

Theoretical Study on the Molecular Mechanism of the [5+2] vs [4+2] Cyclization Mediated by Lewis Acid in the Quinone System

Supporting Information

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- S13** **Figure S1.** Attractor positions and atom numbering of some selected points of the IRC of the one-step mechanism associated with the thermal cyclization of quinone **1**.
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Table S1. B3LYP/6-311G(d,p) total energies, E, enthalpies, H, entropies, S, and free energies, G,^{a,b} associated with the cyclizations of quinones **1** and **1-B**.

	E	H	S	G
<i>E-1</i> ^a	-1042.995174	-1042.51141	226.22	-1042.67477
TS4n	-1042.945473	-1042.46238	214.03	-1042.61694
4n	-1042.988271	-1042.50211	209.43	-1042.65335
TS4x	-1042.939222	-1042.45624	214.63	-1042.61123
4x	-1043.010735	-1042.52438	210.85	-1042.67665
TS5	-1042.936879	-1042.45431	213.00	-1042.60813
5	-1042.962829	-1042.47776	213.14	-1042.63168
<i>E-1B</i> ^b	-1367.664394	-1367.20979	158.76	-1367.25916
TS4n-B	-1367.636773	-1367.18135	143.41	-1367.22595
4n-B	-1367.660090	-1367.20193	142.33	-1367.24619
TS4x-B	-1367.625418	-1367.17021	141.74	-1367.21429
4x-B	-1367.682631	-1367.22462	141.80	-1367.26872
TS5-B	-1367.639506	-1367.18492	143.44	-1367.22953
5-B	-1367.680857	-1367.22288	141.458	-1367.26687

a) in toluene, computed at 180 °C.

b) in dichloromethane, computed at -78 °C.

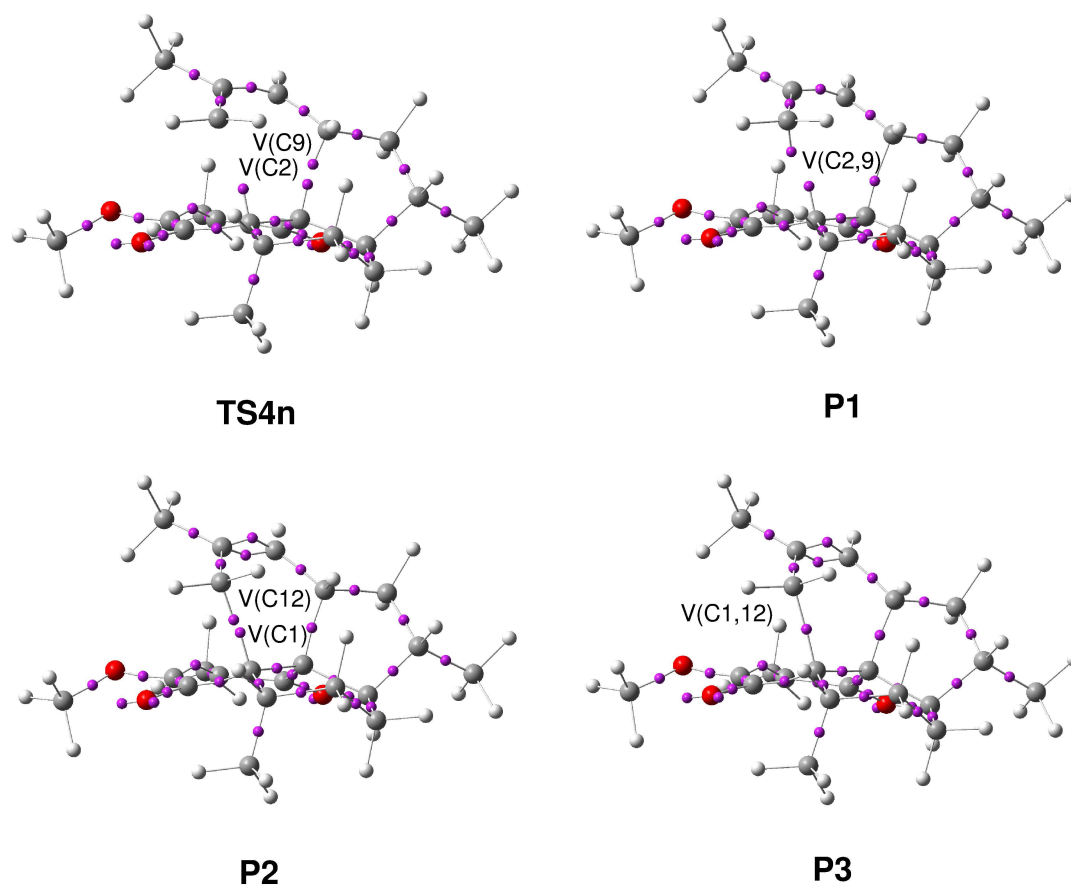


Figure S1. Attractor positions and atom numbering of some selected points of the IRC of the one-step mechanism associated with the thermal cyclization of quinone **1**.

