Supporting Information

Mechanistic investigation of MOF-catalyzed Intramolecular Hydroamination of *o*-Alkynylanilines using Zn-UiO-67-BPY as catalyst

Taotao Liu,[*a] Yintong Yao,[a] Zhipeng Pei,[b] Yuqing Jiang,[c] Jinshuai Song,[*c,d] and Yu Lan[*c,e]

a. College of Chemistry and Chemical Engineering, Henan Institute of Science and Technology, Xinxiang, Henan 453000, China.

b. Institute for Nanoscale Science and Technology, College of Science and Engineering, Flinders University, Bedford Park, South Australia 5042, Australia.

c. Green Catalysis Center, and College of Chemistry, Zhengzhou University Zhengzhou, Henan 450001, China.

d. Laboratory of Synthetic Biology, Zhengzhou University, Zhengzhou 450001, China.

e. School of Chemistry and Chemical Engineering and Chongqing Key Laboratory of Theoretical and Computational Chemistry, Chongqing University, Chongqing 400030, China.

*Corresponding Author(s): Yu Lan: lanyu@cqu.edu.cn; Jinshuai Song: jssong@zzu.edu.cn; Taotao Liu: liutt@hist.edu.cn.

Table S1. The adaption of 27 coordinated anions to the formulars in Fig.5.

Coordination anion	Free energy barrier / kcal/mol	NPA Charge / e
SeO_4^{2-}	24.8	-1.527
$AsBr_6^-$	21.3	-1.632
PF_6^-	18.5	-1.714
ClO_2^-	25.9	-1.482
ClO_4^-	20.5	-1.626
TeO_4^{2-}	24.1	-1.498
BeF_3^-	18.3	-1.668
SrF_3^-	22.0	-1.553
CaF_3^-	19.9	-1.601
BrO_4^-	18.5	-1.636
AsF_6^-	15.8	-1.709
AlF_4^-	17.4	-1.642
MgF_3^-	18.7	-1.603
$AsCl_6^-$	20.5	-1.546
BrO_3^-	23.1	-1.437
PbF_5^-	17.7	-1.665
IO_4^-	17.3	-1.612
GaF_4^-	15.4	-1.615
$SrCl_3^-$	18.9	-1.488
$MgBr_3^-$	16.5	-1.558
$MgCl_3^-$	16.9	-1.543
MgI_3^-	16.6	-1.549
BeI_3^-	15.6	-1.574
$CaCl_3^-$	16.7	-1.54
$CaBr_3^-$	15.6	-1.561
ClO_3^-	18.9	-1.449

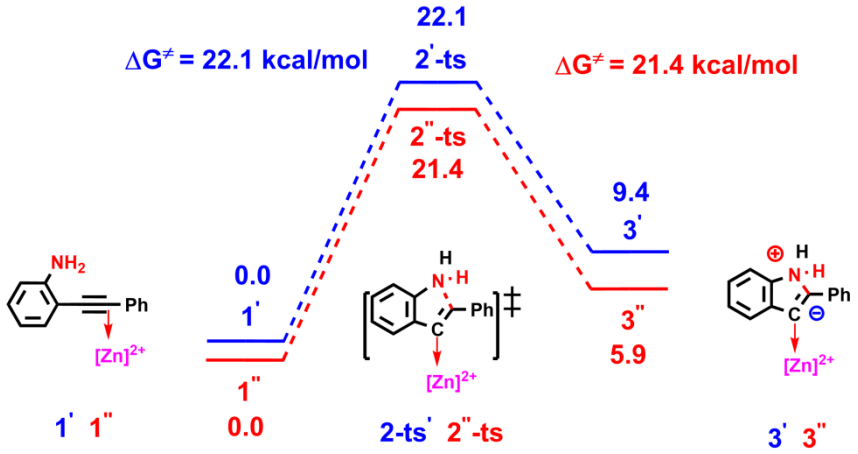
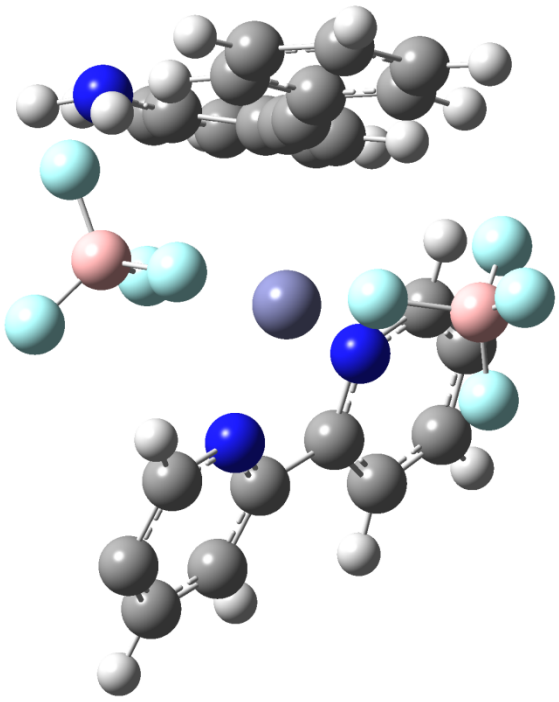


