

Supporting Information
for New Journal of Chemistry

**Mechanism and Diastereoselectivity in Formation of
Trifluoromethyl-Containing Spiro[pyrrolidin-3,2'-oxindole] by a
Catalyst-free and Mutually Activated [3+2]-Cycloaddition Reaction:
A Theoretical Study**

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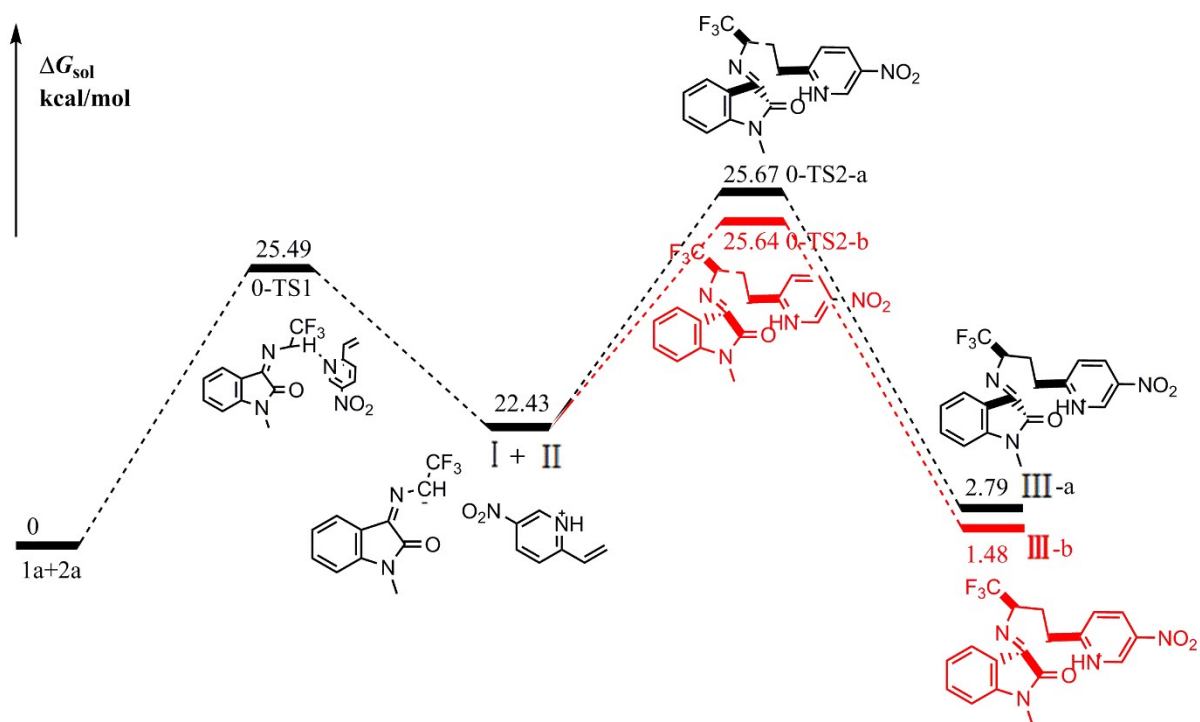


Fig. S1 The mechanism and the free-energy profiles of path 0.

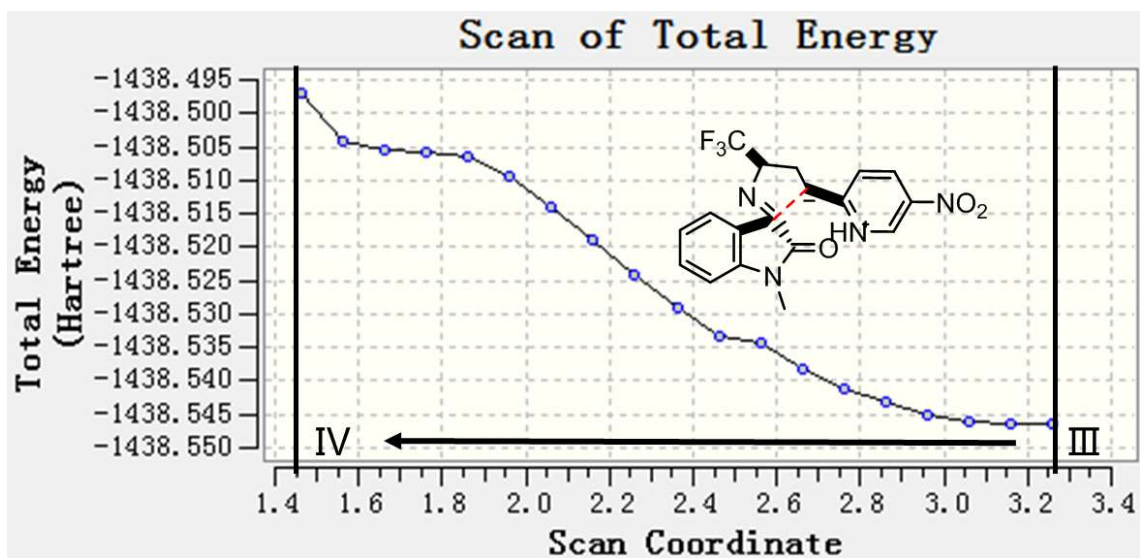


Fig. S2 The relaxed scan analysis from III to IV (The value of abscissa is the length of the red dotted line in the figure).

Cartesian coordinates (Å) for all ground state and transition state geometries as well as the other data

Reaction mechanism

Path 0

1a

0 1

C	1.05097700	0.65136400	-0.00001000
C	2.34515100	0.09165500	0.00000100
C	3.48586500	0.87689100	0.00001200
C	3.31043400	2.26415600	0.00001400
C	2.04080400	2.83900500	-0.00000100
C	0.89772100	2.03473700	-0.00001500
C	0.11605000	-0.48599400	-0.00000100
H	4.47597400	0.43406200	0.00002100
H	4.18710000	2.90431700	0.00002600
H	1.93619500	3.91830000	-0.00000100
H	-0.08324800	2.49508200	-0.00003100
N	2.28750300	-1.30617100	0.00000300
O	0.61323200	-2.89851000	0.00000600
C	0.98888600	-1.74547100	0.00000600
N	-1.14620800	-0.61259200	-0.00000200
C	-1.96007600	0.58298700	-0.00004000
H	-1.78681100	1.19951300	-0.89055800
H	-1.78680700	1.19958700	0.89042700
C	-3.40973500	0.17029800	-0.00000200
F	-3.72054600	-0.56505400	-1.07843200
F	-4.21420300	1.24423900	-0.00019300
F	-3.72057500	-0.56469000	1.07867200
C	3.44521800	-2.17340600	-0.00001300
H	4.05288200	-1.99814200	0.89216000
H	3.08714300	-3.20287100	0.00004200
H	4.05280500	-1.99821600	-0.89225400

2a

0 1

C	-1.65113000	0.26044200	0.00001600
C	-0.86904800	1.42432400	-0.00003400
C	0.51148300	1.31610000	-0.00005300
C	1.04342400	0.03467800	-0.00002400
C	0.21214700	-1.08330800	0.00002200
N	-1.10864500	-0.97136400	0.00004200
H	1.15739000	2.18639400	-0.00008900
H	-1.34801500	2.39719100	-0.00005500
H	0.63761300	-2.08219100	0.00004400

N	2.48898700	-0.15334000	-0.00004100
O	2.91559200	-1.29628200	-0.00002400
O	3.19343000	0.84183600	-0.00006900
C	-3.12023600	0.37095600	0.00004500
H	-3.51531000	1.38371200	0.00000800
C	-3.94170400	-0.67945300	0.00011700
H	-3.55763000	-1.69506200	0.00015700
H	-5.01823100	-0.54398100	0.00013800

3aa

O 1

C	1.81823000	2.49590600	0.31001400
C	0.85997900	1.49384700	0.51112400
C	-0.27608300	1.77031100	1.25406100
C	-0.45021700	3.06059700	1.77073300
C	0.50597300	4.04745600	1.54462300
C	1.66537700	3.78001600	0.80939000
C	2.71639800	0.66806000	-0.72050800
H	-1.02063000	1.00223500	1.44345400
H	-1.33692000	3.29080900	2.35168600
H	0.35661300	5.04294500	1.95100000
H	2.41777200	4.54411600	0.64453900
N	2.89681000	1.99045300	-0.42647100
C	4.06444400	2.75608700	-0.80516400
H	3.77531100	3.61063700	-1.42306500
H	4.58976500	3.11523900	0.08426400
H	4.72022000	2.09890800	-1.37617000
O	3.49035400	-0.03415100	-1.34698700
C	0.50582100	-0.36152300	-1.35039800
C	0.96981500	-1.83339300	-1.39689900
C	1.75782500	-2.05135600	-0.07982500
C	1.39144200	-3.31743400	0.64970700
F	2.19175100	-3.52773100	1.70810000
F	0.13164000	-3.30492500	1.11592600
F	1.50604800	-4.38476200	-0.15626600
C	1.34548700	0.22912000	-0.15365700
N	1.53897300	-0.88357700	0.78184700
C	-0.96601500	-0.21827300	-1.06928200
C	-1.72058300	0.78555300	-1.68751100
C	-2.76787300	-0.92717700	0.16993300
C	-3.05720800	0.92700400	-1.35428200
H	-1.25753500	1.44312100	-2.41499700
C	-3.57006400	0.04893600	-0.40838900
H	-3.17356200	-1.61145000	0.90822700
H	-3.68646600	1.68673800	-1.80330700

N	-1.48487400	-1.05507400	-0.15818100
N	-4.97281900	0.14708800	-0.01569600
O	-5.65009700	1.01408700	-0.54026500
O	-5.38900900	-0.64213100	0.81527500
H	0.11005400	-2.50398200	-1.46306100
H	0.74279000	0.17466700	-2.27251900
H	2.82395300	-2.13439400	-0.30251200
H	1.61743500	-2.01165600	-2.25521100
H	0.64316100	-1.00826300	1.26113400

3ab

0 1

C	2.77489300	-1.85400000	-0.29213300
C	2.55226000	-0.59341100	0.27825300
C	3.53034700	-0.02331700	1.07667300
C	4.73805300	-0.70830200	1.26490700
C	4.94616200	-1.95112800	0.67316400
C	3.95934600	-2.55157100	-0.11549900
C	0.66527600	-1.31376400	-0.97906500
H	3.37634400	0.93596600	1.56208400
H	5.51354700	-0.26613600	1.88141600
H	5.88643900	-2.47041500	0.83014700
H	4.11365700	-3.52524500	-0.56868200
N	1.64723300	-2.26179200	-1.01705400
C	1.56094400	-3.49004100	-1.77690300
H	2.32038400	-3.50616300	-2.56402500
H	1.70400800	-4.35204200	-1.11970500
H	0.56892500	-3.53425300	-2.22612900
O	-0.39424400	-1.35223200	-1.57671800
C	0.27858400	0.14542600	1.18938500
C	0.52652800	1.65534500	1.41124300
C	1.19849300	2.14815500	0.10366300
C	0.61119000	3.42847500	-0.43437700
F	1.29022100	3.87485500	-1.50293600
F	-0.66800500	3.28931200	-0.81679200
F	0.64566200	4.39682000	0.49487000
C	1.15097000	-0.15066600	-0.08891500
N	1.09499700	1.07651600	-0.88871800
C	-1.17412400	-0.17606200	0.94263100
C	-1.73924000	-1.35000200	1.45285900
C	-3.12964300	0.41427900	-0.10429400
C	-3.06208200	-1.64159700	1.16571700
H	-1.14369200	-2.01907300	2.06429500
C	-3.75052400	-0.73524700	0.37077300
H	-3.67428100	1.12069100	-0.72292600

H	-3.54981500	-2.53448200	1.53924300
N	-1.86221600	0.68827000	0.18466200
N	-5.14879400	-0.98232900	0.03433500
O	-5.67234800	-1.98871000	0.48070000
O	-5.71759800	-0.16831100	-0.67371200
H	-0.41638400	2.17569700	1.59200000
H	0.63407200	-0.45645100	2.02764100
H	2.25565200	2.36939900	0.28101000
H	1.18196200	1.82515100	2.26683800
H	0.14867200	1.10241300	-1.28270600

0-ts1

0 1

C	-1.32005700	2.06397900	-0.93434400
C	0.05214000	2.15225000	-0.62630500
C	0.55929600	3.30514000	-0.04122900
C	-0.31408700	4.36644300	0.21752400
C	-1.67002300	4.26540400	-0.09930200
C	-2.19853000	3.10654500	-0.68005400
C	-0.45169300	0.04083000	-1.55884100
H	1.61459900	3.37200700	0.20791300
H	0.06542600	5.27716300	0.66935800
H	-2.33223300	5.09976800	0.10950100
H	-3.25423300	3.02766000	-0.91904100
N	-1.59588000	0.80710000	-1.48350700
C	-2.90953100	0.33019500	-1.85375500
H	-3.58103900	0.34282200	-0.98898100
H	-3.33762700	0.94774900	-2.64844600
H	-2.79914900	-0.69463700	-2.21172000
O	-0.40005700	-1.10774600	-1.99276300
C	1.19871500	0.46586800	2.32692500
C	1.06381400	1.66785100	2.89313000
C	2.26566100	-0.81796700	-0.75020300
H	1.94197200	2.22312600	3.20594900
C	3.71160100	-0.98907600	-0.46953300
F	4.03252300	-2.29388100	-0.35965100
F	4.53795800	-0.48448800	-1.42064700
F	4.09231900	-0.39072800	0.68091700
C	0.64837900	0.86500500	-0.97275900
N	1.84470900	0.47591500	-0.65450500
C	0.07135100	-0.33926000	1.85027100
C	-1.27439600	-0.07546000	2.14252800
C	-0.54540300	-2.19954700	0.54303600
C	-2.26107300	-0.88754300	1.61767700
H	-1.53799000	0.76582400	2.77078500

C	-1.87454300	-1.96738500	0.82644400
H	-0.21343900	-2.98049200	-0.13032000
H	-3.31108800	-0.69830900	1.80881800
N	0.38312200	-1.39493100	1.06375700
N	-2.88199300	-2.81805500	0.20402200
O	-4.05029200	-2.51528600	0.36687000
O	-2.49348900	-3.76971600	-0.44891800
H	0.09983300	2.14027800	3.05689700
H	2.18441400	0.04475900	2.15147900
H	1.87996200	-1.48114200	-1.52492200
H	1.40667000	-1.33255400	0.44002800

Compound I + II

0 1

C	-1.67286500	1.68050500	-0.95276700
C	-0.30762600	1.97758800	-0.69822700
C	0.02268800	3.22471200	-0.16261100
C	-0.99593500	4.14524300	0.09660000
C	-2.33356200	3.83618900	-0.17124800
C	-2.68995800	2.59195200	-0.70251100
C	-0.48955000	-0.20088100	-1.50464400
H	1.06081000	3.47158100	0.04441200
H	-0.74474700	5.11742800	0.51073500
H	-3.10786900	4.56904300	0.03355300
H	-3.72712500	2.34410000	-0.90917700
N	-1.75909200	0.38347800	-1.43733300
C	-2.97562200	-0.29283600	-1.81749200
H	-3.68581100	-0.32572400	-0.98429800
H	-3.45521700	0.20430100	-2.66706700
H	-2.70594200	-1.31082900	-2.10677600
O	-0.29569400	-1.37959100	-1.85141800
C	1.40142600	0.74785400	2.22847100
C	1.23227900	1.96983000	2.74158000
C	2.39820200	-0.46394200	-1.06327300
H	2.09675700	2.57523600	2.99273400
C	3.80109900	-0.57845300	-0.58973000
F	3.88155200	-1.34765100	0.53918200
F	4.60289500	-1.18877900	-1.48460800
F	4.36535000	0.59364800	-0.27680300
C	0.44764400	0.80357600	-1.04516100
N	1.77071400	0.63835200	-0.81702000
C	0.29571500	-0.11818200	1.83802700
C	-1.06566000	0.19682700	1.93994100
C	-0.25250500	-2.22489100	0.86026500
C	-2.01502900	-0.69922100	1.49195000

H	-1.36943500	1.15268300	2.34740100
C	-1.58887400	-1.91185300	0.94741900
H	0.13118900	-3.14278400	0.43654600
H	-3.07365000	-0.46816600	1.54406600
N	0.62716000	-1.33263600	1.33022200
N	-2.55236200	-2.85369000	0.39663200
O	-3.73269500	-2.56790200	0.49072400
O	-2.11875200	-3.86368300	-0.12676400
H	0.25522500	2.40424300	2.92856600
H	2.39974500	0.35655500	2.04973300
H	1.95931300	-1.35960200	-1.49951400
H	1.61957500	-1.56623900	1.25174200