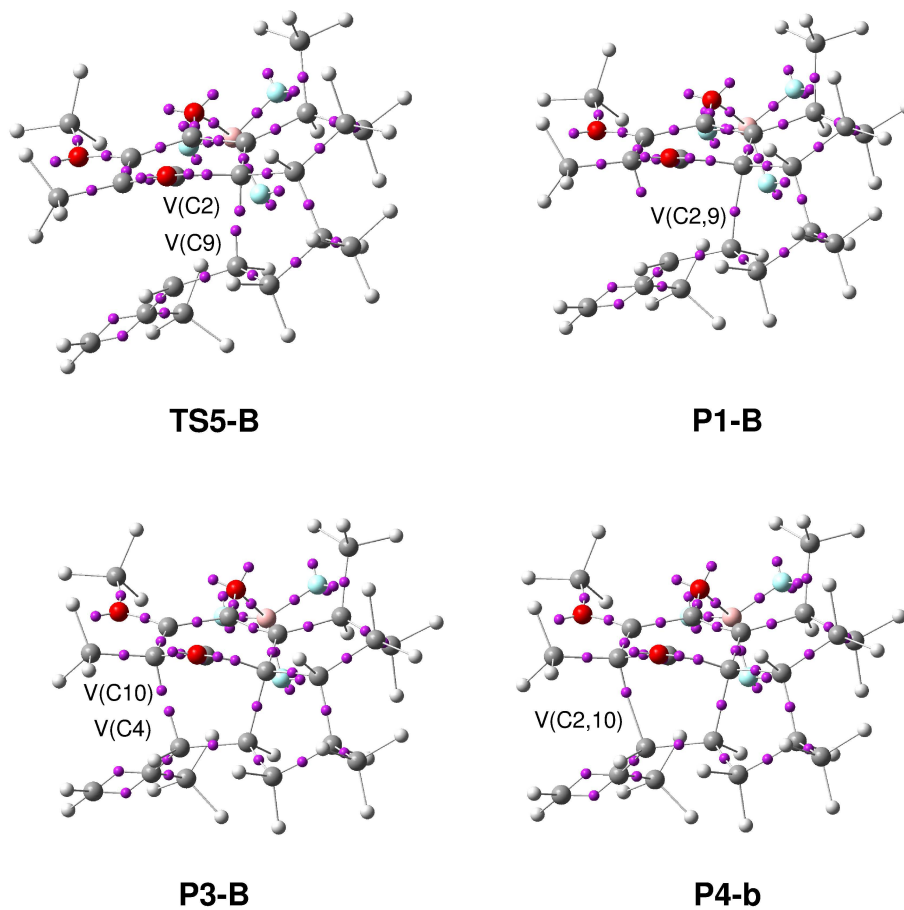


Figure S2. Attractor positions and atom numbering of some selected points of the IRC of the one-step mechanism associated with the LA catalyzed cyclization of quinone **1B**.

B3LYP/6-311G(d,p) computed total energies, unique imaginary frequency, and cartesian coordinates of the stationary points involved in the cyclizations of quinones **1** and **1-B**.

E-1

E(RB3LYP) = -1042.995174 a.u.

C	-3.06621900	-0.34766700	-0.17370100
C	-1.70126000	-0.95072600	-0.17683200
C	-0.62066300	-0.19608100	0.11890800
C	-0.77909400	1.29277200	0.26755600
C	-2.12039900	1.90742900	0.23996200
C	-3.20280800	1.13712500	-0.02861700
C	0.78794300	-0.74010600	0.22671900
C	0.88920000	-2.17392600	-0.33456500
C	-0.32613700	-3.04963800	-0.00346000
C	-1.63884400	-2.42851600	-0.50085300
C	-1.85627900	-2.65809000	-2.01326300
C	1.38082600	-0.54941400	1.66592100
C	0.76184500	-1.44548600	2.74658600
O	0.21382400	2.00598700	0.36806600
C	-2.21935500	3.39096300	0.44792000
O	-4.41456900	1.72627400	-0.04676500
C	-5.53474800	1.20236200	-0.78793600
O	-4.05901300	-1.05634600	-0.25105700
C	2.92325400	-0.69826000	1.66924100
C	3.64020500	0.27670200	0.78145000
C	4.53041600	-0.05776000	-0.16340700
C	5.25737900	0.86946500	-1.03663400
C	6.12538000	0.39250800	-1.94271600
C	5.00881000	2.35110000	-0.89443900
H	1.40358000	-0.09108400	-0.40430200
H	0.99870100	-2.11258500	-1.42216600
H	1.80171800	-2.65338500	0.02809500
H	-0.20243300	-4.04010000	-0.45291400
H	-0.39312200	-3.20484700	1.07513200
H	-2.47682900	-2.90709200	0.01368400
H	-2.14904300	3.92319900	-0.50755800
H	-3.17289700	3.65703200	0.90321600
H	-1.39755100	3.74054400	1.07196600
H	-6.02496500	0.39914000	-0.24289900
H	-6.20718400	2.05140600	-0.90400600
H	-5.22478800	0.84316700	-1.77038600
H	-1.87733400	-3.73037300	-2.22666600
H	-2.80511900	-2.23237100	-2.34390700
H	-1.05517500	-2.20863700	-2.60598900
H	1.17346800	0.48831400	1.93756300
H	1.12315500	-1.14269900	3.73367600
H	-0.32880500	-1.37466800	2.75924400
H	1.03184500	-2.49666700	2.61103100
H	3.21263600	-1.72288400	1.41189500
H	3.25327200	-0.54046600	2.70511300
H	3.39795900	1.32469900	0.94302700
H	4.75484300	-1.11267000	-0.31543200
H	6.30554700	-0.67242400	-2.04628400
H	6.67799200	1.05065900	-2.60359600
H	3.95418200	2.59328800	-1.05924500

H	5.26135300	2.69799300	0.11275600
H	5.60634600	2.91766200	-1.61004100

E-1B

E(RB3LYP) = -1367.664394 a.u.

C	-2.23058700	0.51872600	-0.16156600
C	-1.06569300	-0.36931000	-0.28744500
C	0.15131900	0.12669600	0.05489600
C	0.30885200	1.60070300	0.34796400
C	-0.85919100	2.50418500	0.28702700
C	-2.06597800	1.98925600	-0.05060300
C	1.41715000	-0.69109700	0.08649700
C	1.26846900	-2.01428800	-0.68890700
C	-0.09159900	-2.68778100	-0.48598700
C	-1.26677400	-1.76749100	-0.84384300
C	-1.50360700	-1.68223400	-2.36851500
C	1.97318100	-0.82981400	1.55169800
C	1.15985900	-1.74901100	2.47180900
O	1.42036200	2.06223400	0.56104900
C	-0.65633000	3.96108400	0.56460900
O	-3.13466600	2.80200800	-0.08171500
C	-4.23138200	2.59985500	-1.00634300
O	-3.42009000	0.12722700	-0.11666900
B	-4.33232100	-1.19420500	0.23620900
F	-3.67181900	-1.84076800	1.25179500
F	-5.50862600	-0.61301400	0.62382400
F	-4.43054900	-1.91149000	-0.92727500
C	3.46233900	-1.25985900	1.54342600
C	4.38119700	-0.29437800	0.85433200
C	5.20535300	-0.60764800	-0.15637500
C	6.12481000	0.30881400	-0.83942900
C	6.89794900	-0.14435500	-1.83948200
C	6.17985900	1.75119800	-0.39858600
H	2.17169800	-0.08488700	-0.42472000
H	1.41282700	-1.80716500	-1.75399800
H	2.06901700	-2.70208100	-0.40796700
H	-0.15291500	-3.59116900	-1.09968800
H	-0.20174000	-3.00900400	0.55097000
H	-2.16114000	-2.19716000	-0.40175900
H	-0.48450200	4.50713400	-0.36999200
H	-1.53840300	4.39204800	1.03760600
H	0.21731900	4.10917200	1.19730800
H	-4.98625000	1.95332000	-0.56552800
H	-4.63699900	3.59450800	-1.18074000
H	-3.87595100	2.17952800	-1.94809100
H	-1.71903700	-2.67938000	-2.75980000
H	-2.35687000	-1.04411100	-2.60673800
H	-0.62695000	-1.28854000	-2.88911500
H	1.94506600	0.17534500	1.97913900
H	1.52745000	-1.66032500	3.49797600
H	0.09832300	-1.48904300	2.47876600
H	1.25062100	-2.79990800	2.18456700
H	3.57142300	-2.25920300	1.10947200
H	3.76782200	-1.34776800	2.59450700
H	4.35744400	0.72644400	1.22903800
H	5.21391000	-1.63399100	-0.52065900
H	6.86011700	-1.18117600	-2.15719000
H	7.58758500	0.50638500	-2.36522400
H	5.20111100	2.23201000	-0.49433800