Fig. S1 Potential energy diagrams (in kcal/mol) for the 5-*endo* cyclization step when: the substrate acting as a co-catalyst is present within the octahedral cage during the reaction (blue), and the QM region of the octahedral cage additionally includes two Zr_6 clusters connected to the Zn(II)-bipyridine moiety (red).

Geometrical structure of QM region, energy and coordinates of QM region in intermediate 1



Thermal correction to Gibbs Free Energy= 0.323852 a.u.

ONIOM: gridpoint 1 method: low system: model energy: 0.444352938959 a.u.

ONIOM: gridpoint 2 method: high system: model energy: -3719.635537770234 a.u.

ONIOM: gridpoint 3 method: low system: real energy: 9.260978421385 a.u.

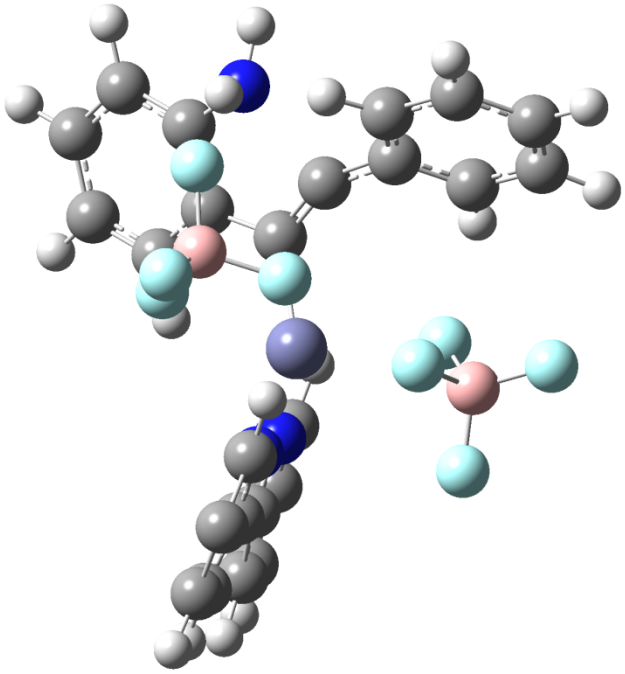
ONIOM: extrapolated energy = -3710.818912287808a.u.