0-TS2-a

0 1

C	1.16014500	1.34865000	0.96958100
C	0.04240400	0.49319800	1.16937300
C	0.20757100	-0.63603800	1.97519200
C	1.46174300	-0.90488500	2.53387400
C	2.54695900	-0.05813200	2.30486300
C	2.40578800	1.09348500	1.52332900
C	-0.55774900	2.35211800	-0.16096600
H	-0.61854200	-1.30811700	2.18011300
H	1.59005900	-1.78769700	3.15256200
H	3.51489000	-0.29085900	2.73911500
H	3.24455400	1.75926400	1.34399200
N	0.79316100	2.41588700	0.16399700
C	1.68308400	3.45857200	-0.28543400
H	2.52675100	3.03167300	-0.83770200
H	1.11153800	4.11410300	-0.94341200
H	2.06897700	4.03925300	0.55843400
O	-1.13989500	3.18169900	-0.84917700
C	-1.21646600	-0.54045200	-2.09908100
C	-2.26055000	-1.31297100	-1.67801000
C	-2.80637500	-0.42559200	0.49925300
C	-4.28198500	-0.61186000	0.40048000
F	-4.92623000	-0.34308800	1.56047300
F	-4.84771300	0.17113700	-0.53103200
F	-4.59475700	-1.88880400	0.09688400
C	-1.06629200	1.09802500	0.44456800
N	-2.34100000	0.77899500	0.27925100
C	0.14250200	-0.71465300	-1.72616500
C	1.16474300	0.19482100	-2.10293800
C	1.77596400	-1.98431700	-0.50708700
C	2.44503600	0.03645600	-1.64936300

H	0.89073200	1.04270300	-2.72038300
C	2.74552100	-1.07787100	-0.83383300
H	1.94877300	-2.85441500	0.11311700
H	3.22660000	0.74494300	-1.89863900
N	0.52855400	-1.78410700	-0.96444300
N	4.06359300	-1.23813700	-0.26404200
O	4.87720100	-0.35268800	-0.47281500
O	4.28930500	-2.23940000	0.39846900
H	-3.25306000	-1.10342400	-2.06110100
H	-1.41417800	0.36146900	-2.66939600
H	-2.28415800	-1.22913800	1.01638300
H	-2.13780300	-2.28358700	-1.20646100
H	-0.17211900	-2.46605100	-0.68452000

0-TS2-b

0 1

C	0.99374900	1.97967200	0.61695600
C	-0.32019300	2.07980600	0.10694700
C	-0.67979900	3.19594600	-0.64742400
C	0.26903000	4.19474000	-0.86802600
C	1.56279600	4.08371400	-0.34612700
C	1.94536000	2.97049200	0.40688200
C	-0.06946700	0.06126300	1.27331400
H	-1.68496900	3.28096900	-1.05071200
H	0.00096200	5.07026800	-1.45110500
H	2.28465100	4.87398700	-0.52707000
H	2.94762200	2.88354200	0.81532100
N	1.12278000	0.77857100	1.30778000
C	2.28689800	0.39389200	2.07051400
H	2.38509000	1.00496900	2.97405500
H	2.17728600	-0.65434700	2.35526400
H	3.19274600	0.51764400	1.46776100
O	-0.22404400	-1.04749600	1.79627700
C	-1.04292000	-0.93834900	-1.90977000
C	-2.11353200	-1.68106600	-1.52192700
C	-2.85518600	-0.52216200	0.54137200
C	-4.32339000	-0.64677900	0.31727500
F	-5.05801300	-0.23230600	1.37563900
F	-4.75584800	0.06312300	-0.73690300
F	-4.67500000	-1.93216800	0.10750900
C	-1.02044800	0.87608500	0.50020600
N	-2.31179100	0.63523700	0.27367600
C	0.30051100	-1.08928100	-1.45609200
C	1.33738400	-0.20631100	-1.85492500
C	1.88931600	-2.30642000	-0.14245800

C	2.61268900	-0.36089400	-1.38451400
H	1.08185700	0.61357300	-2.51606200
C	2.88185400	-1.43858500	-0.51382300
H	2.03803300	-3.13712400	0.53548500
H	3.40686900	0.32268700	-1.66170400
N	0.65584500	-2.11903800	-0.63066500
N	4.20161500	-1.61634700	0.05293400
O	5.05274600	-0.79027600	-0.23568000
O	4.38776600	-2.56975800	0.79230400
H	-3.07757100	-1.49409700	-1.98191800
H	-1.19725300	-0.08057800	-2.55714000
H	-2.39231600	-1.30539100	1.13701300
H	-2.03638600	-2.59619200	-0.94166700
H	-0.06567500	-2.75106200	-0.29329600

III-a

0 1

C	1.42780800	2.61685300	-0.38820700
C	1.07118000	1.26055500	-0.53197900
C	-0.13522700	0.93992700	-1.15032900
C	-0.96566100	1.96681500	-1.60227100
C	-0.59467800	3.30091100	-1.43872500
C	0.61290900	3.64821300	-0.82983200
C	3.20307700	1.52536000	0.54051300
H	-0.44687300	-0.08812500	-1.28819900
H	-1.90686600	1.72116900	-2.08244700
H	-1.25395800	4.08798400	-1.79137500
H	0.90311000	4.68606800	-0.70666800
N	2.67060700	2.75044500	0.23980400
C	3.32265000	4.01252100	0.51271600
H	2.69979700	4.63183300	1.16377900
H	4.26645800	3.79418200	1.01242300
H	3.51881000	4.55135300	-0.41854900
O	4.26766000	1.31213300	1.08110800
C	-0.11751300	-1.12160200	1.72983700
C	0.74077200	-2.21792700	1.17516700
C	1.52019600	-1.78304200	-0.08996400
C	2.33750300	-2.94937000	-0.61240200
F	3.09295700	-2.59236800	-1.66192100
F	3.16333800	-3.44967400	0.31793800
F	1.53827700	-3.95021100	-1.01731100
C	2.18122800	0.48279900	0.06367400
N	2.45671500	-0.74025300	0.26165200
C	-1.36123300	-0.82132000	1.30267500
C	-2.15424500	0.29061200	1.81533400

C	-3.21850500	-1.29888600	-0.19662800
C	-3.38644000	0.56995700	1.34744200
H	-1.70273100	0.89382700	2.59540500
C	-3.94633500	-0.25811100	0.30983200
H	-3.59071000	-1.94427900	-0.98276800
H	-3.96716300	1.40059200	1.72984800
N	-1.99176600	-1.55385200	0.27330300
N	-5.24687800	-0.00919900	-0.20726300
O	-5.87753600	0.93552700	0.26027900
O	-5.68814800	-0.74131100	-1.09182200
H	1.47660700	-2.52618200	1.92298300
H	0.29674800	-0.48688100	2.50568000
H	0.82841300	-1.51521300	-0.89592900
H	0.15670300	-3.10978800	0.91817800
H	-1.49095700	-2.33262700	-0.14083900

III-b

0 1

C	-1.42294100	2.65771800	0.34808700
C	-2.38355100	1.67615300	0.06605300
C	-3.63377300	2.02555600	-0.41872400
C	-3.91847600	3.38096500	-0.60157900
C	-2.95400800	4.34848900	-0.31526200
C	-1.68404300	4.00581200	0.16287400
C	-0.37087100	0.69922000	0.90398800
H	-4.36859900	1.25769100	-0.64152900
H	-4.89241200	3.68521900	-0.96941600
H	-3.19066800	5.39702700	-0.46753900
H	-0.93859300	4.76420000	0.37723900
N	-0.24355000	2.06080000	0.81973700
C	0.91778800	2.79114100	1.28086100
H	0.64492600	3.46512300	2.09796100
H	1.64596000	2.06325400	1.63914900
H	1.35162500	3.37147500	0.46204400
O	0.43850600	-0.05980000	1.40637000
C	0.00509700	-0.98875500	-1.79987400
C	-0.81967000	-2.15742500	-1.35235400
C	-1.44459900	-1.94197100	0.05886700
C	-2.34640000	-3.10677200	0.40280000
F	-2.90590000	-2.95773600	1.61395800
F	-3.34838800	-3.25802900	-0.47673500
F	-1.65722400	-4.25990600	0.42230300
C	-1.75442200	0.37078000	0.30819600
N	-2.26888300	-0.75341500	0.01463200
C	1.25741400	-0.71245400	-1.37567800

C	1.98515900	0.50372600	-1.71775900
C	3.14095500	-1.30711700	0.03782400
C	3.19251800	0.78830900	-1.18896700
H	1.49964100	1.19116400	-2.40203200
C	3.79482300	-0.14609700	-0.27504200
H	3.55198000	-2.04309800	0.71777500
H	3.72068700	1.70240100	-1.43223000
N	1.94965800	-1.57331300	-0.50307100
N	5.06031400	0.11520800	0.31483200
O	5.62466500	1.16608700	0.02031300
O	5.53945900	-0.71003200	1.09154500
H	-1.63903100	-2.31968700	-2.05746400
H	-0.45206700	-0.26151600	-2.46212500
H	-0.65704800	-1.90821700	0.81737400
H	-0.24134200	-3.08803500	-1.31317500
H	1.49873200	-2.43463700	-0.21636500

Paths A-E

Path A

A-TS1

0 1

C	-1.45431300	-0.78202500	-0.13290700
C	-2.38636800	0.26424500	-0.00554700
C	-3.74660600	0.03627500	0.13097800
C	-4.16451200	-1.29622400	0.15035800
C	-3.25255100	-2.34959500	0.02737900
C	-1.88840000	-2.10283200	-0.12384000
C	-0.15178600	-0.15326100	-0.30793300
H	-4.45378300	0.85344400	0.22882900
H	-5.22136600	-1.51517900	0.26398100
H	-3.61329300	-3.37263900	0.04692300
H	-1.17704400	-2.91560900	-0.23149300
N	-1.70743600	1.50104900	-0.03204600
O	0.52022100	2.16449900	-0.15770900
C	-0.40246500	1.28413500	-0.24583000
N	1.04863900	-0.63196500	-0.12851200
C	2.09854600	0.21630900	-0.38134900
H	2.16606100	0.65856700	-1.37970300
H	1.48029000	1.50865500	-0.02574700
C	3.40878100	-0.31980900	0.07535800
F	3.40623600	-0.62224000	1.38717900
F	4.39326800	0.57382500	-0.12873700
F	3.78361900	-1.45358500	-0.56023800
C	-2.32200900	2.79401400	0.21138200

H	-2.72601100	2.82852400	1.22559000
H	-1.55920400	3.56324000	0.09555600
H	-3.12385600	2.96203200	-0.51048400

INT1

0 1

C	-1.32000900	-0.73775500	0.00883500
C	-2.44658900	0.11292500	0.00578700
C	-3.75189000	-0.37558700	-0.00851000
C	-3.91377900	-1.75643500	-0.01065000
C	-2.80472600	-2.62007200	-0.00335300
C	-1.50769300	-2.12437900	0.00646900
C	-0.15028900	0.10459200	0.00645300
H	-4.60754900	0.29170200	-0.02273200
H	-4.91598400	-2.17264700	-0.02169900
H	-2.96836900	-3.69321400	-0.00762100
H	-0.65142400	-2.79210300	0.00933000
N	-1.99075100	1.42837500	0.01597600
O	0.11326300	2.52125800	-0.00495600
C	-0.62917900	1.41147800	-0.00014500
N	1.13996500	-0.37898200	-0.01581100
C	2.17081500	0.36670600	0.03878000
H	2.18684200	1.45432700	0.12082800
C	3.52162600	-0.28373000	0.00116400
F	3.46372700	-1.60998900	-0.13682300
F	4.21634500	-0.02571000	1.12652500
F	4.26218400	0.19714700	-1.01549700
C	-2.82546800	2.61696000	0.01769200
H	-3.75711400	2.39102400	0.53698500
H	-2.32767800	3.41844300	0.56793200
H	-3.04659100	2.94810200	-1.00032400
H	-0.39995400	3.29729400	-0.28717700

A-TS2

0 1

C	0.98085300	1.36866900	1.02714700
C	-0.09623300	0.48868200	1.26466100
C	0.11907700	-0.62417200	2.07942200
C	1.39112900	-0.83400800	2.61017100
C	2.44578300	0.04236900	2.33562400
C	2.25190000	1.17212900	1.53969000
C	-0.76025000	2.28079400	-0.00742000
H	-0.68158300	-1.32063700	2.30253600
H	1.56785500	-1.70024600	3.23962600
H	3.42949000	-0.15109300	2.75168900
H	3.06326900	1.86114100	1.32699000

N	0.53941400	2.43357500	0.21156000
C	1.37909100	3.51462000	-0.27969600
H	1.64081700	4.18511600	0.54177800
H	2.28537500	3.08942000	-0.71401300
H	0.83150300	4.06325200	-1.04502700
O	-1.45631400	3.13309400	-0.72104800
C	-2.77062000	-0.58373600	0.24548300
C	-4.23708000	-0.91289100	0.19005200
F	-4.83164400	-0.77418900	1.38939700
F	-4.90385400	-0.12626000	-0.66716500
F	-4.43239700	-2.18512100	-0.19466900
C	-1.25214000	1.06329500	0.57605300
N	-2.50894400	0.73515600	0.34940700
H	-2.37050500	2.78277500	-0.76509100
H	-2.22865200	-1.31053200	0.85493700
C	-1.00545500	-0.27447200	-1.85191800
C	-2.10409300	-1.06951500	-1.46028600
C	0.35690500	-0.58155300	-1.60080400
C	1.37953900	0.32001800	-2.01643300
C	1.91014800	-1.92761900	-0.55410600
C	2.68030200	0.09540100	-1.64102800
H	1.11092700	1.19606100	-2.59881800
C	2.94433200	-1.04074400	-0.86685000
H	2.12983300	-2.82325800	0.02110700
H	3.48214600	0.77613100	-1.90468300
N	0.65743300	-1.72056900	-0.91208300
N	4.25909500	-1.27161500	-0.34245500
O	5.13816700	-0.45568100	-0.59859300
O	4.44784900	-2.26773600	0.34843900
H	-3.01274400	-0.91276700	-2.03773900
H	-1.19457100	0.65214700	-2.38834400
H	-1.88781800	-2.11423800	-1.24698300

INT2+2a

0 1			
C	-1.40949200	1.32798400	-1.20364500
C	-0.38983600	0.36765900	-1.42536500
C	-0.74128400	-0.85112900	-2.02056200
C	-2.07385300	-1.08298900	-2.34756200
C	-3.06370500	-0.11904000	-2.10735800
C	-2.74214300	1.10716400	-1.53321800
C	0.46091700	2.19962300	-0.39471600
H	0.00071200	-1.61763700	-2.21517300
H	-2.35344600	-2.03103000	-2.79632800
H	-4.09603900	-0.33388300	-2.36419200

H	-3.50144800	1.85871700	-1.33947000
N	-0.85494500	2.44077900	-0.57568300
C	-1.59783200	3.58972100	-0.09457400
H	-2.06557000	4.11407100	-0.93093200
H	-2.36996500	3.26313600	0.60776100
H	-0.90927800	4.26381500	0.41383400
O	1.22728100	3.07869000	0.23971200
C	2.53737500	-0.62744700	-0.97129500
C	3.95074700	-0.97081400	-0.61261100
F	4.70171800	-1.22637100	-1.70095100
F	4.56506100	-0.00518900	0.07727600
F	3.99029500	-2.08946600	0.14047200
C	0.82562100	0.95617900	-0.90433500
N	2.11256200	0.54124600	-0.69442200
H	2.10731800	2.66495800	0.32713600
H	1.96852600	-1.43604100	-1.43048800
C	1.26068500	0.65182600	2.54543700
C	2.46710800	0.08660500	2.47207800
C	0.02631100	0.01612100	2.05333300
C	-1.18300400	0.72484500	2.11262900
C	-0.99762500	-1.79958800	1.08964200
C	-2.34008100	0.13624100	1.62993100
H	-1.20102600	1.72892900	2.52422300
C	-2.22848400	-1.14735400	1.11336400
H	-0.91952200	-2.80230800	0.68047400
H	-3.29681000	0.64592400	1.64365500
N	0.10819800	-1.23122200	1.55179100
N	-3.40451200	-1.81846000	0.58208100
O	-4.47099000	-1.22825900	0.63562800
O	-3.26421700	-2.93711900	0.11457800
H	3.34892500	0.60139300	2.83991600
H	1.13985600	1.64477900	2.97227800
H	2.59983900	-0.90213600	2.04338500

A-TS3

0 1

C	0.76799100	1.48465500	1.04879500
C	-0.30331800	0.61558100	1.31989400
C	-0.14843200	-0.35346800	2.30399200
C	1.06619600	-0.42263800	2.99187000
C	2.11819300	0.44428600	2.69211300
C	1.98456600	1.42383600	1.70321200
C	-0.84550000	2.12851100	-0.33362800
H	-0.94782200	-1.04944200	2.53483100
H	1.19641400	-1.17175600	3.76597400