H	6.47164500	1.83141400	0.65348100
H	6.89789000	2.31482200	-0.99579500

TS4n

E(RB3LYP) = -1042.945473 a.u.

1 imaginary frequency found: -434.08 cm⁻¹

C	1.49236500	1.07440500	-0.22403600
C	0.05439300	1.10796300	0.09426000
C	-0.81799200	0.02562200	-0.28813900
C	-0.20653200	-1.05036600	-1.15208800
C	1.25744500	-1.21633900	-1.18408500
C	2.05598600	-0.20885100	-0.75002500
C	-2.31380500	0.26696200	-0.64630600
C	-2.77785400	1.72297200	-0.44006600
C	-2.02386600	2.41586000	0.69620400
C	-0.52314200	2.49914600	0.37405500
C	-0.27346400	3.47365100	-0.80326500
C	-3.25629100	-0.73810600	0.10455300
C	-4.34765900	-1.30504700	-0.80383700
O	-0.91951200	-1.79862500	-1.81559300
C	1.80316700	-2.47703800	-1.79078100
O	3.39318500	-0.41623700	-0.76547900
C	4.35685100	0.62857800	-1.02009500
O	2.22826600	2.05279500	-0.08134700
C	-2.40604400	-1.81816200	0.78946700
C	-1.20869600	-1.09200600	1.32456800
C	-0.00335100	-1.68019200	1.76093300
C	1.04090300	-0.87808400	2.21444100
C	0.85163500	0.50811500	2.24945400
C	2.41328200	-1.46373600	2.46131000
H	-2.38870100	0.02635000	-1.70822500
H	-2.63492800	2.29495000	-1.36016500
H	-3.85473500	1.73163900	-0.24586300
H	-2.41275700	3.42696800	0.85053400
H	-2.18641800	1.88094300	1.63966200
H	0.00236600	2.92044700	1.23614600
H	1.14753200	-2.81430500	-2.59358100
H	2.81366000	-2.32453500	-2.16713400
H	1.84344600	-3.28127100	-1.04706900
H	4.51318700	1.24797900	-0.14048200
H	5.27081900	0.09507900	-1.28124100
H	4.04127100	1.25699500	-1.85293800
H	-0.79283400	4.41764500	-0.61175100
H	0.78890400	3.67942200	-0.91085700
H	-0.64094300	3.07572800	-1.75219500
H	-3.74596400	-0.17388400	0.90952400
H	-5.02285800	-1.96195200	-0.24707400
H	-4.95277400	-0.50718500	-1.24506200
H	-3.90161900	-1.88232300	-1.61813600
H	-2.11735700	-2.60407900	0.08849500
H	-2.96677900	-2.28805100	1.60601700
H	-1.50421800	-0.21354300	1.88920900
H	0.18280100	-2.73194400	1.56156700
H	-0.10864400	0.93092900	2.50421500
H	1.69634800	1.16518300	2.42177400
H	2.39858200	-2.55096000	2.36397000
H	3.14276700	-1.07412700	1.74579600
H	2.77034400	-1.21763900	3.46507600

4n

E(RB3LYP) = -1042.988271 a.u.

C	-3.26633800	-0.69059600	0.21661200
C	-2.28355100	0.26889100	-0.56003000
C	-0.82848300	-0.07850700	-0.02544600
C	-1.20184200	-0.70496100	1.38960400
C	-2.39956000	-1.59961700	1.11488800
C	-0.00552100	-1.14989600	2.16586100
C	0.94668400	-0.22796100	2.34890100
C	0.68550200	1.12639900	1.72542400
C	0.23414000	1.07203100	0.19391300
C	-0.29328600	-1.22370400	-0.90243200
C	1.15092600	-1.49276300	-1.03476900
C	2.05400200	-0.50094100	-0.83323000
C	1.59623300	0.86936000	-0.48937500
C	-2.72376000	1.75271000	-0.46347000
C	-1.75507600	2.65071500	0.30828300
C	-0.31762500	2.48244400	-0.20395000
C	2.21368600	-0.44822100	3.12452100
O	-1.06486800	-1.98702800	-1.47068100
C	1.55101200	-2.84012500	-1.55998400
O	3.34627500	-0.75155600	-1.12787800
C	4.43491400	0.03514500	-0.60696900
O	2.34183800	1.81770300	-0.67337800
C	-0.24799900	2.77788000	-1.71616300
C	-4.23636100	-1.43916400	-0.69714600
H	-2.31153000	-0.01969600	-1.60992200
H	-2.83956600	2.15764500	-1.47181200
H	-3.71602200	1.81084700	-0.00684700
H	-2.05516500	3.69731500	0.19139200
H	-1.80931500	2.44096100	1.38155100
H	0.31809200	3.21732600	0.29768100
H	1.41024600	-2.88689700	-2.64498500
H	2.59870900	-3.04427900	-1.34601600
H	0.91989100	-3.61877300	-1.12920200
H	4.29050400	0.26484700	0.45000800
H	5.31244300	-0.59950300	-0.72387800
H	4.55201100	0.95919300	-1.16757800
H	-0.81715300	3.68398400	-1.94410200
H	0.77811400	2.93843500	-2.04042000
H	-0.66873700	1.96802800	-2.31857300
H	-3.85862600	-0.06060800	0.89118200
H	-4.91619000	-2.06987800	-0.11518800
H	-4.84945000	-0.74381300	-1.27945000
H	-3.68546500	-2.07562400	-1.39274100
H	-2.11958700	-2.52061000	0.60023700
H	-2.92020500	-1.87424500	2.03690500
H	-1.61557000	0.15902000	1.92895500
H	0.07672800	-2.16232500	2.54995400
H	-0.11685700	1.62671500	2.27909300
H	1.55818900	1.77771500	1.79728900
H	2.25872700	-1.46016000	3.53254300
H	3.10146100	-0.29234500	2.50079300
H	2.29220300	0.25905800	3.95837300

