-0.83326400
H	-4.16055800	-2.27721800	1.25389800
C	0.94182800	1.49547400	0.33046800
C	1.90390700	1.48662000	1.34395700
C	2.94874600	2.41058200	1.26335900
H	1.83380800	0.79251300	2.17555600
C	1.98965700	3.18272400	-0.80130100
C	2.99059300	3.27822600	0.17650400
H	3.71137000	2.44588400	2.03511200
H	2.00682700	3.83002500	-1.67498900
H	3.78608700	4.00877200	0.07063500
O	-1.38958100	1.21849500	0.17449800
N	0.98546100	2.30937700	-0.73555800
C	1.23310700	-1.50149800	-0.57038400
C	2.47886800	-1.24006800	-1.15650400
C	1.13668000	-2.49662600	0.41336800
C	3.60337200	-1.97501500	-0.78011700
H	2.56558700	-0.46895300	-1.91761000
C	2.26273300	-3.22589100	0.79348500
H	0.18055700	-2.71676300	0.88509200
C	3.49823700	-2.96777400	0.19520200
H	4.56025600	-1.77220300	-1.25173700
H	2.17472700	-3.99684200	1.55320300
H	4.37388100	-3.53910400	0.48815400
H	-1.37231100	-2.35700900	-0.86724700

17

E(RB3LYP) = -902.677141 a.u.

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.48841100
C	2.37014000	0.00000000	1.32606900
C	0.94057500	1.18588700	-0.44378400
C	2.34872300	1.10214100	0.21709300
H	2.35916800	-0.97572000	0.82481000
H	0.49023100	-0.92962800	-0.34218300
H	1.01917200	1.17387000	-1.53379200
H	3.04776200	0.71280600	-0.53191200
C	-1.19091100	0.03700100	2.23752300
C	-2.38959300	0.07466300	1.56057500
H	-3.31133600	0.10771900	2.13578300
C	-2.47986200	0.08483700	0.12642700
H	-3.45915800	0.11926700	-0.33889100
C	-1.35115000	0.04758400	-0.62099700
H	-1.13486200	0.05243600	3.32042000
H	-1.39483000	0.04486700	-1.70673300
C	3.53100100	0.04050600	2.29533100
C	4.69095400	-0.68244800	2.01011800
C	5.75960800	-0.59371600	2.90307500
H	4.76111900	-1.30355300	1.12089600
C	4.40539200	0.86380700	4.24001300
C	5.61545700	0.19385900	4.04268700
H	6.67954200	-1.13916200	2.71533100
H	4.25218700	1.48133900	5.12214600
H	6.41686900	0.28598200	4.76857900
O	1.13319000	0.03435800	2.12179100
N	3.37987200	0.80056000	3.38459100
C	2.84971300	2.47838300	0.63108100
C	3.96245800	3.02279700	-0.01995600
C	2.20837600	3.23568700	1.62235200
C	4.42729100	4.29826500	0.30677000
H	4.47028000	2.44949000	-0.79257600
C	2.67253900	4.50784600	1.95110300
H	1.35835400	2.82706800	2.16164900
C	3.78172200	5.04392600	1.29239700
H	5.29030400	4.70614700	-0.21122400
H	2.16985300	5.08013400	2.72540200
H	4.13942600	6.03705900	1.54765200
H	0.45020800	2.12066600	-0.16260300

18

E(RB3LYP) = -902.685576 a.u.

C	-2.50821400	-0.81707000	0.33526700
C	-2.49799900	0.66234600	0.18084100
C	-0.11193200	0.51895300	0.45348100
C	-1.40227500	-1.44493600	-0.59353700
C	-0.07455700	-0.63555500	-0.57054200
H	-0.14868000	0.14349300	1.48199200
H	-2.17586700	-1.01867100	1.37082500
H	-1.79741900	-1.48753500	-1.61173400
H	0.05021600	-0.14069500	-1.53758100
C	-3.67262000	1.39573400	-0.07679200
C	-4.85907700	0.70924200	-0.20442800
H	-5.76575800	1.27140800	-0.41303500
C	-4.95536200	-0.71982300	-0.08428800
H	-5.92413100	-1.19360200	-0.20162500
C	-3.84519700	-1.45103300	0.17307600
H	-3.61143000	2.47286200	-0.18600300
H	-3.89293600	-2.53201800	0.27343400
C	1.00448000	1.52331600	0.29063400
C	1.79378700	1.90954600	1.37288500
C	2.80538100	2.84686600	1.15207400
H	1.62890700	1.48964000	2.36085000
C	2.12451400	2.90823000	-1.14753200
C	2.97303400	3.35938800	-0.13124100
H	3.44479900	3.16904200	1.96833300
H	2.22678100	3.28635800	-2.16227600
H	3.74416400	4.09134300	-0.34891900
O	-1.37139100	1.29907700	0.26659600
N	1.16051000	2.00506300	-0.95053300
C	1.14715400	-1.51009000	-0.31473400
C	2.20087500	-1.52635800	-1.23575400
C	1.24449700	-2.30193300	0.83925200
C	3.32700100	-2.31996800	-1.01122300
H	2.14082600	-0.91273800	-2.13064900
C	2.37089400	-3.09217900	1.06711000
H	0.43720500	-2.31405600	1.57041200
C	3.41509400	-3.10333600	0.14009200
H	4.13399100	-2.32599600	-1.73804700
H	2.43146300	-3.70037200	1.96498400
H	4.29078600	-3.72151400	0.31406800
H	-1.24222700	-2.47304700	-0.26192000