H	3.05425300	0.36446000	3.23505800
H	2.79520400	2.10481200	1.46423600
N	0.39291200	2.39350500	0.01850300
C	1.25611100	3.42923500	-0.53139200
H	2.19569400	2.97521900	-0.85122700
H	0.75606100	3.88324500	-1.38596100
H	1.44793500	4.18593900	0.23161100
O	-1.52293200	2.79006700	-1.22535400
C	-0.86286000	-0.40546600	-1.20609400
C	-1.91250100	-1.36491700	-0.75249700
C	-2.91360600	-0.66233300	0.28972100
C	-4.34792300	-0.95092000	-0.07850900
F	-5.21521400	-0.40999800	0.79367600
F	-4.67026500	-0.47434600	-1.29298700
F	-4.58813800	-2.27589900	-0.10107400
C	-1.38316000	0.95788700	0.35724000
N	-2.68638100	0.74130600	0.25307900
C	0.54233500	-0.68813100	-1.15043600
C	1.45322300	0.15923800	-1.83388200
C	2.28231800	-1.83418100	-0.16097100
C	2.80825300	0.00069600	-1.64971500
H	1.07043800	0.93457300	-2.49105000
C	3.22319800	-1.01100400	-0.78202800
H	2.61433000	-2.63111800	0.49883200
H	3.53481600	0.63240600	-2.14811900
N	0.98063600	-1.68682700	-0.33940200
N	4.62976400	-1.22337500	-0.53319900
O	5.43034400	-0.47235000	-1.07333300
O	4.95479700	-2.14184700	0.20753700
H	-2.50532700	-1.69605900	-1.61031400
H	-1.14730200	0.25047700	-2.02690200
H	-2.41394100	2.36026600	-1.22516400
H	-2.75552000	-1.14510600	1.26610300
H	-1.45938300	-2.24016100	-0.28421800

Path B
B-TS2

0 1

C	-1.34607500	-0.75825400	-0.00022400
C	-2.44352200	0.15123200	-0.00000200
C	-3.75958300	-0.28040500	0.00019400
C	-3.98976700	-1.65865400	0.00021300
C	-2.92672700	-2.56626200	0.00002100
C	-1.60190500	-2.13003800	-0.00020500

C	-0.18587500	0.08762300	-0.00040400
H	-4.58200500	0.42821700	0.00034900
H	-5.01073400	-2.02609000	0.00038500
H	-3.13491000	-3.63160100	0.00005300
H	-0.78447900	-2.84380900	-0.00036300
N	-1.97232400	1.47793800	-0.00000300
O	0.25975400	2.35869700	-0.00005900
C	-0.62464400	1.43695300	-0.00017900
N	1.16236600	0.12746800	-0.00032700
C	2.07975600	-0.77354400	-0.00018100
H	1.87147600	-1.83856100	-0.00010700
H	1.18013800	1.41531100	-0.00017500
C	3.50554400	-0.33902900	0.00008300
F	4.16471400	-0.80561300	-1.07509500
F	4.16423800	-0.80571300	1.07551800
F	3.62846900	0.99452700	0.00015500
C	-2.80044600	2.66752200	0.00015800
H	-3.43081400	2.68999500	0.89235100
H	-2.14335200	3.53732900	0.00015900
H	-3.43097100	2.69011900	-0.89192200

Path C

C-TS1

0 1

C	1.10493900	0.66268400	-0.04977700
C	2.38828800	0.06637300	0.01138800
C	3.54938700	0.82032900	0.05584500
C	3.41864100	2.21322900	0.04126000
C	2.16547500	2.82058700	-0.01257000
C	0.99838600	2.05158700	-0.05898700
C	0.16479700	-0.44492000	-0.06862100
H	4.52448300	0.34653000	0.10255000
H	4.31270900	2.82799800	0.07251600
H	2.09091300	3.90286300	-0.02094500
H	0.03487600	2.54628700	-0.09833100
N	2.27352100	-1.32269700	0.01741800
O	0.53998900	-2.85978500	-0.04333200
C	0.94703800	-1.70916800	-0.03009100
N	-1.14306000	-0.50738000	-0.08502500
C	-2.03998400	0.50181000	-0.31773700
H	-1.77248400	-0.65904000	-1.07619100
C	-3.46215200	0.19882800	0.02558200
F	-3.76020000	0.55795700	1.28969300
F	-3.75464300	-1.10425100	-0.08601700

F	-4.30017800	0.88171500	-0.76739800
C	3.38404400	-2.24522000	0.07572400
H	4.06117700	-2.08617000	-0.76839100
H	3.93983900	-2.12405900	1.01028600
H	2.97469800	-3.25455400	0.02600000
H	-1.77731900	1.55344900	-0.38618000

Path D

D-TS1

0 1

C	-3.11665400	0.75808900	-0.16798900
C	-3.07038200	0.17189200	-1.44624800
C	-4.18006400	-0.42596300	-2.02354900
C	-5.36642400	-0.43037400	-1.28017000
C	-5.42861200	0.14486200	-0.01008000
C	-4.30061500	0.74779800	0.55592600
C	-1.78093700	1.29086300	0.11448800
H	-4.13003400	-0.87594400	-3.00993800
H	-6.25359900	-0.89001900	-1.70464400
H	-6.36237500	0.12566800	0.54271800
H	-4.34299900	1.20117000	1.54224900
N	-1.77831200	0.29552500	-1.96516500
O	0.25463700	1.12942700	-1.26199100
C	-0.94971900	0.96425800	-1.08960000
N	-1.40564100	1.70968200	1.28274000
C	-0.17099500	2.15105200	1.66932700
H	-0.16513900	2.50061000	2.70196400
H	0.57385400	0.69282100	1.69498500
C	0.61874300	3.11642200	0.82888100
F	1.79639700	2.67059900	0.34354600
F	0.95466800	4.19393700	1.58465100
F	-0.06925000	3.59921000	-0.22140100
C	-1.31870600	-0.31672500	-3.19133200
H	-1.83480300	0.11027400	-4.05620800
H	-0.24862400	-0.11958300	-3.27484700
H	-1.48964900	-1.39676200	-3.16330100
C	2.64361900	-0.26415600	0.04057600
C	2.98969900	-0.85584100	-1.18869700
C	4.21287800	-0.61387800	-1.78734900
C	5.09324300	0.23471800	-1.10772800
C	4.77370400	0.80953300	0.12637600
C	3.53977100	0.55762900	0.71906200
C	1.34408800	-0.77324400	0.39016700
H	4.48265600	-1.06606600	-2.73524500

H	6.06186400	0.44179100	-1.55225000
H	5.49400700	1.44874100	0.62401700
H	3.27464400	0.98439800	1.68089200
N	1.96271800	-1.69191800	-1.64205600
O	-0.10425500	-2.35222000	-0.84872400
C	0.93945500	-1.74325200	-0.74426900
N	0.59191600	-0.42139100	1.37420100
C	-0.63100000	-1.12240700	1.73384100
H	-1.21740700	-0.46874800	2.38290700
H	-1.22156400	-1.39963100	0.85743100
C	-0.28281900	-2.37132100	2.51428600
F	0.53521500	-3.18529500	1.83117400
F	-1.39180700	-3.05748200	2.80839200
F	0.33439100	-2.07509900	3.66625900
C	1.97861600	-2.41087800	-2.90042200
H	1.02481900	-2.92857700	-3.00185900
H	2.10519700	-1.70877300	-3.72811200
H	2.79346500	-3.13960100	-2.90964000

Compound INT4+INT5

0 1

C	-3.17625100	0.56247100	-0.25496000
C	-3.07472900	-0.18345800	-1.45472500
C	-4.15936500	-0.85912600	-2.00436600
C	-5.37575500	-0.79432800	-1.32188100
C	-5.49472900	-0.06739800	-0.12972600
C	-4.40559400	0.61794700	0.40667900
C	-1.88621700	1.15900600	-0.00846500
H	-4.06085300	-1.42089700	-2.92862500
H	-6.24027100	-1.31419000	-1.72318600
H	-6.45210900	-0.03497800	0.38212200
H	-4.50323000	1.18792200	1.32672300
N	-1.77248100	-0.09644000	-1.90439300
O	0.23883000	0.81142800	-1.19289200
C	-1.00357700	0.69231200	-1.04384700
N	-1.66478300	1.89849000	1.11540000
C	-0.74338600	2.73693500	1.41557500
H	-0.76575400	3.20358600	2.39970400
H	1.28255800	0.47133000	2.07540300
C	0.35572800	3.27168100	0.54562300
F	1.47982400	2.52475400	0.55048500
F	0.72872800	4.48606900	1.00638700
F	-0.01331500	3.44200300	-0.72941200
C	-1.23994700	-0.78421200	-3.05613700
H	-1.73366600	-0.44735100	-3.97341900

H	-0.17584200	-0.54840900	-3.11279200
H	-1.36751200	-1.86624700	-2.95571800
C	2.71048900	-0.14331400	-0.09307700
C	2.95011300	-0.88127300	-1.26841000
C	4.13532800	-0.74456100	-1.97293600
C	5.08278000	0.14433000	-1.45886700
C	4.86556800	0.86606700	-0.27966700
C	3.67111000	0.72615300	0.41768300
C	1.41165500	-0.54789600	0.37814700
H	4.32320200	-1.30603900	-2.88120400
H	6.02081400	0.27170700	-1.99033500
H	5.63163200	1.53825400	0.08943600
H	3.48636300	1.28324800	1.33070300
N	1.87881300	-1.72882200	-1.55033100
O	-0.13995800	-2.23094100	-0.53391200
C	0.89902000	-1.61065800	-0.60402200
N	0.83335900	-0.23955600	1.49761600
C	-0.37503400	-0.84626000	2.04292800
H	-0.89524300	-0.10198100	2.64729500
H	-1.01949500	-1.20169600	1.24174200
C	0.01433700	-2.01883400	2.91707100
F	0.69496300	-2.93998800	2.21965300
F	-1.07138300	-2.60465600	3.42798100
F	0.79840200	-1.63817800	3.93617900
C	1.81152200	-2.63376000	-2.68011600
H	0.88048500	-3.19503700	-2.60243000
H	1.82358900	-2.07320400	-3.61862200
H	2.65665400	-3.32660800	-2.65689300

D-TS2

0 1

C	2.90651400	-0.27722000	0.35152700
C	3.50553200	-1.35468100	-0.34512200
C	4.80339400	-1.28216000	-0.82849300
C	5.50972800	-0.09134200	-0.61794700
C	4.93122300	0.98170400	0.06257200
C	3.62898700	0.89358900	0.56482800
C	1.58248100	-0.71506300	0.71545000
H	5.25317000	-2.11627700	-1.35839600
H	6.52577800	-0.00608600	-0.99074200
H	5.50203800	1.89262500	0.21403100
H	3.18580100	1.72114000	1.11109400
N	2.59026100	-2.39461000	-0.43949400
O	0.36062000	-2.73561800	0.12413400
C	1.37782600	-2.04721700	0.15753500

N	0.61990800	0.11304500	1.14196800
C	-0.57542400	-0.08976100	1.62988100
H	-1.19023000	0.78665400	1.80788300
H	-1.57808400	2.84681200	-0.00258400
C	-1.10393500	-1.35003300	2.23492500
F	-1.92863900	-2.04302900	1.43294200
F	-1.84800700	-1.01703000	3.31403100
F	-0.14430500	-2.17253400	2.66804500
C	2.80045400	-3.62293100	-1.16692200
H	3.62534600	-4.19739800	-0.73438900
H	1.88077500	-4.20535200	-1.09919800
H	3.02204900	-3.41981600	-2.21956100
C	-3.03507400	0.75381000	-0.71105200
C	-3.16964900	-0.57876800	-1.15267600
C	-4.38899100	-1.23611200	-1.09234300
C	-5.47753300	-0.52316500	-0.58379200
C	-5.35624800	0.79955400	-0.14558600
C	-4.12646700	1.45087300	-0.20125000
C	-1.63448500	1.07316000	-0.86155600
H	-4.49295700	-2.26309800	-1.42513800
H	-6.44423700	-1.01375000	-0.52688200
H	-6.22489100	1.31952500	0.24299700
H	-4.01868900	2.47681900	0.13937300
N	-1.94661600	-1.07033100	-1.60560400
O	0.20525600	-0.21330400	-1.82108000
C	-0.96129500	-0.12296400	-1.48077200
N	-0.99939500	2.13896800	-0.46518500
C	0.39278000	2.30119800	-0.33163000
H	0.70269600	1.26320200	0.68430200
H	0.96271900	1.89891500	-1.16613600
C	0.74647200	3.70521100	0.00486400
F	0.60328300	4.57679900	-1.01782600
F	2.02287100	3.79794700	0.40314300
F	-0.03154800	4.18032300	1.00076400
C	-1.72146100	-2.42254200	-2.06877000
H	-0.66209100	-2.52012900	-2.30172700
H	-1.97210800	-3.13053800	-1.27529500
H	-2.32508100	-2.62450100	-2.95778800

Path E

E-TS1

0 1

C	-1.32005700	2.06397900	-0.93434400
C	0.05214000	2.15225000	-0.62630500
C	0.55929600	3.30514000	-0.04122900

C	-0.31408700	4.36644300	0.21752400
C	-1.67002300	4.26540400	-0.09930200
C	-2.19853000	3.10654500	-0.68005400
C	-0.45169300	0.04083000	-1.55884100
H	1.61459900	3.37200700	0.20791300
H	0.06542600	5.27716300	0.66935800
H	-2.33223300	5.09976800	0.10950100
H	-3.25423300	3.02766000	-0.91904100
N	-1.59588000	0.80710000	-1.48350700
C	-2.90953100	0.33019500	-1.85375500
H	-3.58103900	0.34282200	-0.98898100
H	-3.33762700	0.94774900	-2.64844600
H	-2.79914900	-0.69463700	-2.21172000
O	-0.40005700	-1.10774600	-1.99276300
C	1.19871500	0.46586800	2.32692500
C	1.06381400	1.66785100	2.89313000
C	2.26566100	-0.81796700	-0.75020300
H	1.94197200	2.22312600	3.20594900
C	3.71160100	-0.98907600	-0.46953300
F	4.03252300	-2.29388100	-0.35965100
F	4.53795800	-0.48448800	-1.42064700
F	4.09231900	-0.39072800	0.68091700
C	0.64837900	0.86500500	-0.97275900
N	1.84470900	0.47591500	-0.65450500
C	0.07135100	-0.33926000	1.85027100
C	-1.27439600	-0.07546000	2.14252800
C	-0.54540300	-2.19954700	0.54303600
C	-2.26107300	-0.88754300	1.61767700
H	-1.53799000	0.76582400	2.77078500
C	-1.87454300	-1.96738500	0.82644400
H	-0.21343900	-2.98049200	-0.13032000
H	-3.31108800	-0.69830900	1.80881800
N	0.38312200	-1.39493100	1.06375700
N	-2.88199300	-2.81805500	0.20402200
O	-4.05029200	-2.51528600	0.36687000
O	-2.49348900	-3.76971600	-0.44891800
H	0.09983300	2.14027800	3.05689700
H	2.18441400	0.04475900	2.15147900
H	1.87996200	-1.48114200	-1.52492200
H	1.40667000	-1.33255400	0.44002800

E-TS1'

O 1

C	-2.35738500	-0.76990600	0.99189600
C	-1.46532000	-1.69387400	0.41602100

C	-1.95390300	-2.74861400	-0.34236300
C	-3.33593800	-2.86801500	-0.51221700
C	-4.20703800	-1.93939500	0.06098700
C	-3.73031600	-0.86901800	0.82499800
C	-0.27432500	0.00788600	1.54810800
H	-1.26843400	-3.45970000	-0.79469700
H	-3.73687000	-3.68745900	-1.10032200
H	-5.27712200	-2.04641600	-0.08807500
H	-4.40692100	-0.14167100	1.26245600
N	-1.63499600	0.21814700	1.67052700
C	-2.21681100	1.39236000	2.27975400
H	-1.39782700	2.02008900	2.63314700
H	-2.80984600	1.94620600	1.54341200
H	-2.85667100	1.11943300	3.12369800
O	0.59507900	0.75085800	1.99328900
C	3.01984200	2.33797500	0.00488700
C	3.51182200	3.38665100	0.66735800
C	2.19264300	-1.09963700	0.33452300
H	4.55784200	3.40667200	0.95436500
C	3.32995400	-1.89622600	-0.18717600
F	4.43848700	-1.12981700	-0.29234700
F	3.68835600	-2.95014200	0.58914700
F	3.08729900	-2.41301900	-1.40625700
C	-0.11331600	-1.22935800	0.72499800
N	0.98018400	-1.70298100	0.20667600
C	1.62430900	2.21269300	-0.42380600
C	0.64027000	3.19328800	-0.27220500
C	0.05782700	0.73983600	-1.39607600
C	-0.67073700	2.90314100	-0.61183500
H	0.89333700	4.16233900	0.13969200
C	-0.94740700	1.66489400	-1.18153300
H	-0.11325800	-0.22673500	-1.85659900
H	-1.46769600	3.62025000	-0.44947600
N	1.29940500	1.02885400	-0.99251500
N	-2.32128900	1.28614400	-1.49891000
O	-3.21173600	2.00337600	-1.07622300
O	-2.49111100	0.27634800	-2.15529900
H	2.90832100	4.24543000	0.94547000
H	3.65816200	1.49440900	-0.24630500
H	2.43533600	-0.49918500	1.21227900
H	1.92834700	0.07923200	-0.64642300