TS4x

E(RB3LYP) = -1042.939222 a.u.

1 imaginary frequency found: -459.60 cm^{-1}

C	1.82288100	-0.56848500	0.58638000
C	0.34258800	-0.70453500	0.53518100
C	-0.47327200	0.46320400	0.35722500
C	0.24550700	1.78243100	0.29788300
C	1.68573900	1.83032400	-0.03062200
C	2.43513200	0.70793400	0.09029700
C	-1.89357500	0.60082700	0.95173100
C	-2.34400900	-0.62347700	1.77607400
C	-1.75656800	-1.92842700	1.23709900
C	-0.22137500	-1.90737200	1.31068600
C	0.24698800	-1.91253500	2.78677300
C	-2.97215400	0.97439700	-0.12252700
C	-4.02806600	1.93494300	0.42877100
O	-0.35113100	2.83904400	0.49275000
C	2.28281900	3.16852700	-0.35802400
O	3.77084900	0.80850500	-0.07990300
C	4.57862400	-0.31063800	-0.49366900
O	2.55062600	-1.46142800	1.00516300
C	-2.29374400	1.50804700	-1.39979800
C	-1.15797500	0.57609000	-1.71276700
C	-1.45465900	-0.74161800	-2.09208300
C	-0.54506800	-1.79111900	-2.02542100
C	0.73542000	-1.52890700	-1.52874300
C	-0.98256400	-3.21320500	-2.28905000
H	-1.83286500	1.46295500	1.61940100
H	-2.04720100	-0.49906300	2.82060400
H	-3.43717700	-0.67363200	1.77979400
H	-2.12803000	-2.77991600	1.81610300
H	-2.08276400	-2.08592700	0.20584900
H	0.16651300	-2.82281400	0.85753900
H	2.52049400	3.72084500	0.55765400
H	3.20598200	3.05187400	-0.92456400
H	1.57233200	3.77799500	-0.91750600
H	4.08714300	-0.88128500	-1.28444200
H	5.49173300	0.13645600	-0.88511600
H	4.79985500	-0.96478700	0.34567800
H	-0.29996200	-2.68247600	3.33987200
H	1.31044200	-2.12854000	2.85655200
H	0.06469900	-0.95489100	3.28072300
H	-3.47754200	0.04021500	-0.39999000
H	-3.57157300	2.89115200	0.70044500
H	-4.81091600	2.12881100	-0.31062100
H	-4.51123700	1.52688700	1.32138900
H	-1.93759700	2.52607600	-1.24532800
H	-3.01799600	1.53070300	-2.22265900
H	-0.20346600	0.99285700	-2.02068200
H	-2.50219000	-0.99569000	-2.23918100
H	1.21087600	-0.59171700	-1.78862400
H	1.41696200	-2.35274700	-1.34549800
H	-2.07033500	-3.30257600	-2.32317100
H	-0.59058200	-3.56455000	-3.24926800
H	-0.60437300	-3.89362500	-1.52141500

4x

E(RB3LYP) = -1043.010735 a.u.

C	-0.07438000	-0.36113100	2.29864000
C	-0.12823000	0.37859600	0.88323200

C	0.65940400	-0.39218600	-0.22244200
C	2.12213200	-0.78702000	0.19351900
C	2.40414000	-0.72881100	1.69840900
C	1.18795400	-1.23583500	2.46949800
C	0.84017700	0.45101800	-1.55885700
C	2.28204100	0.11941600	-2.01456300
C	3.07465700	0.02249900	-0.70797000
C	0.43477400	1.80981600	1.06354200
C	0.52298600	2.57800100	-0.23061700
C	0.66494800	1.93580000	-1.39097600
C	-1.61085000	0.56666900	0.50480800
C	-2.25801300	-0.40130500	-0.43084800
C	-1.58835800	-1.48455400	-0.90325500
C	-0.13708300	-1.64052500	-0.64598900
C	4.46579300	-0.59289700	-0.85937100
C	0.43222900	4.07569000	-0.13134900
O	0.39523700	-2.71391900	-0.88209100
C	-2.26982900	-2.58088100	-1.66721500
O	-3.58473600	-0.31615700	-0.67220900
C	-4.24988000	0.95471700	-0.83139000
O	-2.28278900	1.43366200	1.03609100
C	-1.30701300	-1.19504000	2.69053100
H	2.22441000	-1.83426900	-0.10637200
H	3.27200500	-1.35472900	1.92716700
H	2.66978000	0.28398700	2.01948200
H	0.96708200	-2.25451900	2.12857200
H	1.40697900	-1.31386400	3.53920000
H	-0.01320100	0.45633700	3.02414200
H	-2.46769500	-3.43543900	-1.01070100
H	-3.22044100	-2.24000100	-2.07304300
H	-1.62548300	-2.94686000	-2.46810300
H	-3.61751800	1.66392600	-1.36806600
H	-5.13539700	0.73232300	-1.42621200
H	-4.53142600	1.37210900	0.13202600
H	-1.15370900	-1.59976900	3.69508200
H	-2.22486800	-0.60543200	2.71336600
H	-1.45797400	-2.04494600	2.02017600
H	3.18291400	1.03437900	-0.29585600
H	4.40004100	-1.60827100	-1.26441500
H	5.08725500	-0.00082700	-1.53798900
H	4.98874600	-0.64854300	0.09976200
H	2.29953700	-0.84955500	-2.52603400
H	2.67419900	0.86787000	-2.70856400
H	0.13022700	0.11616900	-2.32213200
H	0.70966700	2.50940200	-2.31529800
H	-0.22824200	2.33879100	1.75187300
H	1.41410900	1.77844800	1.54848000
H	0.54580000	4.55505000	-1.10592700
H	-0.53148600	4.37683000	0.29495200
H	1.20738600	4.47049600	0.53606400

TS5

E(RB3LYP) = -1042.936879 a.u.