C	8.47911400	3.79916100	-1.63971000
C	9.37465500	4.42767500	-0.76065300
H	9.92344200	5.32313100	-1.06798400
C	9.59282800	3.91575300	0.51408700
H	10.27708600	4.41863200	1.19584000
C	8.95066900	2.73886600	0.89068400
C	7.79043200	2.68438700	-1.14918600
H	7.01414800	2.17765400	-1.71768200
C	9.44791400	0.83885100	4.68585300
C	8.47909200	0.48595300	3.72899200

H	7.76492200	-0.32376700	3.89282800
C	9.20203700	2.08931800	2.20634600
C	10.35405400	1.84055600	4.32404600
H	11.15060800	2.15270300	5.00335400
C	10.22838400	2.47020000	3.08087800
H	10.93151300	3.25244400	2.79601500
N	8.37104000	1.08697400	2.54093200
N	8.05705500	2.15709500	0.05918700
Zn	7.24210900	0.42740900	0.85443900
F	5.45880400	3.17847600	1.28791400
F	3.42098500	2.13652400	1.00763900
F	4.96889500	2.14152500	-0.68963500
F	5.35390900	0.87895800	1.20544600
F	8.95018100	-1.02293800	0.71784400
F	9.02355200	-2.27622200	2.65616000
F	8.12999900	-3.18076900	0.73894700
F	7.03798300	-1.44755500	1.82108800
B	8.32676900	-2.05153700	1.50966400
B	4.74540000	2.16782500	0.68996800
C	9.96073100	0.93005500	-4.01333800
C	8.77532900	0.68252400	-3.33630600
C	8.59583500	-0.46755700	-2.53350900
C	9.64459000	-1.43547500	-2.45528500
C	10.84233700	-1.16468500	-3.15104300
C	10.99857300	-0.00652900	-3.90445200
H	10.07580100	1.83160400	-4.61492800
H	7.94873100	1.38179200	-3.43494700
H	11.65563700	-1.89433000	-3.08867000
H	11.94367400	0.16929100	-4.42448000
N	9.48049600	-2.61734200	-1.78244500
H	8.76478600	-2.67775700	-1.06429700

H	10.32836600	-3.11111200	-1.53071800
C	7.37731100	-0.69069800	-1.83709200
C	6.33665900	-0.97313400	-1.24930900
C	5.07555500	-1.46790600	-0.77511200
C	5.00741700	-2.71622800	-0.12115600
C	3.89697800	-0.71861900	-0.95913500
C	3.78065900	-3.20243300	0.32708400
H	5.92155800	-3.28246800	0.05307300
C	2.67814000	-1.21415300	-0.50226700
H	3.95768100	0.26405800	-1.42273300
C	2.61323400	-2.45561000	0.13795100
H	3.74303700	-4.16473200	0.84304900
H	1.77554100	-0.61182500	-0.63070100
H	1.65460000	-2.83582200	0.50291900

Geometrical structure of QM region, energy and coordinates of QM region in 2-ts



Thermal correction to Gibbs Free Energy= 0.323888 a.u.

ONIOM: gridpoint 1 method: low system: model energy: 0.486117579157 a.u.

ONIOM: gridpoint 2 method: high system: model energy: -3719.595402533309 a.u.

ONIOM: gridpoint 3 method: low system: real energy: 9.300710848457 a.u.

ONIOM: extrapolated energy = -3710.780809264009 a.u.