Compound INT6+INT7

0 1

C	3.63035200	-1.09916200	-0.27724400
C	2.26653500	-0.90742000	0.07413300
C	1.52664200	-2.01363200	0.49608400
C	2.13797200	-3.26941800	0.55066100
C	3.47789000	-3.43484100	0.19387000
C	4.24489700	-2.34204000	-0.22456600
C	3.21894300	1.13620000	-0.55521500
H	0.48584200	-1.90756000	0.78861500
H	1.55997700	-4.12820000	0.87819700
H	3.93351000	-4.41873300	0.24384200
H	5.28891600	-2.45979100	-0.49917100
N	4.17424700	0.12021600	-0.64951100
C	5.53916100	0.33578700	-1.06178900
H	6.23857000	0.05442100	-0.26800300
H	5.77492700	-0.24204500	-1.96112300
H	5.65048500	1.39887600	-1.27863900
O	3.44424300	2.32270900	-0.82768200
C	-1.23453100	-0.26783700	2.74674400
C	-1.54857300	-0.68919100	3.97347200
C	0.61952600	2.40256800	-0.05693500
H	-0.89879600	-0.45607300	4.81012500
C	-0.75863200	2.90914300	0.16836500
F	-1.63161200	2.55912200	-0.81091100
F	-1.31405700	2.43814700	1.31010400
F	-0.78088800	4.24669200	0.23742100
C	1.99740600	0.49973400	-0.10411100
N	0.81648100	1.12639500	0.08938300
C	-2.04655800	-0.54564100	1.56114000
C	-3.32413700	-1.11582200	1.56747900
C	-2.09497800	-0.41333000	-0.80395800
C	-3.98168300	-1.34470600	0.37314100
H	-3.79927700	-1.36782900	2.50685600
C	-3.34624900	-0.98849900	-0.81390900
H	-1.56205000	-0.10511200	-1.69612900
H	-4.97170400	-1.78546100	0.35170900
N	-1.49564200	-0.21604200	0.37187300
N	-4.00791700	-1.20677200	-2.09877600
O	-5.10228400	-1.73658200	-2.08114400
O	-3.42146100	-0.84363500	-3.10158500
H	-2.43751300	-1.27497100	4.18735600
H	-0.32418900	0.30006300	2.57329500
H	1.38563300	3.10767800	-0.35809700
H	-0.50340700	0.27121200	0.33997300

E-TS2

0 1

C	3.56868900	-1.12554900	-0.22073900
C	2.20382100	-0.91316700	0.11325600
C	1.45534100	-1.99809300	0.57380000
C	2.05989000	-3.25354100	0.68137600
C	3.40082200	-3.43978200	0.34001000
C	4.17625900	-2.36846100	-0.11542300
C	3.17998400	1.09981000	-0.58591100
H	0.41424800	-1.87741100	0.85667700
H	1.47501800	-4.09528300	1.03920200
H	3.85091900	-4.42316000	0.43176800
H	5.22146200	-2.50165500	-0.37781400
N	4.12565000	0.07480500	-0.63508700
C	5.49606400	0.26334800	-1.04402400
H	5.73299700	-0.35111600	-1.91823000
H	5.61874300	1.31628500	-1.30038700
H	6.18567200	0.00646700	-0.23369300
O	3.41234900	2.27412600	-0.89872300
C	-1.22568700	-0.09644000	2.75814500
C	-1.60116800	-0.35483600	4.01222400
C	0.59306100	2.41847300	-0.15353000
H	-0.96559400	-0.06130200	4.84075400
C	-0.77952900	2.95013200	0.05006700
F	-1.33466000	2.54222500	1.21489000
F	-0.78068200	4.28901100	0.05518700
F	-1.65715400	2.56481600	-0.90933800
C	1.94959600	0.48925400	-0.12095700
N	0.77952500	1.14433600	0.03798700
C	-2.00894200	-0.45753300	1.57315600
C	-3.26146600	-1.08299500	1.59366500
C	-2.02936100	-0.43474900	-0.78534600
C	-3.89488300	-1.39100700	0.40415900
H	-3.73355700	-1.32563900	2.53720400
C	-3.25851600	-1.05936100	-0.78862400
H	-1.50012400	-0.15185900	-1.68877100
H	-4.86307200	-1.87784400	0.39090800
N	-1.44711900	-0.15861500	0.38190400
N	-3.88803100	-1.36751800	-2.07030500
O	-4.95047700	-1.95943300	-2.04533500
O	-3.30920500	-1.01284300	-3.08106900
H	-2.53136700	-0.85736700	4.25942500
H	-0.28241600	0.40661400	2.56151600
H	1.37386200	3.09807500	-0.47156500
H	-0.39968300	0.39186500	0.31404000

Compound INT3+2a

0 1

C	1.22361200	1.61987700	-0.79951600
C	0.36595400	0.61114500	-1.30105500
C	0.87153900	-0.35781400	-2.16500200
C	2.22382200	-0.31137800	-2.50926900
C	3.05757200	0.69164800	-2.00749200
C	2.56658900	1.67596500	-1.14416200
C	-0.81391100	2.03253900	0.16045300
H	0.22781900	-1.14172400	-2.55442500
H	2.63193600	-1.06566500	-3.17429300
H	4.10728400	0.70477800	-2.28399200
H	3.21605500	2.45009400	-0.74700900
N	0.50855700	2.44814600	0.05854800
C	1.06718900	3.54724700	0.80947100
H	1.90601200	3.20455400	1.42419700
H	1.41565000	4.34158200	0.14260100
H	0.28099000	3.93865700	1.45614000
O	-1.68176900	2.56981000	0.85224900
C	-1.12064400	-0.40497900	2.42515600
C	-2.21854100	-1.11867900	2.16270100
C	-3.21529800	0.31368900	-0.28516900
C	-4.29204900	-0.66197500	-0.58900900
F	-5.31767700	-0.09723000	-1.24761700
F	-3.84101000	-1.67613100	-1.34769500
F	-4.81486900	-1.19681500	0.52714800
C	-0.91584700	0.86691100	-0.70138500
N	-2.03812400	0.13800300	-0.83410100
C	0.20708400	-0.69687300	1.86311200
C	1.29158400	0.12838100	2.19774000
C	1.51838300	-1.99563400	0.49704200
C	2.53365700	-0.12421200	1.64048700
H	1.14591900	0.96167200	2.87729600
C	2.63231900	-1.20546200	0.77572500
H	1.60449500	-2.83887900	-0.18156900
H	3.39957500	0.49158300	1.85561200
N	0.33015600	-1.74826800	1.02999100
N	3.89839700	-1.50456100	0.12920000
O	4.84886500	-0.77726800	0.36901800
O	3.94691700	-2.46817200	-0.61920600
H	-2.18674200	-1.98602800	1.50887700
H	-1.17151900	0.46333200	3.07739400
H	-3.40087200	1.16420100	0.35484700
H	-3.17259400	-0.85759700	2.60881400

H	-1.94509100	-0.68955500	-1.43192300
E- TS3			
0 1			
C	-1.18017600	1.73012800	0.77077000
C	-0.38643300	0.67032000	1.26378400
C	-0.95169500	-0.31058900	2.07753400
C	-2.30948500	-0.22470300	2.37870000
C	-3.08716400	0.82251600	1.87213900
C	-2.53293800	1.82287400	1.06807800
C	0.91016900	2.11016200	-0.08803500
H	-0.34719100	-1.12982300	2.45775900
H	-2.77117600	-0.98315700	3.00219400
H	-4.14542400	0.86476000	2.11095000
H	-3.14040500	2.63366500	0.67862600
N	-0.39980600	2.56356000	-0.02529400
C	-0.87075200	3.76023800	-0.68456900
H	-1.70799700	3.52394300	-1.34795600
H	-1.19298500	4.50708400	0.04707100
H	-0.04377300	4.16235100	-1.27056100
O	1.83666800	2.68200400	-0.65724900
C	1.16619500	-0.11974100	-2.08361300
C	2.32972200	-0.78674700	-1.80303000
C	3.07511100	0.07090000	0.07307700
C	4.16225500	-0.86721900	0.47910000
F	4.94693800	-0.36590900	1.44917800
F	3.65620200	-2.02198300	0.94842800
F	4.96126000	-1.15645500	-0.55418700
C	0.91522600	0.85866200	0.68832600
N	1.97018500	0.04987000	0.82674300
C	-0.15471600	-0.56766400	-1.70228700
C	-1.28343500	0.19003900	-2.09168600
C	-1.47312600	-2.03627700	-0.52220700
C	-2.53259000	-0.16852800	-1.63498700
H	-1.14895800	1.06668200	-2.71691000
C	-2.61955000	-1.29638800	-0.81988500
H	-1.55056400	-2.92611400	0.09624300
H	-3.42046400	0.40494100	-1.87594100
N	-0.27040700	-1.69230300	-0.95415500
N	-3.88172200	-1.67100200	-0.23260400
O	-4.87234100	-1.01326600	-0.52277500
O	-3.90408200	-2.62717500	0.53186700
H	2.28777000	-1.79727300	-1.40465600
H	1.20883700	0.81690300	-2.63284400
H	3.36376800	1.00984700	-0.38007500

H	3.24322700	-0.49866700	-2.31309000
H	1.81631400	-0.78729600	1.39358100

Analysis of of the favored path E

NBO

1a

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.12589	1.99898	4.11159	0.01532	6.12589
C	2	0.19503	1.99900	3.78938	0.01659	5.80497
C	3	-0.28953	1.99903	4.27801	0.01249	6.28953
C	4	-0.20789	1.99917	4.19519	0.01353	6.20789
C	5	-0.26783	1.99915	4.25529	0.01339	6.26783
C	6	-0.18120	1.99906	4.16885	0.01328	6.18120
C	7	0.20307	1.99911	3.77274	0.02508	5.79693
H	8	0.25508	0.00000	0.74369	0.00123	0.74492
H	9	0.25296	0.00000	0.74591	0.00114	0.74704
H	10	0.25422	0.00000	0.74467	0.00111	0.74578
H	11	0.26791	0.00000	0.73065	0.00144	0.73209
N	12	-0.46599	1.99925	5.45532	0.01142	7.46599
O	13	-0.59769	1.99980	6.57747	0.02043	8.59769
C	14	0.67495	1.99932	3.28520	0.04052	5.32505
N	15	-0.38869	1.99933	5.36448	0.02488	7.38869
C	16	-0.41156	1.99917	4.39573	0.01667	6.41156
H	17	0.27519	0.00000	0.72217	0.00264	0.72481
H	18	0.27521	0.00000	0.72214	0.00265	0.72479
C	19	1.15631	1.99919	2.77253	0.07197	4.84369
F	20	-0.37637	1.99992	7.36952	0.00692	9.37637
F	21	-0.37868	1.99992	7.37214	0.00661	9.37868
F	22	-0.37642	1.99992	7.36957	0.00692	9.37642
C	23	-0.49733	1.99950	4.48556	0.01227	6.49733
H	24	0.24124	0.00000	0.75732	0.00143	0.75876
H	25	0.27263	0.00000	0.72526	0.00211	0.72737
H	26	0.24125	0.00000	0.75731	0.00143	0.75875
* Total *		0.00000	33.98881	89.66771	0.34348	124.00000

2a

Summary of Natural Population Analysis:

Natural Population						
Atom	No	Natural Charge	Core	Valence	Rydberg	Total

C	1	0.20798	1.99908	3.77123	0.02171	5.79202
C	2	-0.26444	1.99906	4.25342	0.01195	6.26444
C	3	-0.18334	1.99905	4.16915	0.01513	6.18334
C	4	-0.00126	1.99875	3.98432	0.01819	6.00126
C	5	0.05507	1.99914	3.92332	0.02246	5.94493
N	6	-0.45155	1.99942	5.42973	0.02241	7.45155
H	7	0.28779	0.00000	0.71061	0.00160	0.71221
H	8	0.26024	0.00000	0.73854	0.00122	0.73976
H	9	0.26818	0.00000	0.73007	0.00175	0.73182
N	10	0.54663	1.99955	4.39974	0.05409	6.45337
O	11	-0.39538	1.99982	6.37878	0.01678	8.39538
O	12	-0.39804	1.99982	6.38137	0.01685	8.39804
C	13	-0.28499	1.99911	4.27101	0.01487	6.28499
H	14	0.24038	0.00000	0.75830	0.00132	0.75962
C	15	-0.36318	1.99917	4.35329	0.01072	6.36318
H	16	0.24478	0.00000	0.75376	0.00146	0.75522
H	17	0.23112	0.00000	0.76788	0.00100	0.76888
* Total *		0.00000	21.99197	55.77452	0.23351	78.00000

E-TS1

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
C	1	0.17449	1.99900	3.80969	0.01682	5.82551
C	2	-0.09511	1.99899	4.08001	0.01611	6.09511
C	3	-0.21883	1.99906	4.20587	0.01391	6.21883
C	4	-0.27064	1.99914	4.25806	0.01344	6.27064
C	5	-0.23832	1.99916	4.22538	0.01377	6.23832
C	6	-0.29075	1.99903	4.27919	0.01253	6.29075
C	7	0.65623	1.99928	3.30251	0.04198	5.34377
H	8	0.26099	0.00000	0.73747	0.00153	0.73901
H	9	0.24764	0.00000	0.75122	0.00114	0.75236
H	10	0.24771	0.00000	0.75113	0.00116	0.75229
H	11	0.24999	0.00000	0.74874	0.00126	0.75001
N	12	-0.46407	1.99924	5.45337	0.01147	7.46407
C	13	-0.49684	1.99950	4.48494	0.01240	6.49684
H	14	0.22882	0.00000	0.76929	0.00189	0.77118
H	15	0.24445	0.00000	0.75409	0.00146	0.75555
H	16	0.26980	0.00000	0.72783	0.00237	0.73020
O	17	-0.65250	1.99978	6.63318	0.01954	8.65250

C	18	-0.29142	1.99910	4.27545	0.01688	6.29142
C	19	-0.34339	1.99917	4.33336	0.01086	6.34339
C	20	-0.44666	1.99909	4.42245	0.02512	6.44666
H	21	0.24957	0.00000	0.74946	0.00097	0.75043
C	22	1.13422	1.99900	2.79591	0.07087	4.86578
F	23	-0.38473	1.99993	7.37841	0.00639	9.38473
F	24	-0.38409	1.99993	7.37773	0.00643	9.38409
F	25	-0.38990	1.99992	7.38353	0.00645	9.38990
C	26	0.05682	1.99904	3.91746	0.02668	5.94318
N	27	-0.36450	1.99935	5.34507	0.02007	7.36450
C	28	0.25798	1.99909	3.72216	0.02077	5.74202
C	29	-0.25173	1.99905	4.24033	0.01234	6.25173
C	30	0.10572	1.99910	3.87150	0.02369	5.89428
C	31	-0.16076	1.99906	4.14612	0.01558	6.16076
H	32	0.27453	0.00000	0.72429	0.00118	0.72547
C	33	0.00405	1.99873	3.97797	0.01925	5.99595
H	34	0.30615	0.00000	0.69174	0.00212	0.69385
H	35	0.29684	0.00000	0.70155	0.00161	0.70316
N	36	-0.49610	1.99932	5.48120	0.01557	7.49610
N	37	0.55563	1.99955	4.39886	0.04596	6.44437
O	38	-0.39780	1.99981	6.37416	0.02382	8.39780
O	39	-0.37836	1.99982	6.35462	0.02392	8.37836
H	40	0.22503	0.00000	0.77373	0.00124	0.77497
H	41	0.27956	0.00000	0.71768	0.00277	0.72044
H	42	0.26557	0.00000	0.73175	0.00268	0.73443
H	43	0.42470	0.00000	0.57029	0.00501	0.57530

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* Total *	0.00000	55.98026	145.42874	0.59100	202.00000
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Structures of E-TS1-CH₃

1a-CH₃

0 1

C	1.44939300	0.31292900	0.00001500
C	0.57078400	-0.78065100	-0.00001500
C	1.05843000	-2.07761700	-0.00002700
C	2.44291800	-2.26797700	-0.00001300
C	3.30576300	-1.17084500	0.00001300
C	2.82510000	0.14339900	0.00002700
C	-0.62394400	1.28577500	-0.00002300
H	0.37326500	-2.92007100	-0.00004900
H	2.85034900	-3.27325000	-0.00002400
H	4.37853300	-1.33722200	0.00002200
H	3.50134200	0.99168300	0.00004500
N	0.72813100	1.51574200	0.00002600