1 imaginary frequency found: -411.11 cm⁻¹

C	0.12251500	-0.56083700	1.48858800
C	0.94995300	0.02372900	0.35149000
C	0.43152200	1.29376700	-0.08973100
C	-0.97556000	1.58710900	-0.06893200
C	-1.83355700	0.61645300	0.61903800

C	-1.33626300	-0.55307400	1.21009800
C	2.47979100	-0.15690000	0.51457500
C	3.27592400	1.12579700	0.23593000
C	2.73522700	1.84860300	-0.99962700
C	1.30000400	2.33825300	-0.76003000
C	1.29117000	3.65870600	0.05007100
C	2.94222500	-1.33405800	-0.38439900
C	4.16239200	-2.07437200	0.16579300
O	-1.47109400	2.58600400	-0.64674400
O	-3.16178200	0.73996100	0.68227100
C	-3.89138200	1.96081100	0.40741000
C	-2.23972200	-1.39151800	2.07143000
O	0.60074100	-1.07803100	2.47403000
C	1.72064400	-2.23442600	-0.56557900
C	0.51709700	-1.33235000	-0.81735600
C	-0.78329200	-1.88297900	-0.49744200
C	-1.94384200	-1.86555900	-1.38351500
C	-2.90204800	-2.79969200	-1.22258600
C	-2.04354200	-0.83431500	-2.48242100
H	2.63606800	-0.45831600	1.55393900
H	3.22634100	1.79253100	1.10230600
H	4.33279000	0.87318100	0.10518400
H	3.36992800	2.70151400	-1.25776800
H	2.76224200	1.17389900	-1.86265500
H	0.82466200	2.57306500	-1.72076400
H	-1.67872200	-2.20565200	2.52962500
H	-2.68451300	-0.78886200	2.86857900
H	-3.06393700	-1.79863200	1.48069000
H	-3.85424300	2.21227700	-0.64788800
H	-4.90833500	1.72996100	0.72263900
H	-3.49169000	2.78764400	0.99102000
H	1.85538100	4.42461300	-0.49043600
H	0.27085700	4.01381700	0.18391700
H	1.75085400	3.52819700	1.03338200
H	3.20439300	-0.92685200	-1.36949200
H	4.47538600	-2.87671500	-0.50898000
H	5.01531500	-1.40221500	0.29384100
H	3.93881400	-2.52016000	1.14022200
H	1.55254600	-2.82504300	0.34215100
H	1.85290800	-2.94277700	-1.38997100
H	0.56795900	-0.82728400	-1.77829300
H	-0.76861700	-2.72409000	0.18990000
H	-2.83163200	-3.55823700	-0.45124300
H	-3.76818600	-2.83904100	-1.87276800
H	-2.01704800	0.18567200	-2.09152800
H	-1.21421500	-0.92676900	-3.19077300
H	-2.97375900	-0.95809100	-3.03812200

5

E(RB3LYP) = -1042.962829 a.u.

C	-0.94896500	-1.72171200	-0.02407300
C	-1.36220000	-0.55423700	0.97547700
C	0.05347100	-0.19549600	1.51900900
C	0.92926300	-0.07592100	0.25673100
C	0.43327200	-1.31899400	-0.59104400
C	0.47677400	1.22191400	-0.34257300
C	-0.90450000	1.51432500	-0.53149300
C	-1.79012800	0.70959600	0.29598300
C	1.45019900	2.25349200	-0.85386600

C	2.88586900	1.72034600	-0.97148700
C	3.31155400	0.96196200	0.28671900
C	2.44877100	-0.28719300	0.51429300
C	1.56107500	-2.34755600	-0.43452300
C	2.84406800	-1.50466800	-0.36408000
O	-3.03364700	1.03931000	0.55886100
C	-3.61309400	2.35285500	0.29981600
C	-2.32194900	-1.02219700	2.06430400
O	0.37262500	-0.09409500	2.66899900
O	-1.33814200	2.45790500	-1.25557400
C	1.37191400	3.54548300	-0.00281200
C	4.06096100	-2.27218500	0.15202200
C	-2.01354500	-2.14339500	-1.01887400
C	-2.30783600	-1.27234500	-2.21665100
C	-2.66925300	-3.29256900	-0.82971500
H	2.55230700	-0.58688200	1.56295200
H	3.23626000	1.62296500	1.15619800
H	4.36393300	0.66803600	0.22057700
H	3.56440900	2.55785000	-1.15971400
H	2.96224300	1.06145100	-1.84352800
H	1.08010900	2.53235600	-1.84777500
H	-1.87977300	-1.86401000	2.60039800
H	-2.52115300	-0.22782500	2.78373600
H	-3.27014200	-1.34240200	1.63175700
H	-3.42197300	2.65687000	-0.72213800
H	-4.66927900	2.22102400	0.52311800
H	-3.16811800	3.07117200	0.98887000
H	2.01734300	4.31446100	-0.43719300
H	0.34852500	3.92068600	0.00419200
H	1.69171800	3.37091300	1.02749700
H	3.06602300	-1.14317700	-1.37666400
H	4.29898100	-3.11792900	-0.49973900
H	4.94922900	-1.63618500	0.20067400
H	3.87524800	-2.66432500	1.15745400
H	1.43934000	-2.90289700	0.50422100
H	1.57667900	-3.08075700	-1.24524300
H	0.35851000	-1.01528000	-1.63565100
H	-0.79081100	-2.57372500	0.64384300
H	-2.45856400	-3.93763100	0.01658600
H	-3.43686800	-3.62711000	-1.51933600
H	-2.57609300	-0.25015000	-1.93747700
H	-1.43832200	-1.19115800	-2.87648300
H	-3.13078000	-1.69033700	-2.79839900

TS4n-B

E(RB3LYP) = -1367.636773 a.u.

1 imaginary frequency found: -116.15 cm⁻¹

C	-1.92701500	-0.45444300	1.34582700
C	-1.46106000	0.06060300	-0.18224600
C	-2.75870600	0.85126600	-0.61231100
C	-3.92036900	0.39948400	0.33633700
C	-3.39653300	-0.78844900	1.15346600
C	-2.61607000	2.38703300	-0.63895400
C	-1.51576400	2.89221500	0.29514500
C	-0.15149600	2.33160900	-0.13283300
C	-0.15861300	0.80328100	-0.14552500
C	-1.36540900	-1.25492500	-0.96413400
C	-0.08001200	-1.98470300	-0.98196400
C	1.07194800	-1.28979700	-0.78909700

C	1.05500300	0.14455600	-0.45758800
C	0.25395400	2.89310400	-1.52100000
O	2.15998700	0.81250500	-0.64266000
B	3.36539400	1.10554400	0.23575400
F	4.39596900	1.42535000	-0.63440100
O	2.26663500	-1.92477900	-0.86364900
C	3.13044600	-1.65834500	-1.99534900
C	-0.10879500	-3.42475800	-1.39652400
O	-2.33736600	-1.73422700	-1.52308500
C	-5.22779300	0.12837400	-0.40711700
C	-1.01212600	-1.45268500	1.91083900
C	0.27407500	-1.11006300	2.23044800
C	1.31724200	-2.12855900	2.61979900
F	3.66461200	-0.01596100	1.01468800
F	3.03953800	2.18530700	1.07011000
C	0.65993400	0.23442700	2.01049200
H	-2.99764100	0.50426900	-1.61745200
H	-2.40381500	2.72673900	-1.65491100
H	-3.57676400	2.83428100	-0.36925400
H	-1.46862700	3.98415900	0.27027800
H	-1.74069400	2.62348300	1.33346100
H	0.61698200	2.65975700	0.57033600
H	-0.43290800	-3.51238400	-2.43745100
H	0.87367100	-3.87927100	-1.29134500
H	-0.83346300	-3.98053800	-0.79681500
H	3.53882400	-0.65141000	-1.95101300
H	3.93131400	-2.39091900	-1.92171900
H	2.57918200	-1.80813600	-2.92705100
H	0.11228600	3.97722500	-1.52071600
H	1.29797000	2.68256900	-1.73784300
H	-0.35176400	2.47519900	-2.32751300
H	-4.09502000	1.21885800	1.04462000
H	-6.02467600	-0.15024900	0.28858500
H	-5.56218200	1.01362700	-0.95620100
H	-5.09828700	-0.68689000	-1.12417200
H	-3.52519200	-1.73140400	0.61737700
H	-3.90397700	-0.87995700	2.11747800
H	-1.86768400	0.47255500	1.91884900
H	-1.33043700	-2.48959000	1.96884300
H	-0.03187200	1.04025600	2.20939900
H	1.70268800	0.51362400	2.06990700
H	0.89373300	-3.13345200	2.65060000
H	2.14484600	-2.11636300	1.90621800
H	1.73436100	-1.89936100	3.60406100

4n-B

E(RB3LYP) = -1367.660090 a.u.

C	-0.26398600	-2.07980200	-0.24495900
C	-0.05538200	-0.60841700	0.24406600
C	1.42376700	-0.10381900	-0.03326500
C	2.50376500	-1.09278600	-0.64471000
C	2.19499100	-2.61096700	-0.55175500
C	0.91175700	-2.95690000	0.20508800
C	2.12516200	0.24529600	1.35683100
C	3.58293700	0.47774200	0.99412900
C	3.86680900	-0.71656600	0.05662200
C	-0.37128300	-0.49724400	1.82015000
C	0.05723300	0.81898600	2.42799800
C	1.32034300	1.19105500	2.18654800

C	-1.16329600	0.27702400	-0.29529200
C	-0.93379900	1.67943100	-0.64235600
C	0.32676200	2.13896300	-0.84124600
C	1.45815700	1.17312300	-0.87188500
C	5.01937800	-0.49615000	-0.92317200
C	-0.94443700	1.61875500	3.21018600
O	2.41711700	1.46320300	-1.56846900
C	0.62462900	3.56081800	-1.18252900
O	-1.97983800	2.53911100	-0.66650400
C	-3.06026300	2.34942400	-1.61624600
O	-2.36863900	-0.07023700	-0.32613200
B	-3.50739400	-1.19074900	0.01216800
F	-3.19226500	-1.76654700	1.22210300
C	-0.46647400	-2.17605800	-1.76961200
F	-3.48876000	-2.06945600	-1.03890200
F	-4.64047800	-0.41917800	0.06320500
H	2.59901500	-0.83864000	-1.69918700
H	2.12134000	-3.01699300	-1.56352300
H	3.03734300	-3.12890500	-0.08588400
H	0.65344000	-4.00534600	0.02724100
H	1.06394000	-2.86583400	1.28473700
H	-1.16519400	-2.45341900	0.24137500
H	-0.28770700	4.13340000	-1.32799000
H	1.20249100	4.01837000	-0.37157700
H	1.25112800	3.60397900	-2.07482100
H	-3.80876400	1.66988500	-1.21640400
H	-3.48672300	3.33999900	-1.76478300
H	-2.67271200	1.97317600	-2.56516100
H	-0.51055700	-3.22764500	-2.06579700
H	-1.40241800	-1.71784000	-2.08307400
H	0.34903900	-1.71079900	-2.32809500
H	4.13442300	-1.56011800	0.70270300
H	5.94533500	-0.26127000	-0.38882900
H	5.20388200	-1.39149300	-1.52505200
H	4.79352900	0.33049200	-1.60029800
H	3.73730200	1.43387700	0.48859500
H	4.22578900	0.46190100	1.87810500
H	2.11315900	-0.72166100	1.87711300
H	1.73729100	2.12645700	2.54701900
H	0.17762200	-1.31820700	2.29138400
H	-1.42592100	-0.69933900	1.98549800
H	-0.49926600	2.53218100	3.60962000
H	-1.79886900	1.89900500	2.58330100
H	-1.34718200	1.03710200	4.04658600

TS4x-B

E(RB3LYP) = -1367.625418 a.u.