C	1.33168700	2.83039300	0.00005300
H	1.95018600	2.96562500	0.89184300
H	1.95000500	2.96576700	-0.89184200
H	0.52712900	3.56610800	0.00019000
O	-1.49749800	2.13337300	-0.00008000
C	-3.16651800	-0.22556900	-0.00004800
C	-4.28930200	-1.24825900	0.00011800
C	-0.79600300	-0.23737700	-0.00002600
N	-1.87187800	-0.90876000	-0.00005400
H	-3.23499800	0.43122000	-0.87521000
H	-3.23492800	0.43143200	0.87494500
H	-5.26163100	-0.74826100	0.00002100
H	-4.23143300	-1.88720600	-0.88572800
H	-4.23145200	-1.88690400	0.88618400

E-TS1-CH₃

0 1

C	-2.20865200	-1.39658700	-0.59667400
C	-2.44936700	-0.02218000	-0.38622000
C	-3.56895300	0.37572700	0.33667700
C	-4.43931200	-0.60237600	0.82762600
C	-4.19041300	-1.95811500	0.60167500
C	-3.06443700	-2.37758900	-0.11599900
C	-0.44579400	-0.31384500	-1.58270800
H	-3.75675400	1.43133900	0.51384100
H	-5.31761700	-0.30574200	1.39254200
H	-4.87861900	-2.70205500	0.99090400
H	-2.86571200	-3.43118000	-0.28610700
N	-1.02307700	-1.54789700	-1.31349300
C	-0.42019600	-2.81240500	-1.66175600
H	-0.17920300	-3.38957800	-0.76312900
H	-1.08958900	-3.40275100	-2.29460700
H	0.49829500	-2.59776800	-2.20920300
O	0.62871400	-0.16702600	-2.17080400
C	-0.43108100	1.65663300	2.09414600
C	-1.32762300	1.17867000	2.95910600
C	-0.08075900	2.64511000	-1.39964000
H	-2.18144100	1.78040400	3.25294100
C	-0.12331800	4.15439300	-1.42475700
C	-1.34960700	0.70358700	-1.00477900
N	-1.18895100	2.00688000	-0.96371500
C	0.73414000	0.89310000	1.63139100
C	1.28009700	-0.20722000	2.30701600
C	2.35787000	0.70855700	-0.05786600
C	2.39587400	-0.84013600	1.79077000

H	0.83911800	-0.54512100	3.23677200
C	2.93722000	-0.35681000	0.60285500
H	2.71338100	1.07744600	-1.01277800
H	2.85018900	-1.68653600	2.29311400
N	1.29824700	1.30665400	0.47911700
N	4.11975500	-0.98548400	0.02578500
O	4.59206300	-1.94311700	0.61091500
O	4.56168800	-0.51577300	-1.00793300
H	-1.25369200	0.18199600	3.38509800
H	-0.55657500	2.64125300	1.65195700
H	0.53516000	2.15711100	-2.16252500
H	0.71074700	2.11255400	-0.27959700
H	0.88323300	4.57845600	-1.35523300
H	-0.57479300	4.54245500	-2.34741300
H	-0.71181100	4.53289500	-0.58302700

Origin of diastereoselectivity

Structures of paths E-a/b/c/d

E-a

E-TS3-a

0 1

C	-1.18017600	1.73012800	0.77077000
C	-0.38643300	0.67032000	1.26378400
C	-0.95169500	-0.31058900	2.07753400
C	-2.30948500	-0.22470300	2.37870000
C	-3.08716400	0.82251600	1.87213900
C	-2.53293800	1.82287400	1.06807800
C	0.91016900	2.11016200	-0.08803500
H	-0.34719100	-1.12982300	2.45775900
H	-2.77117600	-0.98315700	3.00219400
H	-4.14542400	0.86476000	2.11095000
H	-3.14040500	2.63366500	0.67862600
N	-0.39980600	2.56356000	-0.02529400
C	-0.87075200	3.76023800	-0.68456900
H	-1.70799700	3.52394300	-1.34795600
H	-1.19298500	4.50708400	0.04707100
H	-0.04377300	4.16235100	-1.27056100
O	1.83666800	2.68200400	-0.65724900
C	1.16619500	-0.11974100	-2.08361300
C	2.32972200	-0.78674700	-1.80303000
C	3.07511100	0.07090000	0.07307700
C	4.16225500	-0.86721900	0.47910000
F	4.94693800	-0.36590900	1.44917800
F	3.65620200	-2.02198300	0.94842800

F	4.96126000	-1.15645500	-0.55418700
C	0.91522600	0.85866200	0.68832600
N	1.97018500	0.04987000	0.82674300
C	-0.15471600	-0.56766400	-1.70228700
C	-1.28343500	0.19003900	-2.09168600
C	-1.47312600	-2.03627700	-0.52220700
C	-2.53259000	-0.16852800	-1.63498700
H	-1.14895800	1.06668200	-2.71691000
C	-2.61955000	-1.29638800	-0.81988500
H	-1.55056400	-2.92611400	0.09624300
H	-3.42046400	0.40494100	-1.87594100
N	-0.27040700	-1.69230300	-0.95415500
N	-3.88172200	-1.67100200	-0.23260400
O	-4.87234100	-1.01326600	-0.52277500
O	-3.90408200	-2.62717500	0.53186700
H	2.28777000	-1.79727300	-1.40465600
H	1.20883700	0.81690300	-2.63284400
H	3.36376800	1.00984700	-0.38007500
H	3.24322700	-0.49866700	-2.31309000
H	1.81631400	-0.78729600	1.39358100

E-TS3-b

0 1

C	-1.31781800	2.61978500	-0.42862800
C	-2.03730900	1.41554200	-0.21813900
C	-3.30237000	1.46813300	0.36450300
C	-3.82712000	2.71227200	0.72266400
C	-3.10228000	3.88507600	0.51248200
C	-1.83014600	3.85442300	-0.06896300
C	0.05236200	0.99596800	-1.25160300
H	-3.87913100	0.56830700	0.54896200
H	-4.81213200	2.76334600	1.17470600
H	-3.52816000	4.83977400	0.80434600
H	-1.26488000	4.76563700	-0.23631300
N	-0.08456000	2.34502400	-1.02613100
C	0.93398800	3.32448200	-1.33122400
H	0.56204000	4.05790900	-2.05199200
H	1.25150600	3.84185800	-0.42100200
H	1.78340500	2.79318400	-1.76224100
O	1.00172500	0.42001300	-1.76969900
C	-0.52143700	-0.33849600	1.86930500
C	-1.23876400	-1.51039300	1.88321100
C	-2.11160200	-1.72672500	-0.12010100
C	-2.05713100	-3.18744200	-0.41428500
F	-2.78703500	-3.53715400	-1.48885700

F	-0.79707800	-3.58779100	-0.65387200
F	-2.52826900	-3.89650200	0.61883700
C	-1.16046200	0.37123000	-0.69704100
N	-1.28027000	-0.94820100	-0.82037200
C	0.84446800	-0.27985600	1.38941300
C	1.62575500	0.88686200	1.56782600
C	2.57372900	-1.33837700	0.29484400
C	2.91768300	0.91725300	1.09415300
H	1.19604800	1.74543300	2.07371700
C	3.39813400	-0.23030100	0.45913600
H	2.94364400	-2.22008600	-0.22044400
H	3.55273700	1.78825000	1.21038400
N	1.32709700	-1.36915800	0.74747900
N	4.74617100	-0.26131600	-0.05951100
O	5.43627800	0.74025100	0.07038000
O	5.13446000	-1.28631200	-0.60361800
H	-0.70683600	-2.44972000	1.76420800
H	-0.94659600	0.57886600	2.26423000
H	-3.07968600	-1.33580200	0.16134500
H	-2.18964200	-1.55069800	2.40503100
H	-0.44770900	-1.38590600	-1.23198900

E-C

E-TS3-c

0 1

C	3.83101700	-1.20794300	0.09873600
C	3.44144600	0.11360300	-0.20160400
C	4.30911000	0.95879800	-0.88209500
C	5.56899300	0.47331800	-1.24074400
C	5.94090300	-0.83827500	-0.93852000
C	5.07379200	-1.70413400	-0.26475200
C	1.72691100	-1.00655400	0.97286900
H	4.01571000	1.97611100	-1.12637400
H	6.26330500	1.12160600	-1.76509600
H	6.92242300	-1.19673500	-1.23232800
H	5.36267800	-2.72349800	-0.02995800
N	2.80058300	-1.85353500	0.78092200
C	2.85185500	-3.21238500	1.27179600
H	3.01438600	-3.91133700	0.44677600
H	3.65429900	-3.32857900	2.00590400
H	1.89426800	-3.42701900	1.74673600
O	0.71207000	-1.27831800	1.61068800
C	-0.44566600	0.44847500	-1.34427800
C	0.66608900	-0.34650100	-1.52799200
C	0.10753500	1.46785800	0.68725800

C	-0.50898300	2.82123900	0.76221900
F	-0.49670700	3.33885600	2.00410100
F	0.13808300	3.69571000	-0.02825300
F	-1.78782900	2.78040800	0.37394400
C	2.07192000	0.24269500	0.26474300
N	1.41891300	1.40627900	0.47395600
C	-1.76386800	-0.07750000	-0.95812600
C	-1.91606000	-1.24669300	-0.18855100
C	-4.04458700	0.20864800	-1.09737000
C	-3.18615300	-1.69429900	0.11663000
H	-1.04164800	-1.76888000	0.18432200
C	-4.26079200	-0.94581800	-0.35448500
H	-4.88559900	0.79419600	-1.45639900
H	-3.35359200	-2.58849900	0.70619500
N	-2.82222000	0.63538000	-1.39272100
N	-5.62189100	-1.36345300	-0.06175500
O	-5.77898900	-2.36361900	0.61999000
O	-6.53763500	-0.69323000	-0.51283400
H	0.62602500	-1.41686800	-1.34346900
H	-0.48849000	1.41729700	-1.83584500
H	-0.37760500	0.65830000	1.21547100
H	1.46866500	-0.00531100	-2.17228500
H	1.87122600	2.24590500	0.10825400

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C	3.90871100	-1.10481300	-0.01273200
C	3.20076700	-0.09928600	-0.67972400
C	3.81719500	0.65338000	-1.66136700
C	5.15771600	0.38580600	-1.96995500
C	5.84798500	-0.62148100	-1.29884000
C	5.23316400	-1.39006400	-0.30374900
C	1.82997900	-1.17363500	0.92618600
H	3.27180800	1.43614800	-2.18252800
H	5.66011900	0.96418200	-2.73805800
H	6.88524800	-0.81939600	-1.55077600
H	5.77139700	-2.17488300	0.21743200
N	3.07946600	-1.72447300	0.93359500
C	3.48644500	-2.81338900	1.79472700
H	3.78953400	-3.67803100	1.19767400
H	4.32026900	-2.50460500	2.43109700
H	2.63244200	-3.08087600	2.41676400
O	0.89642000	-1.51666400	1.63468900
C	-0.47616400	0.71917300	-0.68994500
C	0.64096300	-0.25599300	-1.13844800

C	0.06572900	1.27604200	0.65407600
C	-0.39811400	2.68522500	0.92190200
F	0.00470700	3.13079000	2.11923200
F	0.07538400	3.54728600	0.00268900
F	-1.73681100	2.76398200	0.88878300
C	1.80196200	-0.04442700	-0.12583800
N	1.52180600	1.21853700	0.58228700
C	-1.85217600	0.11600300	-0.57114900
C	-2.07173900	-1.01744300	0.22424900
C	-4.06847300	0.23912300	-1.15760900
C	-3.35095000	-1.53733500	0.31611500
H	-1.24190600	-1.47257900	0.75832400
C	-4.35095400	-0.88628900	-0.39510000
H	-4.85618200	0.74489200	-1.70672200
H	-3.57778800	-2.41233800	0.91408500
N	-2.83452600	0.73191400	-1.24345100
N	-5.72046900	-1.38895800	-0.34413100
O	-5.93002900	-2.40420300	0.29707500
O	-6.57950400	-0.76742000	-0.94651100
H	0.30596400	-1.29627400	-1.15047100
H	-0.54515200	1.54573000	-1.40249900
H	-0.28159500	0.65889300	1.48935200
H	0.97938600	-0.00249800	-2.14485600
H	1.84561500	1.97668900	-0.02206600

E-d

E-TS3-d

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C	3.46964100	-1.47399000	0.20407000
C	3.30922700	-0.11623000	-0.14151000
C	4.33015900	0.56278900	-0.79475900
C	5.51560500	-0.12270000	-1.07537600
C	5.66164300	-1.46600700	-0.72581300
C	4.63624100	-2.16695700	-0.08239800
C	1.38558300	-0.92330500	0.97227400
H	4.21030500	1.60539000	-1.07638300
H	6.32801800	0.39396000	-1.57555300
H	6.58821200	-1.98209500	-0.95684700
H	4.75061500	-3.21181800	0.18755200
N	2.31970800	-1.93476200	0.84476300
C	2.15551900	-3.25874000	1.40112900
H	2.23531000	-4.01723700	0.61739500
H	2.91194100	-3.45172900	2.16756700
H	1.16382500	-3.30675800	1.85175600
O	0.32926800	-0.99927100	1.58628000

C	-0.41871100	0.67196100	-1.45588500
C	0.70319100	-0.10921600	-1.63390900
C	0.18535800	1.74668800	0.60706900
C	-0.21807700	3.17894300	0.62326200
F	-0.12981200	3.74406100	1.84130300
F	0.55416200	3.91114400	-0.19931900
F	-1.48980000	3.32165800	0.22773100
C	1.95035500	0.23540600	0.23956200
N	1.47779800	1.48754500	0.42944400
C	-1.70991000	0.09745900	-1.06522400
C	-2.86942000	0.89829200	-1.06733100
C	-2.90734900	-1.73744500	-0.36196100
C	-4.07962300	0.34842800	-0.69586100
H	-2.80267500	1.93892900	-1.36242500
C	-4.08457600	-0.99445800	-0.33064800
H	-2.91919300	-2.78873500	-0.09008500
H	-4.99529300	0.92806000	-0.68487100
N	-1.74811500	-1.20573700	-0.72232400
N	-5.32353300	-1.63273300	0.07427100
O	-6.34186000	-0.95871700	0.07354200
O	-5.28615900	-2.81106300	0.39497300
H	0.63272000	-1.18714800	-1.52556400
H	-0.45566400	1.67267500	-1.87777800
H	-0.43475100	1.02750100	1.12234000
H	1.53415200	0.26764500	-2.22060600
H	2.06138800	2.24631600	0.07449300

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C	4.05221900	-0.92920900	-0.14851300
C	3.11997100	-0.06628000	-0.73599900
C	3.46863500	0.69781200	-1.83366900
C	4.76982500	0.58922000	-2.34222500
C	5.68648100	-0.27589000	-1.74891900
C	5.34378800	-1.05464200	-0.63682300
C	2.16488900	-1.20901800	1.10830400
H	2.74549700	1.36898200	-2.29095500
H	5.06318300	1.18003800	-3.20343700
H	6.69033900	-0.35277000	-2.15506000
H	6.06065400	-1.72767700	-0.17799800
N	3.46993300	-1.59121200	0.94086900
C	4.15549600	-2.54403100	1.78554000
H	4.53082000	-3.38062900	1.18944300
H	4.99208000	-2.06623100	2.30323800
H	3.43750800	-2.91365800	2.51778900

O	1.40429900	-1.61443700	1.96756400
C	-0.45746400	0.52170400	-0.57193400
C	0.56861100	-0.60649700	-0.78829000
C	0.01932900	1.10190400	0.77652100
C	-0.49041100	2.49608400	1.03859700
F	-0.08352300	2.96958300	2.22323300
F	-0.06247400	3.36209200	0.10031600
F	-1.83179300	2.53227300	1.02734800
C	1.82465900	-0.16480400	0.02420100
N	1.47677700	1.09562300	0.71639200
C	-1.88994000	0.05798000	-0.56577400
C	-2.83414700	0.62520800	-1.42694600
C	-3.45387600	-1.33749500	0.37176900
C	-4.14465500	0.17709200	-1.38123200
H	-2.53780700	1.40612000	-2.11840900
C	-4.43892000	-0.82007900	-0.46277800
H	-3.69193000	-2.11394000	1.09201200
H	-4.91453200	0.58019900	-2.02888100
N	-2.19966200	-0.90234200	0.31743600
N	-5.80106800	-1.33574800	-0.36444300
O	-6.64910600	-0.84300900	-1.08801400
O	-6.01484100	-2.23037000	0.43612800
H	0.17371500	-1.54147700	-0.38187800
H	-0.33015900	1.29500000	-1.33702300
H	-0.32514100	0.46138000	1.59668700
H	0.80128700	-0.75095000	-1.84416000
H	1.77300500	1.86401100	0.11239800

Bond lengths of E-TS3-a/b/c/d

E-TS3-a(C2-C5)

Bond Length (18C, 25C) along IRC

X-Axis: Intrinsic Reaction Coordinate

Y-Axis: Bond Length (Angstroms)