1 imaginary frequency found: -48.04 cm⁻¹

C	1.86943900	0.14676700	1.41248900
C	1.36962300	0.34397400	-0.21161900
C	2.63069900	-0.17852100	-1.00149500
C	3.76982600	-0.42736100	0.02940700
C	3.37850300	0.34334300	1.29374800
C	0.04548500	-0.26649000	-0.52936600
C	-0.02951400	-1.61670300	-1.23610400
C	1.33060700	-2.32884800	-1.28229700
C	2.39166000	-1.41370600	-1.88475800
C	-1.14274200	0.46344700	-0.35668600
C	-1.09901700	1.89362400	0.05368300

C	0.07319000	2.57885700	0.10147800
C	1.31793900	1.89365500	-0.27360900
C	-0.59501800	-1.45024100	-2.67361800
O	2.31174100	2.53726500	-0.56611900
C	0.15698800	4.04188700	0.42626000
O	-2.22692800	2.51517200	0.45042200
C	-3.43282200	2.54170000	-0.35736800
O	-2.31455200	0.02743200	-0.75733000
B	-3.33020000	-0.94166800	-0.19831600
F	-2.72602800	-2.16540700	0.14145400
C	5.15727300	-0.07705400	-0.50809000
C	1.48392800	-1.14965500	1.97781900
C	0.17664200	-1.52117000	2.16813800
C	-0.22509900	-2.92809100	2.54507000
F	-3.88562600	-0.37615400	0.96276400
F	-4.27898500	-1.10800700	-1.19249800
C	-0.81799200	-0.55990700	1.91050200
H	2.94312300	0.65183400	-1.63448700
H	2.08633100	-1.11016500	-2.88903500
H	3.33843800	-1.94824300	-2.00651100
H	1.22323200	-3.24195700	-1.87400600
H	1.63227600	-2.64901000	-0.28078600
H	-0.74005000	-2.23979600	-0.69373100
H	0.71269000	4.56775900	-0.35274600
H	-0.83541400	4.47576200	0.52504400
H	0.70033600	4.20067700	1.36354900
H	-4.11039400	1.75554000	-0.03721600
H	-3.87294100	3.52180100	-0.17521400
H	-3.19630200	2.43227600	-1.41463600
H	-0.54496100	-2.41620600	-3.18340400
H	-1.63167200	-1.12415500	-2.65917300
H	-0.02035200	-0.73027500	-3.26010500
H	3.76246300	-1.49769600	0.27537200
H	5.21918000	0.98792200	-0.75072000
H	5.93290300	-0.30336200	0.22910700
H	5.38817200	-0.64370300	-1.41470500
H	3.61689000	1.40225600	1.18324600
H	3.89525100	-0.02178800	2.18508500
H	1.36575800	0.95782400	1.94882800
H	2.26787500	-1.88294200	2.14329600
H	-0.60615500	0.48521400	2.08084200
H	-1.86289500	-0.83787500	1.90911200
H	0.62091100	-3.61426800	2.49182800
H	-0.62477400	-2.95483700	3.56259600
H	-1.01282700	-3.28413100	1.87737000

4x-B

E(RB3LYP) = -1367.682631 a.u.

C	-1.05832800	-0.07691800	0.22617700
C	0.33510000	0.20715600	0.78056700
C	1.44004400	-0.32568400	-0.19438800
C	1.10945000	-1.75275300	-0.62633700
C	-0.30307100	-2.05116600	-1.02556100
C	-1.32224800	-1.26424700	-0.59305100
C	1.50299400	0.49476100	-1.56298200
C	3.02142000	0.64593200	-1.82642400
C	3.63179600	0.83309300	-0.43427200
C	2.89297300	-0.23883700	0.39005100
C	0.44326200	-0.43937400	2.24530900

C	1.86755000	-0.93544400	2.56691300
C	2.97046200	-0.10492800	1.91580000
C	0.45330300	1.74576400	0.91559200
C	0.38052400	2.44664500	-0.41887900
C	0.82311900	1.83518600	-1.51926700
C	5.15488000	0.71235000	-0.39152700
C	-0.23251900	3.81839700	-0.42882400
C	-0.56595200	-1.54482000	2.59422600
O	1.93507800	-2.64012100	-0.73260900
C	-0.52649700	-3.26858200	-1.86057900
O	-2.61037400	-1.51864900	-0.93787700
C	-3.33726600	-2.43245800	-0.08397900
O	-1.96755200	0.71469300	0.55341200
B	-3.45273700	1.17652900	0.02697300
F	-3.38383500	1.20938800	-1.33912100
F	-4.35828600	0.28940200	0.55052900
F	-3.54544100	2.42891600	0.59208300
H	3.35443900	-1.19753700	0.13493000
H	3.94736900	-0.45746300	2.25792400
H	2.89923100	0.94063400	2.23299500
H	1.97271900	-1.97663200	2.23932300
H	1.97879800	-0.94553900	3.65537300
H	0.22446000	0.39956500	2.91224400
H	-0.37004000	-4.17081700	-1.26045000
H	-1.53358300	-3.28532200	-2.27146500
H	0.20671900	-3.30761100	-2.66887900
H	-3.48171900	-2.00012300	0.90570100
H	-4.30447600	-2.57056800	-0.56093500
H	-2.81572200	-3.38975500	-0.01510000
H	-0.41314700	-1.83964000	3.63564800
H	-1.60278300	-1.21325600	2.50549600
H	-0.43133700	-2.44099300	1.98326600
H	3.34972500	1.82704000	-0.06407100
H	5.47806100	-0.27171600	-0.74711400
H	5.62625300	1.46969800	-1.02458100
H	5.54010600	0.84584300	0.62323500
H	3.41646400	-0.27031200	-2.27971500
H	3.23208100	1.47136900	-2.51068800
H	1.04960900	-0.07924800	-2.37848100
H	0.74062600	2.33768000	-2.48053000
H	-0.35303800	2.09943600	1.55952900
H	1.38342100	1.99928600	1.42893300
H	-0.21704300	4.26098900	-1.42659900
H	-1.27034100	3.77200900	-0.08118000
H	0.30171600	4.48918700	0.25410400

TS5-B

E(RB3LYP) = -1367.639506 a.u.