#	X	Y
	0.000000000	2.9502379038
	0.1675100000	2.9397601245
	0.3350000000	2.9295348561
	0.5025000000	2.9196654789
	0.6700000000	2.9102941641
	0.8375200000	2.9016583795
	1.0050500000	2.8930448590
	1.1725700000	2.8844231011
	1.3401000000	2.8758280155
	1.5076300000	2.8672024439
	1.6751500000	2.8584739098

1. 8426800000	2. 8495548520
2. 0102000000	2. 8403214338
2. 1777100000	2. 8306196988
2. 3452000000	2. 8202295558
2. 5126600000	2. 8088735955
2. 6800600000	2. 7961967122
2. 8473700000	2. 7818425211
3. 0145900000	2. 7656270437
3. 1818100000	2. 7477109216
3. 3491000000	2. 7285016772
3. 5164600000	2. 7083361470
3. 6838200000	2. 6874212607
3. 8508100000	2. 6658369017
4. 0168000000	2. 6436888167
4. 1834600000	2. 6212619580
4. 3504900000	2. 5983291045
4. 5175600000	2. 5751559876
4. 6844600000	2. 5519171595
4. 8516100000	2. 5285501500
5. 0189000000	2. 5051288181
5. 1862900000	2. 4817405324
5. 3532500000	2. 4582504623
5. 5207100000	2. 4346849965
5. 6881100000	2. 4109248077
5. 8553200000	2. 3866700640
6. 0228300000	2. 3623027637
6. 1903400000	2. 3372553164
6. 3578400000	2. 3117889371
6. 5253100000	2. 2857959097
6. 6927500000	2. 2593343593
6. 8601300000	2. 2323424818
7. 0273200000	2. 2048073930
7. 1948200000	2. 1770352051
7. 3623300000	2. 1484527350
7. 5298100000	2. 1196661041
7. 6972600000	2. 0904103318
7. 8646200000	2. 0610730818
8. 0317400000	2. 0312136496
8. 1992400000	2. 0012540234
8. 3667600000	1. 9714383756
8. 5342600000	1. 9416980395
8. 7017600000	1. 9123674826
8. 8692500000	1. 8832371684
9. 0367300000	1. 8548028971

9. 2041800000	1. 8269027340
9. 3716000000	1. 8002713486
9. 5389800000	1. 7748443101
9. 7062900000	1. 7517141089
9. 8735000000	1. 7308983401
10. 0403600000	1. 7137206487
10. 2076700000	1. 6983727738
10. 3749800000	1. 6901247773
10. 5422500000	1. 6805848484
10. 7092700000	1. 6756974524
10. 8767100000	1. 6711459822
11. 0440900000	1. 6676416805
11. 2111400000	1. 6647194585
11. 3785600000	1. 6623203739
11. 5456900000	1. 6601253756
11. 7131500000	1. 6577895255
11. 8804600000	1. 6569943399
12. 0472200000	1. 6548756006
12. 2145900000	1. 6523569589
12. 3815500000	1. 6519024394
12. 5488200000	1. 6505551489
12. 7161300000	1. 6494876388
12. 8834000000	1. 6484600531
13. 0506300000	1. 6475256856
13. 2177800000	1. 6466731742
13. 3849100000	1. 6458892445
13. 5519700000	1. 6451576848
13. 7190500000	1. 6444640603
13. 8860900000	1. 6437965462
14. 0530900000	1. 6431431935
14. 2201600000	1. 6424872297
14. 3871900000	1. 6418173108
14. 5543900000	1. 6411484926
14. 7216900000	1. 6404937416
14. 8890800000	1. 6381727526
15. 0557300000	1. 6385696641
15. 2228200000	1. 6380934657
15. 3901200000	1. 6378014018
15. 5575600000	1. 6382391914
15. 7246900000	1. 6372637098
15. 8919600000	1. 6367090477
16. 0593400000	1. 6357015470
16. 2260800000	1. 6357173931
16. 3931100000	1. 6353804829

16.5602900000 1.6350503644
16.7275200000 1.6346558550

E-TS3-a(C1-C3)

Bond Length (19C, 20C) along IRC

X-Axis: Intrinsic Reaction Coordinate

Y-Axis: Bond Length (Angstroms)

#	X	Y
0.0000000000		2.1933856509
0.1675100000		2.1621251073
0.3350000000		2.1303984114
0.5025000000		2.0982177309
0.6700000000		2.0656184848
0.8375200000		2.0324895141
1.0050500000		1.9994168151
1.1725700000		1.9664132267
1.3401000000		1.9334735987
1.5076300000		1.9006517639
1.6751500000		1.8680226734
1.8426800000		1.8356808030
2.0102000000		1.8037599840
2.1777100000		1.7724594454
2.3452000000		1.7420729018
2.5126600000		1.7130657649
2.6800600000		1.6861602951
2.8473700000		1.6623890187
3.0145900000		1.6428628827
3.1818100000		1.6280656232
3.3491000000		1.6172375738
3.5164600000		1.6093043817
3.6838200000		1.6028466427
3.8508100000		1.5977562597
4.0168000000		1.5943833120
4.1834600000		1.5904440041
4.3504900000		1.5871604827
4.5175600000		1.5842479373
4.6844600000		1.5817450073
4.8516100000		1.5796848798
5.0189000000		1.5778126049
5.1862900000		1.5762713234
5.3532500000		1.5742745612
5.5207100000		1.5725577296
5.6881100000		1.5707882578
5.8553200000		1.5693719905
6.0228300000		1.5680043648

6. 1903400000	1. 5658517304
6. 3578400000	1. 5651270344
6. 5253100000	1. 5622463392
6. 6927500000	1. 5625387601
6. 8601300000	1. 5583509439
7. 0273200000	1. 5584584627
7. 1948200000	1. 5571842784
7. 3623300000	1. 5547661465
7. 5298100000	1. 5535299987
7. 6972600000	1. 5519265661
7. 8646200000	1. 5496313707
8. 0317400000	1. 5487304824
8. 1992400000	1. 5476811679
8. 3667600000	1. 5451074678
8. 5342600000	1. 5446220922
8. 7017600000	1. 5419233734
8. 8692500000	1. 5419732382
9. 0367300000	1. 5389875516
9. 2041800000	1. 5396577419
9. 3716000000	1. 5362790598
9. 5389800000	1. 5377611601
9. 7062900000	1. 5338240055
9. 8735000000	1. 5365365096
10. 0403600000	1. 5337530817
10. 2076700000	1. 5326015000
10. 3749800000	1. 5342955978
10. 5422500000	1. 5316498897
10. 7092700000	1. 5331293833
10. 8767100000	1. 5341120169
11. 0440900000	1. 5319285551
11. 2111400000	1. 5331899284
11. 3785600000	1. 5345834149
11. 5456900000	1. 5334810115
11. 7131500000	1. 5328675162
11. 8804600000	1. 5346164584
12. 0472200000	1. 5338218093
12. 2145900000	1. 5333467337
12. 3815500000	1. 5340407616
12. 5488200000	1. 5342043401
12. 7161300000	1. 5343382863
12. 8834000000	1. 5344079790
13. 0506300000	1. 5344380032
13. 2177800000	1. 5344261422
13. 3849100000	1. 5343620971

13. 5519700000	1. 5342421873
13. 7190500000	1. 5340773082
13. 8860900000	1. 5338902158
14. 0530900000	1. 5337001899
14. 2201600000	1. 5335322933
14. 3871900000	1. 5334010239
14. 5543900000	1. 5333141877
14. 7216900000	1. 5332621237
14. 8890800000	1. 5337236431
15. 0557300000	1. 5336681983
15. 2228200000	1. 5335463474
15. 3901200000	1. 5333615864
15. 5575600000	1. 5329635117
15. 7246900000	1. 5328844361
15. 8919600000	1. 5329157485
16. 0593400000	1. 5328058763
16. 2260800000	1. 5327937390
16. 3931100000	1. 5326794608
16. 5602900000	1. 5326497037
16. 7275200000	1. 5326714536

E-TS3-b(C2-C5)

Bond Length (18C, 25C) along IRC

X-Axis: Intrinsic Reaction Coordinate

Y-Axis: Bond Length (Angstroms)

#	X	Y
0. 0000000000		2. 7382833559
0. 1671900000		2. 7255679496
0. 3343600000		2. 7131024167
0. 5015400000		2. 7008620401
0. 6687300000		2. 6888896122
0. 8359300000		2. 6775825072
1. 0031300000		2. 6661750568
1. 1703300000		2. 6545016486
1. 3375400000		2. 6425582436
1. 5047400000		2. 6302523760
1. 6719400000		2. 6174771015
1. 8391400000		2. 6041100951
2. 0063300000		2. 5899942146
2. 1735100000		2. 5749302473
2. 3406800000		2. 5586802569
2. 5078300000		2. 5409611654
2. 6749400000		2. 5214666100
2. 8420200000		2. 4999502494
3. 0090700000		2. 4763527464

3. 1761300000	2. 4508480641
3. 3432200000	2. 4237868400
3. 5103400000	2. 3955090254
3. 6774800000	2. 3663217704
3. 8446400000	2. 3363559451
4. 0117600000	2. 3059149237
4. 1787900000	2. 2748629564
4. 3458400000	2. 2436431652
4. 5129800000	2. 2119979482
4. 6801700000	2. 1801163448
4. 8473600000	2. 1478698595
5. 0145600000	2. 1155674542
5. 1817400000	2. 0830226482
5. 3489100000	2. 0504625140
5. 5160500000	2. 0177247112
5. 6831900000	1. 9851595598
5. 8503400000	1. 9525395763
6. 0175100000	1. 9201428001
6. 1847000000	1. 8878434530
6. 3519000000	1. 8558629509
6. 5190900000	1. 8242703390
6. 6862800000	1. 7931768346
6. 8534600000	1. 7629999034
7. 0205800000	1. 7336975186
7. 1875700000	1. 7068206097
7. 3545100000	1. 6821061716
7. 5209000000	1. 6609761512
7. 6874200000	1. 6463990850
7. 8535500000	1. 6352393036
8. 0195400000	1. 6291384434
8. 1863500000	1. 6244259348
8. 3533800000	1. 6219749079
8. 5203300000	1. 6188380040
8. 6870300000	1. 6177315965
8. 8531200000	1. 6159335192
9. 0179700000	1. 6141565431
9. 1830000000	1. 6134400239
9. 3490100000	1. 6119791345
9. 5160500000	1. 6112241721
9. 6830700000	1. 6100448848
9. 8500200000	1. 6112283855
10. 0164600000	1. 6082094693
10. 1828200000	1. 6088738804
10. 3492800000	1. 6089228400

10. 5163700000	1. 6074266831
10. 6834900000	1. 6078897342
10. 8505500000	1. 6063363364
11. 0174200000	1. 6073857298
11. 1842900000	1. 6065732028
11. 3511700000	1. 6064590678
11. 5183000000	1. 6060271116
11. 6854100000	1. 6052247765
11. 8524200000	1. 6052789039
12. 0191700000	1. 6047643478
12. 1856200000	1. 6047746757
12. 3524900000	1. 6040983559
12. 5195200000	1. 6036931154
12. 6866000000	1. 6034835948
12. 8537600000	1. 6038081701
13. 0209300000	1. 6037759252
13. 1880300000	1. 6034423209
13. 3551600000	1. 6026586476
13. 5220600000	1. 6031117684
13. 6885200000	1. 6019497024
13. 8545600000	1. 6026217502
14. 0206600000	1. 6012712874
14. 1871300000	1. 6023531807
14. 3538900000	1. 6017008316
14. 5207200000	1. 6015604510
14. 6878900000	1. 6012709749
14. 8549900000	1. 6010631499
15. 0220500000	1. 6003237359
15. 1888300000	1. 6001837477
15. 3557300000	1. 5997357990
15. 5226100000	1. 5995296930
15. 6897800000	1. 5993968968
15. 8568700000	1. 5989082346
16. 0240400000	1. 5987168720
16. 1911700000	1. 5993414689
16. 3582100000	1. 5981470750
16. 5252800000	1. 5979729116
16. 6922900000	1. 5975921305

E-TS3-b(C1-C3)

Bond Length (19C, 20C) along IRC

X-Axis: Intrinsic Reaction Coordinate

Y-Axis: Bond Length (Angstroms)

#	X	Y
	0. 0000000000	2. 1958835757

0. 1671900000	2. 1649813513
0. 3343600000	2. 1336530003
0. 5015400000	2. 1019642015
0. 6687300000	2. 0700179868
0. 8359300000	2. 0375814655
1. 0031300000	2. 0052216873
1. 1703300000	1. 9730396553
1. 3375400000	1. 9410484780
1. 5047400000	1. 9093317562
1. 6719400000	1. 8779865810
1. 8391400000	1. 8471327357
2. 0063300000	1. 8169251123
2. 1735100000	1. 7875770798
2. 3406800000	1. 7593808177
2. 5078300000	1. 7327400032
2. 6749400000	1. 7081822735
2. 8420200000	1. 6863244899
3. 0090700000	1. 6676636229
3. 1761300000	1. 6523902695
3. 3432200000	1. 6401399794
3. 5103400000	1. 6304448356
3. 6774800000	1. 6224072747
3. 8446400000	1. 6160678213
4. 0117600000	1. 6098785441
4. 1787900000	1. 6059285875
4. 3458400000	1. 6005933850
4. 5129800000	1. 5968656868
4. 6801700000	1. 5921309726
4. 8473600000	1. 5891487108
5. 0145600000	1. 5851388630
5. 1817400000	1. 5823627215
5. 3489100000	1. 5787896320
5. 5160500000	1. 5762638483
5. 6831900000	1. 5729851704
5. 8503400000	1. 5705808256
6. 0175100000	1. 5676397348
6. 1847000000	1. 5652527105
6. 3519000000	1. 5626353179
6. 5190900000	1. 5603035494
6. 6862800000	1. 5578908894
6. 8534600000	1. 5556719497
7. 0205800000	1. 5534015568
7. 1875700000	1. 5514791646
7. 3545100000	1. 5494102796

7. 5209000000	1. 5475500286
7. 6874200000	1. 5471165703
7. 8535500000	1. 5451810619
8. 0195400000	1. 5457915288
8. 1863500000	1. 5462178660
8. 3533800000	1. 5454438176
8. 5203300000	1. 5469037232
8. 6870300000	1. 5448127522
8. 8531200000	1. 5482517421
9. 0179700000	1. 5445902918
9. 1830000000	1. 5468847377
9. 3490100000	1. 5463123235
9. 5160500000	1. 5469485084
9. 6830700000	1. 5465477035
9. 8500200000	1. 5479561013
10. 0164600000	1. 5475118176
10. 1828200000	1. 5477895404
10. 3492800000	1. 5474826567
10. 5163700000	1. 5476830000
10. 6834900000	1. 5475471019
10. 8505500000	1. 5480509501
11. 0174200000	1. 5474819834
11. 1842900000	1. 5476290800
11. 3511700000	1. 5475658400
11. 5183000000	1. 5476060292
11. 6854100000	1. 5478579172
11. 8524200000	1. 5476398127
12. 0191700000	1. 5477176670
12. 1856200000	1. 5475806205
12. 3524900000	1. 5476290008
12. 5195200000	1. 5476211521
12. 6866000000	1. 5475893060
12. 8537600000	1. 5474990334
13. 0209300000	1. 5474346021
13. 1880300000	1. 5473828917
13. 3551600000	1. 5473730425
13. 5220600000	1. 5473791769
13. 6885200000	1. 5472542427
13. 8545600000	1. 5473991071
14. 0206600000	1. 5471704630
14. 1871300000	1. 5473767857
14. 3538900000	1. 5473129059
14. 5207200000	1. 5473275406
14. 6878900000	1. 5473287918

14.8549900000	1.5472827708
15.0220500000	1.5472145210
15.1888300000	1.5470938311
15.3557300000	1.5471100484
15.5226100000	1.5470892598
15.6897800000	1.5471597246
15.8568700000	1.5470055930
16.0240400000	1.5470629556
16.1911700000	1.5473760432
16.3582100000	1.5469931218
16.5252800000	1.5470687854
16.6922900000	1.5470317079

E-TS3-c(C2-C3)

Bond Length (18C, 20C) along IRC

X-Axis: Intrinsic Reaction Coordinate

Y-Axis: Bond Length (Angstroms)

#	X	Y
0.0000000000	2.3392972377	
0.3361600000	2.2910331245	
0.6403900000	2.2470525960	
0.9760600000	2.1959595901	
1.3118800000	2.1456164870	
1.6478400000	2.0957640317	
1.9838400000	2.0465345680	
2.3198900000	1.9981561988	
2.6559600000	1.9506509193	
2.9920300000	1.9040472229	
3.3281200000	1.8583325920	
3.6642000000	1.8136723752	
4.0002700000	1.7703577181	
4.3363300000	1.7288569605	
4.6723500000	1.6897321739	
5.0082400000	1.6543717040	
5.3437800000	1.6248597973	
5.6787900000	1.6046350905	
6.0132300000	1.5911766456	
6.3333600000	1.5869843362	
6.6543200000	1.5728946400	
6.9826400000	1.5838964785	
7.2849000000	1.5729309890	
7.6075400000	1.5546990690	
7.9250200000	1.5852972403	
8.2373900000	1.5535477281	
8.5314400000	1.5710391952	