1 imaginary frequency found: -361.18 cm⁻¹

C	-1.09962500	-0.35265600	-0.65394800
C	0.12760000	-1.00187800	-0.41937700
C	1.35098100	-0.26253000	-0.49861500
C	1.30691000	0.97415000	-1.37895600
C	0.03738400	1.72626000	-1.36955600
C	-1.13267300	1.01884300	-1.11233500
C	2.71243200	-0.97512700	-0.45563500
C	2.59378700	-2.50255700	-0.55550200
C	1.47557700	-3.01969900	0.34639700
C	0.10645200	-2.49299600	-0.10401100

C	-0.41049700	-3.28305200	-1.33187700
C	3.50041200	-0.54262300	0.81417500
C	5.01715200	-0.63071000	0.63740800
O	2.27395000	1.35146800	-2.01288300
C	-0.02041200	3.08805800	-1.98462900
O	-2.25435400	1.72626700	-1.28754500
C	-3.57158800	1.17759900	-1.55280100
O	-2.26404700	-0.94948300	-0.50283300
B	-2.88723400	-1.54468400	0.74191900
F	-3.04518600	-2.91715800	0.56027800
F	-4.13267400	-0.92794400	0.90026900
F	-2.06519400	-1.27339600	1.84982000
C	3.03369500	0.86563600	1.17108900
C	1.52147900	0.91747000	1.13750200
C	0.90802700	2.18139600	0.90360800
C	-0.25304200	2.71333700	1.58509700
C	-0.48957200	4.04025600	1.47617200
C	-1.10960700	1.82655900	2.45346200
H	3.26826900	-0.59627900	-1.31678700
H	2.40323900	-2.79479700	-1.59224400
H	3.55077800	-2.95480500	-0.28173300
H	1.45024700	-4.11270400	0.34204900
H	1.66515100	-2.72238800	1.38299000
H	-0.60321500	-2.65958800	0.70512300
H	-0.56699600	3.77824500	-1.33481600
H	0.98345100	3.46944100	-2.16485900
H	-0.56346000	3.05988200	-2.93417300
H	-4.01053100	0.75377200	-0.65508700
H	-4.14326200	2.03703000	-1.89843200
H	-3.52028200	0.42345200	-2.33635900
H	-0.47948900	-4.34249300	-1.07196700
H	-1.40188200	-2.94745800	-1.62985500
H	0.26333800	-3.18383000	-2.18649900
H	3.20940400	-1.20899700	1.63493100
H	5.53326400	-0.35378900	1.56084400
H	5.33405700	-1.64333000	0.37583500
H	5.35584000	0.04378500	-0.15527300
H	3.44419900	1.59465100	0.46484100
H	3.38202200	1.15560100	2.16865100
H	1.02286400	0.27019500	1.85139700
H	1.52035400	2.92030400	0.39582000
H	0.14998500	4.68379900	0.88357300
H	-1.31354300	4.51068000	1.99937200
H	-0.54013500	1.46734300	3.31694600
H	-1.97280100	2.37824000	2.82650400
H	-1.47083000	0.94351000	1.92637900

5-B

E(RB3LYP) = -1367.680857 a.u.

C	-0.43823000	-2.56194800	0.21196300
C	-0.23840500	-1.07153600	0.33516700
C	-1.39708100	-0.11897900	0.35290500
C	-2.84068000	-0.69077500	0.29165700
C	-2.93422100	-2.20714900	0.50267400
C	-1.84366400	-2.94483700	-0.27347800
C	-1.26644400	0.92700700	-0.84058100
C	-2.70960300	1.13868800	-1.31420000
C	-3.40942500	-0.20635900	-1.06963600
C	-0.55148100	2.16998700	-0.26240100

C	0.07738100	1.69059000	1.12135500
C	-1.10471200	0.78495300	1.56939700
C	1.05792200	-0.58308700	0.47873700
C	1.24020700	0.75292500	0.95048800
C	-4.93496600	-0.12214200	-1.10688700
C	0.37425300	2.94009700	-1.18503900
C	1.34900400	2.19473400	-2.06095100
C	0.35712500	2.83859000	2.08391000
O	-1.69861900	0.84980100	2.60251800
O	2.12102300	-1.39285000	0.33896700
B	2.72858200	-1.58139000	-1.01445300
F	1.72409400	-1.82115900	-1.97126000
O	2.35757100	1.26182100	1.37097300
C	3.64195700	0.57589000	1.53974900
C	-0.09200200	-3.23722000	1.56739900
C	0.28917600	4.27350900	-1.22042000
F	3.60636500	-2.65449900	-0.92000200
F	3.42587700	-0.40240700	-1.38189400
H	-3.40902900	-0.19435100	1.08519900
H	-2.85440000	-2.43981400	1.56913500
H	-3.92385800	-2.55335400	0.19164500
H	-1.96371500	-4.02641600	-0.16907100
H	-1.93160300	-2.72769400	-1.34259000
H	0.29874600	-2.91087500	-0.51297200
H	1.10471600	3.51534700	1.67138000
H	-0.56365500	3.39885500	2.25294900
H	0.71623800	2.46991200	3.04519200
H	4.04417800	0.32840300	0.56333600
H	4.25119800	1.31360900	2.05434900
H	3.50439100	-0.31459100	2.14490500
H	-0.20291100	-4.31898600	1.46078600
H	0.93762600	-3.02302200	1.85124800
H	-0.75387700	-2.90275300	2.36887900
H	-3.08124700	-0.90398200	-1.84981900
H	-5.28230400	0.22503100	-2.08399000
H	-5.39784200	-1.09501600	-0.92119200
H	-5.30500100	0.57688600	-0.34966700
H	-3.19498000	1.91772700	-0.71433800
H	-2.75548100	1.45533900	-2.35875500
H	-0.67693700	0.46753400	-1.63332000
H	-1.32667400	2.87032300	0.06196800
H	-0.42472700	4.81814000	-0.61192300
H	0.93160500	4.86272400	-1.86568300
H	2.00456800	1.52184800	-1.50335900
H	0.82860800	1.57349700	-2.79681300
H	1.97996400	2.89741700	-2.60731300