8. 8292900000	1. 5625838977
9. 1471400000	1. 5700901523
9. 4583300000	1. 5606710127
9. 7626800000	1. 5574375625
10. 0704300000	1. 5769320942
10. 3701700000	1. 5531512112
10. 6699700000	1. 5689924421
10. 9690800000	1. 5626812647
11. 2817700000	1. 5625864495
11. 6048100000	1. 5641527875
11. 9245800000	1. 5623913907
12. 2547700000	1. 5622618318
12. 5825500000	1. 5629217066
12. 9110000000	1. 5611274248
13. 2344300000	1. 5626339656
13. 5609000000	1. 5607303090
13. 8857300000	1. 5625058255
14. 2027400000	1. 5605864654
14. 5241700000	1. 5610826446
14. 8450800000	1. 5611928617
15. 1694800000	1. 5604415653
15. 4891600000	1. 5597616151
15. 8087000000	1. 5611649402
16. 1292400000	1. 5583008512
16. 4443500000	1. 5612649096
16. 7480700000	1. 5587106712
17. 0560400000	1. 5597286876
17. 3533900000	1. 5592385466
17. 6665300000	1. 5589326219
17. 9775400000	1. 5592871267
18. 2797800000	1. 5582619176
18. 5876500000	1. 5587603383
18. 9080600000	1. 5575764762
19. 2227000000	1. 5594383497
19. 5239700000	1. 5568203918
19. 8231000000	1. 5580113894
20. 1142700000	1. 5583564265
20. 4202000000	1. 5566435958
20. 7300500000	1. 5579282266
21. 0258400000	1. 5573528869
21. 3162300000	1. 5571010121
21. 6113800000	1. 5568234771
21. 9269800000	1. 5569408605
22. 2253500000	1. 5564998220

22. 5157300000	1. 5571090982
22. 7934600000	1. 5561425753
23. 0785900000	1. 5565291639
23. 3819400000	1. 5562070052
23. 7017400000	1. 5560659657
23. 9944800000	1. 5562985234
24. 2925300000	1. 5553988593
24. 5879000000	1. 5560935530
24. 8749000000	1. 5550922510
25. 1911100000	1. 5555373389
25. 4786600000	1. 5552408583
25. 7651200000	1. 5560449162
26. 0521900000	1. 5556686515
26. 3757500000	1. 5543241456
26. 6689500000	1. 5558793924
26. 9705900000	1. 5540722306
27. 2589100000	1. 5546678758
27. 5567300000	1. 5546250981
27. 8550000000	1. 5547134541
28. 1671100000	1. 5539119229
28. 4732900000	1. 5546352096
28. 7659100000	1. 5537886888
29. 0505200000	1. 5541877483
29. 3458900000	1. 5529762717
29. 6316000000	1. 5534048573
29. 9347900000	1. 5542099870
30. 2319300000	1. 5533323292
30. 5120800000	1. 5538048548
30. 7888800000	1. 5538984829
31. 1047400000	1. 5533616408

E-TS3-c(C1-C5)

Bond Length (19C, 25C) along IRC

X-Axis: Intrinsic Reaction Coordinate

Y-Axis: Bond Length (Angstroms)

#	X	Y
0. 0000000000	2. 3531705223	
0. 3361600000	2. 3060749865	
0. 6403900000	2. 2765263915	
0. 9760600000	2. 2332740184	
1. 3118800000	2. 1876339368	
1. 6478400000	2. 1408427682	
1. 9838400000	2. 0931270773	
2. 3198900000	2. 0445364119	
2. 6559600000	1. 9952892056	

2. 9920300000	1. 9456267064
3. 3281200000	1. 8958762658
3. 6642000000	1. 8462901957
4. 0002700000	1. 7971743118
4. 3363300000	1. 7490247456
4. 6723500000	1. 7029596246
5. 0082400000	1. 6608235282
5. 3437800000	1. 6273486761
5. 6787900000	1. 6049712799
6. 0132300000	1. 6003538503
6. 3333600000	1. 5839732625
6. 6543200000	1. 5933484493
6. 9826400000	1. 5727994645
7. 2849000000	1. 5824142441
7. 6075400000	1. 5844045701
7. 9250200000	1. 5700742990
8. 2373900000	1. 5801274975
8. 5314400000	1. 5776549846
8. 8292900000	1. 5623444383
9. 1471400000	1. 5901940155
9. 4583300000	1. 5582162582
9. 7626800000	1. 5778349347
10. 0704300000	1. 5677008588
10. 3701700000	1. 5666871821
10. 6699700000	1. 5725025167
10. 9690800000	1. 5660519680
11. 2817700000	1. 5678269391
11. 6048100000	1. 5671493614
11. 9245800000	1. 5672429774
12. 2547700000	1. 5668175160
12. 5825500000	1. 5675653481
12. 9110000000	1. 5646867231
13. 2344300000	1. 5675008133
13. 5609000000	1. 5641039934
13. 8857300000	1. 5672144881
14. 2027400000	1. 5637746666
14. 5241700000	1. 5657839600
14. 8450800000	1. 5638872255
15. 1694800000	1. 5650104771
15. 4891600000	1. 5631963089
15. 8087000000	1. 5648087849
16. 1292400000	1. 5620555014
16. 4443500000	1. 5650140427
16. 7480700000	1. 5618142986

17. 0560400000	1. 5640440769
17. 3533900000	1. 5617892957
17. 6665300000	1. 5629298400
17. 9775400000	1. 5614516521
18. 2797800000	1. 5628128365
18. 5876500000	1. 5614861372
18. 9080600000	1. 5615442420
19. 2227000000	1. 5614130579
19. 5239700000	1. 5613354600
19. 8231000000	1. 5609557619
20. 1142700000	1. 5605235204
20. 4202000000	1. 5605479295
20. 7300500000	1. 5599468049
21. 0258400000	1. 5607478231
21. 3162300000	1. 5596177348
21. 6113800000	1. 5599967693
21. 9269800000	1. 5592382172
22. 2253500000	1. 5593863057
22. 5157300000	1. 5597411987
22. 7934600000	1. 5592274865
23. 0785900000	1. 5593017625
23. 3819400000	1. 5589882393
23. 7017400000	1. 5587269946
23. 9944800000	1. 5587983198
24. 2925300000	1. 5588447173
24. 5879000000	1. 5578567511
24. 8749000000	1. 5584647249
25. 1911100000	1. 5575774770
25. 4786600000	1. 5577817669
25. 7651200000	1. 5581351624
26. 0521900000	1. 5579268613
26. 3757500000	1. 5570256141
26. 6689500000	1. 5577676482
26. 9705900000	1. 5573916948
27. 2589100000	1. 5570103603
27. 5567300000	1. 5586069954
27. 8550000000	1. 5563333687
28. 1671100000	1. 5568677529
28. 4732900000	1. 5580414933
28. 7659100000	1. 5536471427
29. 0505200000	1. 5573318924
29. 3458900000	1. 5567600677
29. 6316000000	1. 5550727710
29. 9347900000	1. 5552641896

30.2319300000	1.5556923630
30.5120800000	1.5555614666
30.7888800000	1.5560799062
31.1047400000	1.5545884149

E-TS3-d(C2-C3)

Bond Length (18C, 20C) along IRC

X-Axis: Intrinsic Reaction Coordinate

Y-Axis: Bond Length (Angstroms)

#	X	Y
0.0000000000	2.4032720794	
0.3408600000	2.3586902610	
0.6530300000	2.3163797743	
0.9932800000	2.2695059609	
1.3337800000	2.2240228072	
1.6744400000	2.1790729163	
2.0151600000	2.1338701282	
2.3559200000	2.0880236998	
2.6966800000	2.0413015256	
3.0374500000	1.9936880577	
3.3782200000	1.9451012193	
3.7189800000	1.8954939285	
4.0597200000	1.8449038577	
4.4004100000	1.7938557794	
4.7410200000	1.7436110752	
5.0814900000	1.6972418238	
5.4217600000	1.6592306887	
5.7617300000	1.6338236749	
6.1002300000	1.6176056614	
6.4270800000	1.6086720342	
6.7617300000	1.5934896917	
7.0938000000	1.5986380736	
7.4118100000	1.5822269227	
7.7258900000	1.5890239487	
8.0361500000	1.5656352638	
8.3538500000	1.5938988617	
8.6676000000	1.5741625506	
8.9848400000	1.5737702173	
9.2984700000	1.5737772135	
9.5914100000	1.5869736802	
9.8891700000	1.5588186020	
10.1881400000	1.5846308925	
10.4935800000	1.5746851613	
10.8188200000	1.5747389423	
11.1234900000	1.5755528872	

11. 4455900000	1. 5679557267
11. 7486900000	1. 5768564596
12. 0522300000	1. 5712192272
12. 3717000000	1. 5715323331
12. 6798700000	1. 5732589099
12. 9870500000	1. 5721923803
13. 2957800000	1. 5727739043
13. 6014700000	1. 5727700641
13. 9290000000	1. 5719660270
14. 2352000000	1. 5722593554
14. 5670300000	1. 5725887939
14. 8876400000	1. 5714311743
15. 2117300000	1. 5726867340
15. 5267800000	1. 5721877040
15. 8411700000	1. 5718557599
16. 1727300000	1. 5724746264
16. 4711300000	1. 5718424196
16. 7614200000	1. 5720146888
17. 0730900000	1. 5720544078
17. 4001100000	1. 5711873089
17. 6913400000	1. 5724278856
18. 0196100000	1. 5707185587
18. 3173700000	1. 5724246322
18. 6104200000	1. 5723160807
18. 9433000000	1. 5708270323
19. 2225200000	1. 5738297592
19. 5123500000	1. 5722917229
19. 8400500000	1. 5713599189
20. 1704700000	1. 5728722705
20. 4954000000	1. 5715034010
20. 8163500000	1. 5721949370
21. 1304000000	1. 5723044554
21. 4467200000	1. 5714011988
21. 7556400000	1. 5730250688
22. 0524800000	1. 5719949145
22. 3350900000	1. 5721602937
22. 6616900000	1. 5720983893
22. 9461700000	1. 5725497513
23. 2670000000	1. 5712939569
23. 5568500000	1. 5723524362
23. 8085900000	1. 5730612132
24. 1202000000	1. 5727641268
24. 4275400000	1. 5722058421
24. 7479900000	1. 5725337804

25.0408000000	1.5721754306
25.3514200000	1.5718535627
25.6232100000	1.5726015914
25.9219100000	1.5727254502
26.2070300000	1.5723042845
26.5336300000	1.5722942618
26.8223000000	1.5729286991
27.1323200000	1.5718756930
27.4175000000	1.5716822542
27.7076600000	1.5715231176
28.0063100000	1.5727017736
28.2983100000	1.5727824995
28.6255100000	1.5719087936
28.9262000000	1.5720797400
29.1795900000	1.5725096109
29.4903800000	1.5714063026
29.8066600000	1.5723169893
30.0978000000	1.5721185642
30.3809600000	1.5730102635
30.6722900000	1.5720620020
30.9565800000	1.5716129416
31.2891300000	1.5727142656

E-TS3-d(C1-C5)

Bond Length (19C, 25C) along IRC

X-Axis: Intrinsic Reaction Coordinate

Y-Axis: Bond Length (Angstroms)

#	X	Y
0.0000000000	2.2768565949	
0.3408600000	2.2245514066	
0.6530300000	2.1879264903	
0.9932800000	2.1377042531	
1.3337800000	2.0851715950	
1.6744400000	2.0318396854	
2.0151600000	1.9786437253	
2.3559200000	1.9261386800	
2.6966800000	1.8747939662	
3.0374500000	1.8249713900	
3.3782200000	1.7772263220	
3.7189800000	1.7322808981	
4.0597200000	1.6911937869	
4.4004100000	1.6551347862	
4.7410200000	1.6256686511	
5.0814900000	1.6032791178	
5.4217600000	1.5886591053	

5. 7617300000	1. 5771937472
6. 1002300000	1. 5779692001
6. 4270800000	1. 5669229256
6. 7617300000	1. 5747665612
7. 0938000000	1. 5611727226
7. 4118100000	1. 5681199494
7. 7258900000	1. 5634176635
8. 0361500000	1. 5771543209
8. 3538500000	1. 5517788861
8. 6676000000	1. 5711129763
8. 9848400000	1. 5564224821
9. 2984700000	1. 5626485692
9. 5914100000	1. 5741198665
9. 8891700000	1. 5425487478
10. 1881400000	1. 5734147878
10. 4935800000	1. 5602574363
10. 8188200000	1. 5631384046
11. 1234900000	1. 5585861451
11. 4455900000	1. 5599163787
11. 7486900000	1. 5570381652
12. 0522300000	1. 5599879981
12. 3717000000	1. 5544013568
12. 6798700000	1. 5587691025
12. 9870500000	1. 5565714980
13. 2957800000	1. 5566003440
13. 6014700000	1. 5570780868
13. 9290000000	1. 5547589272
14. 2352000000	1. 5566911813
14. 5670300000	1. 5539991102
14. 8876400000	1. 5563248832
15. 2117300000	1. 5543397730
15. 5267800000	1. 5544826170
15. 8411700000	1. 5539731112
16. 1727300000	1. 5537738076
16. 4711300000	1. 5531652361
16. 7614200000	1. 5539509351
17. 0730900000	1. 5529612390
17. 4001100000	1. 5526821061
17. 6913400000	1. 5527020960
18. 0196100000	1. 5512722303
18. 3173700000	1. 5530058568
18. 6104200000	1. 5512247697
18. 9433000000	1. 5517869953
19. 2225200000	1. 5510078669

19. 5123500000	1. 5512386559
19. 8400500000	1. 5505921775
20. 1704700000	1. 5499878037
20. 4954000000	1. 5501518686
20. 8163500000	1. 5492876138
21. 1304000000	1. 5490971796
21. 4467200000	1. 5487653932
21. 7556400000	1. 5482875751
22. 0524800000	1. 5483339560
22. 3350900000	1. 5479212847
22. 6616900000	1. 5479312387
22. 9461700000	1. 5477250241
23. 2670000000	1. 5475539324
23. 5568500000	1. 5470093768
23. 8085900000	1. 5476082717
24. 1202000000	1. 5469194076
24. 4275400000	1. 5466479980
24. 7479900000	1. 5470390477
25. 0408000000	1. 5467025081
25. 3514200000	1. 5456253885
25. 6232100000	1. 5466254494
25. 9219100000	1. 5459033947
26. 2070300000	1. 5460697362
26. 5336300000	1. 5453672533
26. 8223000000	1. 5463564770
27. 1323200000	1. 5451539610
27. 4175000000	1. 5460649805
27. 7076600000	1. 5451342895
28. 0063100000	1. 5451791875
28. 2983100000	1. 5450958686
28. 6255100000	1. 5450379156
28. 9262000000	1. 5449066060
29. 1795900000	1. 5450855117
29. 4903800000	1. 5449660615
29. 8066600000	1. 5443212592
30. 0978000000	1. 5446016075
30. 3809600000	1. 5444263597
30. 6722900000	1. 5448105247
30. 9565800000	1. 5438914136
31. 2891300000	1. 5440911391

Comparison with the other solvents

THF

1a- THF

O 1

C	1.34127900	-0.74899500	0.00000600
C	2.41236100	0.15722300	0.00001300
C	3.72858600	-0.27425000	-0.00000900
C	3.94621800	-1.65649800	-0.00001000
C	2.88958800	-2.56801100	0.00000300
C	1.56818400	-2.11607300	0.00000900
C	0.10850700	0.04582700	-0.00002200
H	4.55698600	0.42601000	-0.00003400
H	4.96711600	-2.02551500	-0.00001900
H	3.09748900	-3.63247200	0.00000300
H	0.73183500	-2.80853800	0.00002000
N	1.93510000	1.47783400	0.00001700
O	-0.14182700	2.49797000	-0.00004600
C	0.56576200	1.50878700	-0.00003300
N	-1.07873400	-0.39808000	-0.00006200
C	-2.19019700	0.53352300	-0.00020400
H	-2.19206100	1.18005200	-0.88356800
H	-2.19202700	1.18041800	0.88289200
C	-3.46387600	-0.27157300	0.00000100
F	-3.55658000	-1.06369300	-1.07834800
F	-4.53768700	0.53459200	-0.00027800
F	-3.55662600	-1.06297300	1.07888100
C	2.77541300	2.65510600	0.00006000
H	3.40704100	2.67389900	-0.89230400
H	2.12354600	3.52868900	0.00022300
H	3.40721600	2.67369100	0.89230200

2a- THF

O 1

C	-1.65148900	0.26161100	0.00001600
C	-0.86794900	1.42460100	-0.00003300
C	0.51224400	1.31454200	-0.00005200
C	1.04336400	0.03314100	-0.00002400
C	0.21031300	-1.08355900	0.00002200
N	-1.11007000	-0.97005400	0.00004200
H	1.16155500	2.18207500	-0.00008700
H	-1.34529500	2.39824500	-0.00005400
H	0.63492000	-2.08280000	0.00004400
N	2.48994100	-0.15384600	-0.00004100
O	2.91564100	-1.29672400	-0.00002700
O	3.19125100	0.84342700	-0.00006800
C	-3.12043300	0.37188700	0.00004400
H	-3.51782700	1.38380500	0.00000400

C	-3.93943400	-0.67994600	0.00011700
H	-3.55102000	-1.69377000	0.00016100
H	-5.01626900	-0.54754600	0.00013800

E-TS1- THF

0 1

C	-1.29844000	2.09071200	-0.92259400
C	0.07314100	2.15495500	-0.60554200
C	0.59443800	3.29447600	-0.00767700
C	-0.26362400	4.36685800	0.25511800
C	-1.61864500	4.29016700	-0.07053900
C	-2.16152600	3.14504600	-0.66431000
C	-0.45319100	0.05981300	-1.55796500
H	1.64962100	3.33897400	0.24712900
H	0.12768500	5.26876300	0.71481800
H	-2.26841700	5.13385700	0.14066500
H	-3.21673600	3.08655100	-0.91203800
N	-1.58934100	0.84112700	-1.48000300
C	-2.89916600	0.39801500	-1.89786700
H	-3.60574500	0.43438000	-1.06210700
H	-3.28001500	1.02029200	-2.71329300
H	-2.80236400	-0.63156400	-2.24651600
O	-0.41833400	-1.08845300	-1.99392900
C	1.19651500	0.45629900	2.30404800
C	1.06051900	1.66859000	2.84700000
C	2.26310200	-0.82896100	-0.76955100
H	1.93745200	2.22958900	3.15286200
C	3.70403800	-1.01763400	-0.46982100
F	4.00919900	-2.32778600	-0.37588000
F	4.54894100	-0.50534300	-1.39701300
F	4.06761500	-0.44400900	0.69913400
C	0.65320100	0.86487100	-0.96410500
N	1.84752700	0.46016300	-0.65124400
C	0.06680000	-0.34745200	1.83260100
C	-1.27661600	-0.08233100	2.13621900
C	-0.56641000	-2.20401400	0.52516400
C	-2.26881800	-0.88981300	1.61633800
H	-1.53151800	0.75894700	2.76799400
C	-1.89223500	-1.97099500	0.82153400
H	-0.24165300	-2.98109200	-0.15644800
H	-3.31741000	-0.70018400	1.81613800
N	0.36769700	-1.40307100	1.04204800
N	-2.90721400	-2.82206800	0.21091100
O	-4.06883900	-2.47384000	0.32412000
O	-2.52856700	-3.81717500	-0.37892100

H	0.09659800	2.14738800	2.99214200
H	2.18206800	0.03214100	2.13603400
H	1.87323900	-1.48461000	-1.54887200
H	1.38215400	-1.34813200	0.42486200

E-TS3-a- THF

0 1

C	-1.17375200	1.75206700	0.75818200
C	-0.38890500	0.68757000	1.25503800
C	-0.96336100	-0.28706000	2.06914900
C	-2.32151300	-0.19325300	2.36486300
C	-3.09067200	0.85678900	1.85259800
C	-2.52690500	1.85258200	1.04977500
C	0.92414000	2.11896300	-0.09101900
H	-0.36716400	-1.10947800	2.45557900
H	-2.79026400	-0.94812900	2.98711000
H	-4.14969600	0.90471700	2.08612900
H	-3.12854300	2.66664000	0.65813600
N	-0.38484900	2.57993000	-0.03523100
C	-0.84007500	3.78784000	-0.68303400
H	-1.66620500	3.56756900	-1.36603100
H	-1.17230700	4.52437600	0.05471200
H	-0.00089800	4.19666600	-1.24674600
O	1.85668500	2.68374000	-0.65473300
C	1.16217700	-0.11404900	-2.08339700
C	2.32700100	-0.77997400	-1.80795000
C	3.07347800	0.06626000	0.07540500
C	4.14806100	-0.88471200	0.48421100
F	4.93203900	-0.39693400	1.46105500
F	3.62206900	-2.03390700	0.94742000
F	4.94897400	-1.18132000	-0.54470800
C	0.91588100	0.86676800	0.68441400
N	1.96419500	0.04974200	0.82347900
C	-0.15636100	-0.56906100	-1.69974600
C	-1.29102600	0.17592600	-2.09405500
C	-1.46207700	-2.03943800	-0.50856000
C	-2.53732900	-0.19042900	-1.63451800
H	-1.16484700	1.04766500	-2.72776400
C	-2.61486200	-1.31285900	-0.81271100
H	-1.53241600	-2.92456300	0.11744700
H	-3.43147700	0.37189700	-1.87821900
N	-0.26196900	-1.68686800	-0.94108600
N	-3.87604900	-1.69385800	-0.22223200
O	-4.87105400	-1.04911300	-0.52330100
O	-3.88722200	-2.64072300	0.55273100

H	2.28511500	-1.79258800	-1.41500800
H	1.20195600	0.82281300	-2.63256000
H	3.36915200	1.00666200	-0.37012400
H	3.23895900	-0.48997700	-2.31957600
H	1.80092200	-0.79223500	1.37906700

E-TS3-b-THF

0 1

C	-1.35815600	2.60633900	-0.42664800
C	-2.05701600	1.38924900	-0.21819100
C	-3.32275300	1.41929200	0.36384600
C	-3.87084400	2.65344000	0.72090400
C	-3.16755300	3.83873700	0.51067400
C	-1.89421500	3.83091000	-0.06825700
C	0.04268400	1.00645100	-1.24782000
H	-3.88331500	0.50948400	0.55063200
H	-4.85698500	2.68671000	1.17198600
H	-3.61174300	4.78552100	0.80078600
H	-1.34600900	4.75272600	-0.23418000
N	-0.11819200	2.35359100	-1.01872000
C	0.88102800	3.34978000	-1.32919200
H	0.49506600	4.07520300	-2.05090900
H	1.19400600	3.87496200	-0.42164700
H	1.73791100	2.83211400	-1.76202800
O	1.00005300	0.44792900	-1.76668600
C	-0.51670300	-0.33800500	1.86686200
C	-1.22009800	-1.51797400	1.88152600
C	-2.08410700	-1.74831200	-0.12513600
C	-2.01073000	-3.20912500	-0.41470400
F	-2.72477900	-3.56832900	-1.49646500
F	-0.74434000	-3.59493600	-0.63797900
F	-2.48731000	-3.91866900	0.61565300
C	-1.16061000	0.36109300	-0.69536700
N	-1.25846600	-0.95975800	-0.82110000
C	0.85002600	-0.26727200	1.38794100
C	1.62531300	0.90081400	1.57622600
C	2.58230800	-1.30827600	0.28232100
C	2.91747500	0.93981400	1.10269800
H	1.19265600	1.75286100	2.09059100
C	3.40229900	-0.19912500	0.45781800
H	2.95478400	-2.18272600	-0.24318600
H	3.55149200	1.81047800	1.22607800
N	1.33565400	-1.34740100	0.73481900
N	4.75267800	-0.21797400	-0.06150600
O	5.43378200	0.78804700	0.07681500

O	5.14538400	-1.23716300	-0.61102300
H	-0.67584000	-2.45026500	1.76273700
H	-0.95099600	0.57398500	2.26444400
H	-3.05930400	-1.36626700	0.14315600
H	-2.16843700	-1.57023300	2.40698500
H	-0.41099100	-1.38384700	-1.21662200

Toluene

1a-Toluene

0 1

C	1.34272800	-0.74821900	0.00009800
C	2.41408900	0.15736300	-0.00000400
C	3.72957200	-0.27532500	-0.00013300
C	3.94658700	-1.65738900	-0.00011500
C	2.88960100	-2.56734500	0.00001900
C	1.56876700	-2.11469200	0.00012400
C	0.10910000	0.04572700	0.00012900
H	4.55856600	0.42412500	-0.00025500
H	4.96703200	-2.02729600	-0.00020500
H	3.09698400	-3.63174800	0.00003600
H	0.72989200	-2.80368100	0.00022800
N	1.93608200	1.47794700	0.00001100
O	-0.14125000	2.49730300	0.00006300
C	0.56456000	1.50816200	0.00005900
N	-1.07723500	-0.39899400	0.00013000
C	-2.18996000	0.52998100	0.00003300
H	-2.19059700	1.17901900	-0.88166200
H	-2.19073900	1.17902400	0.88172800
C	-3.46508100	-0.27524200	-0.00005100
F	-3.55716600	-1.06349600	-1.07913700
F	-4.53477700	0.53677300	-0.00019200
F	-3.55736700	-1.06336600	1.07911300
C	2.76953000	2.65815200	-0.00003900
H	3.40121700	2.68323000	-0.89262700
H	2.11098200	3.52693900	0.00017100
H	3.40155300	2.68304900	0.89231600

2a-Toluene

0 1

C	-1.65214000	0.26475700	0.00001100
C	-0.86654200	1.42670800	-0.00003300
C	0.51348300	1.31425500	-0.00005000
C	1.04305200	0.03265700	-0.00002400
C	0.20735700	-1.08211900	0.00001700
N	-1.11231600	-0.96657300	0.00003500

H	1.16838500	2.17750100	-0.00008100
H	-1.34169400	2.40147700	-0.00005200
H	0.63176200	-2.08137800	0.00003700
N	2.49103000	-0.15540800	-0.00003800
O	2.91279600	-1.29858300	-0.00002200
O	3.18997500	0.84267900	-0.00006600
C	-3.12115100	0.37242800	0.00004000
H	-3.52385900	1.38223900	-0.00000600
C	-3.93414400	-0.68326400	0.00012200
H	-3.53561000	-1.69284000	0.00017300
H	-5.01163700	-0.55842900	0.00014300

E-TS1-Toluene

O 1

C	-1.45139200	1.91298900	-0.94586000
C	-0.08471100	2.08163500	-0.64322800
C	0.35512400	3.26532700	-0.06517300
C	-0.57855000	4.27269300	0.19525000
C	-1.92688100	4.09230300	-0.11481100
C	-2.38768300	2.90337800	-0.69071800
C	-0.46423100	-0.06447900	-1.54676700
H	1.40800300	3.39257800	0.16891600
H	-0.25082000	5.20806700	0.63750500
H	-2.63549600	4.88847500	0.09055300
H	-3.43744500	2.76401700	-0.92939100
N	-1.65418500	0.63824900	-1.48249900
C	-2.92499800	0.09730900	-1.90156500
H	-3.62022300	0.01989600	-1.05794100
H	-3.37457100	0.72314400	-2.67825900
H	-2.73952000	-0.89917200	-2.30598100
O	-0.35720000	-1.22443200	-1.93748700
C	1.25895300	0.61962400	2.23260100
C	1.10704200	1.82112100	2.79468400
C	2.30554500	-0.73878000	-0.77408500
H	1.97905700	2.40041300	3.07859700
C	3.76047200	-0.83999200	-0.48472500
F	4.13017800	-2.12963500	-0.35205000
F	4.56200400	-0.31399100	-1.43504400
F	4.09933000	-0.21372300	0.66485800
C	0.58446200	0.83320300	-0.98644000
N	1.80886600	0.51622900	-0.67483800
C	0.14631500	-0.21774000	1.78539900
C	-1.21043200	0.07536600	1.99867300
C	-0.43680500	-2.19795400	0.64172200
C	-2.17864000	-0.79248600	1.53911300

H	-1.49258000	0.98884400	2.50628100
C	-1.77078200	-1.95357400	0.88141700
H	-0.09295800	-3.02671600	0.03432700
H	-3.23596000	-0.59139900	1.67061100
N	0.47925300	-1.34498300	1.11170400
N	-2.76199700	-2.87175200	0.33122600
O	-3.92432000	-2.50720500	0.34752700
O	-2.36204300	-3.93140600	-0.11044500
H	0.13936600	2.27541200	2.98269800
H	2.25244500	0.22718100	2.03902900
H	1.93517600	-1.44505000	-1.51735200
H	1.47001400	-1.28906800	0.49169900

E-TS3-a-Toluene

0 1

C	-1.16698500	1.82324600	0.71335500
C	-0.41930800	0.73521100	1.21706700
C	-1.03334700	-0.22219100	2.02224200
C	-2.39235400	-0.09283900	2.29815600
C	-3.12477800	0.97681600	1.77478700
C	-2.52132500	1.95781600	0.98366300
C	0.95806000	2.14447700	-0.08825000
H	-0.47001500	-1.06217900	2.42062700
H	-2.89071100	-0.83651000	2.91031000
H	-4.18570700	1.05145400	1.99043200
H	-3.09453100	2.78907900	0.58585900
N	-0.34223900	2.63639700	-0.05914200
C	-0.73468100	3.88268100	-0.67202900
H	-1.53127200	3.72227400	-1.40518900
H	-1.08101900	4.59590600	0.08223100
H	0.14285800	4.29025900	-1.17532400
O	1.91492400	2.68994300	-0.62667000
C	1.15981000	-0.07333000	-2.07919100
C	2.33372800	-0.72949900	-1.82142300
C	3.05719700	0.05234200	0.09933900
C	4.09201200	-0.94037500	0.51281500
F	4.87488500	-0.49301000	1.50791600
F	3.51187000	-2.07321400	0.95382500
F	4.89762200	-1.25599900	-0.50545700
C	0.90060500	0.88515700	0.67180400
N	1.92772900	0.04255700	0.81796300
C	-0.14767700	-0.56436600	-1.69777500
C	-1.30371800	0.14627600	-2.08850200
C	-1.40502900	-2.06882100	-0.49895900
C	-2.53750200	-0.25425300	-1.62152800

H	-1.20554600	1.01957500	-2.72451600
C	-2.57901100	-1.37706600	-0.80041700
H	-1.44937400	-2.95303300	0.13035200
H	-3.45028400	0.28122000	-1.85561800
N	-0.21681500	-1.68038500	-0.93343900
N	-3.82661400	-1.78409400	-0.19178300
O	-4.83982400	-1.17432400	-0.49871200
O	-3.79909200	-2.71222600	0.60345500
H	2.30093500	-1.75391500	-1.45996600
H	1.18325200	0.87360700	-2.61151400
H	3.38512900	0.99953400	-0.30768300
H	3.24214200	-0.41448000	-2.32415600
H	1.72806100	-0.81893900	1.32690700

E-TS3-b-Toluene

O 1

C	1.48128500	-2.56267200	-0.41862200
C	2.12174400	-1.31280200	-0.21222600
C	3.39076800	-1.28516100	0.36152600
C	4.00250700	-2.49141100	0.70911700
C	3.35723600	-3.70829800	0.49844600
C	2.08090200	-3.75983100	-0.07041300
C	-0.00109500	-1.03054300	-1.22781300
H	3.90904000	-0.34991600	0.54451300
H	4.99236800	-2.47714800	1.15246100
H	3.85040700	-4.63310500	0.77916500
H	1.57727900	-4.70685900	-0.23468400
N	0.22616600	-2.36965000	-0.99884200
C	-0.71751200	-3.41057300	-1.32958300
H	-0.29024500	-4.10839900	-2.05562800
H	-1.01523900	-3.96085200	-0.43162700
H	-1.59431200	-2.93002200	-1.76562700
O	-0.98621600	-0.52115900	-1.74088500
C	0.50076300	0.34834000	1.86741500
C	1.16056700	1.55291500	1.88295300
C	2.00130400	1.82460100	-0.12963500
C	1.85576700	3.28077900	-0.42026200
F	2.53868300	3.66711800	-1.51167000
F	0.57072700	3.60479100	-0.62566300
F	2.31509200	4.01067500	0.60353600
C	1.17279400	-0.32821100	-0.68119600
N	1.20709600	0.99560200	-0.81500800
C	-0.86530700	0.23479800	1.38937200
C	-1.61368900	-0.94558800	1.59774100
C	-2.61524400	1.21486900	0.25744700

C	-2.90433500	-1.02094600	1.12218900
H	-1.16420800	-1.77739400	2.13036900
C	-3.41132500	0.09274400	0.45394300
H	-3.00453400	2.06821500	-0.28961600
H	-3.52355700	-1.89977800	1.26043300
N	-1.37051700	1.28910200	0.71228800
N	-4.76306700	0.06889000	-0.07149900
O	-5.41299700	-0.95461300	0.07779900
O	-5.17754200	1.07105000	-0.63193900
H	0.58065700	2.46336200	1.76508100
H	0.96513500	-0.54666700	2.26951100
H	2.99841200	1.48967700	0.12014000
H	2.10442300	1.64037500	2.41177500
H	0.32737400	1.37736200	-1.18286600