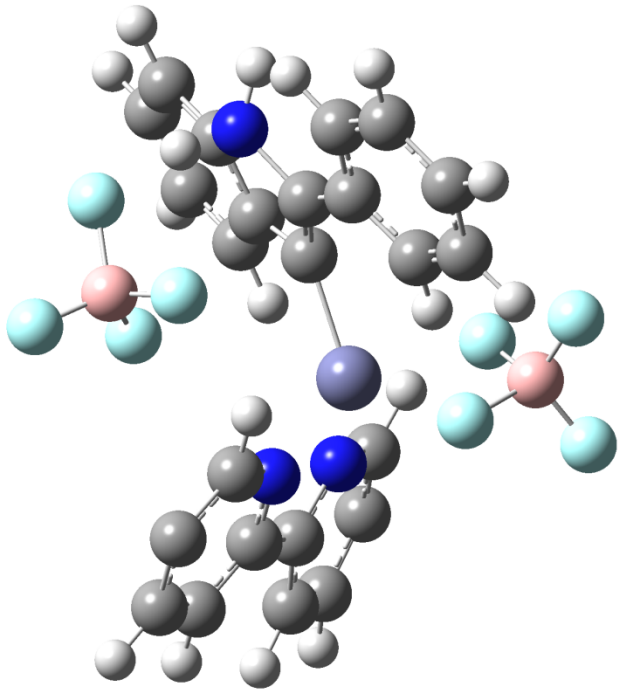
Imaginary frequency: 306.67*i*

C	-8.18915000	3.89300100	2.62875700
C	-9.00890500	4.75232800	1.87735800
H	-9.44006700	5.64969600	2.33160100
C	-9.30577900	4.46849300	0.54976400
H	-9.93817100	5.14450900	-0.02389000
C	-8.81675900	3.28919400	-0.01323800
C	-7.65262400	2.78755500	1.95952900
H	-6.95319200	2.09596300	2.43184000
C	-9.62162400	2.02858400	-4.01356500
C	-8.76659500	1.35355100	-3.12090000

H	-8.22631800	0.44883500	-3.40704900
C	-9.17891300	2.85417100	-1.39107800
C	-10.32873200	3.12283700	-3.50767200
H	-11.03140700	3.67945800	-4.13251500
C	-10.10453200	3.53673000	-2.19170800
H	-10.64022200	4.39928600	-1.79698600
N	-8.56432200	1.75156900	-1.85851000
N	-7.99287900	2.49297300	0.69181000
Zn	-7.32579300	0.78740500	-0.38557300
F	-5.40025700	3.73111300	-0.38607400
F	-3.49647900	2.45951000	-0.67079800
F	-4.92053500	2.04067300	1.07942400
F	-5.57610400	1.54014300	-1.07357300
F	-9.11746900	-0.97682500	-0.62107200
F	-9.09378000	-1.93693000	-2.71249400
F	-7.94042000	-2.93324500	-0.98601600
F	-7.22900900	-0.90052300	-1.86742200
B	-8.38280600	-1.72809700	-1.56635200
B	-4.79821100	2.50292200	-0.23829300
C	-9.52675400	-1.11318700	3.85911900
C	-8.77691700	-0.44015000	2.88917500
C	-7.82436600	-1.13351200	2.13772100
C	-7.65602400	-2.52458400	2.35350700
C	-8.41868600	-3.20010100	3.30029700
C	-9.35067400	-2.48394300	4.06345600
H	-10.24877400	-0.55825600	4.46164200
H	-8.92165100	0.62728400	2.73073300
H	-8.29025000	-4.27654600	3.44430800
H	-9.94353900	-3.00630000	4.81905000
N	-6.66006400	-3.11617400	1.52919600
H	-7.05484000	-3.39929800	0.62065800

H	-6.12460800	-3.87150600	1.95534800
C	-6.90171400	-0.59887200	1.13997400
C	-5.95878000	-1.35598400	0.70028400
C	-4.79648100	-1.60969500	-0.09767100
C	-4.73285500	-2.67918700	-1.01403000
C	-3.72557200	-0.69864700	-0.00573300
C	-3.59946300	-2.84505500	-1.80364800
H	-5.58744400	-3.34323100	-1.13643800
C	-2.61080500	-0.85516200	-0.82793500
H	-3.80057400	0.14436000	0.67953500
C	-2.53999700	-1.93243400	-1.71466800
H	-3.56096300	-3.67376800	-2.51413100
H	-1.80779600	-0.11670300	-0.77986300
H	-1.66160500	-2.05497700	-2.35532800

Geometrical structure of QM region, energy and coordinates of QM region in intermediate 3



Thermal correction to Gibbs Free Energy= 0.327500 a.u.

ONIOM: gridpoint 1 method: low system: model energy: 47.111459736876 a.u.

ONIOM: gridpoint 2 method: high system: model energy: -3719.621455727259 a.u.

ONIOM: gridpoint 3 method: low system: real energy: 55.929279975151 a.u.

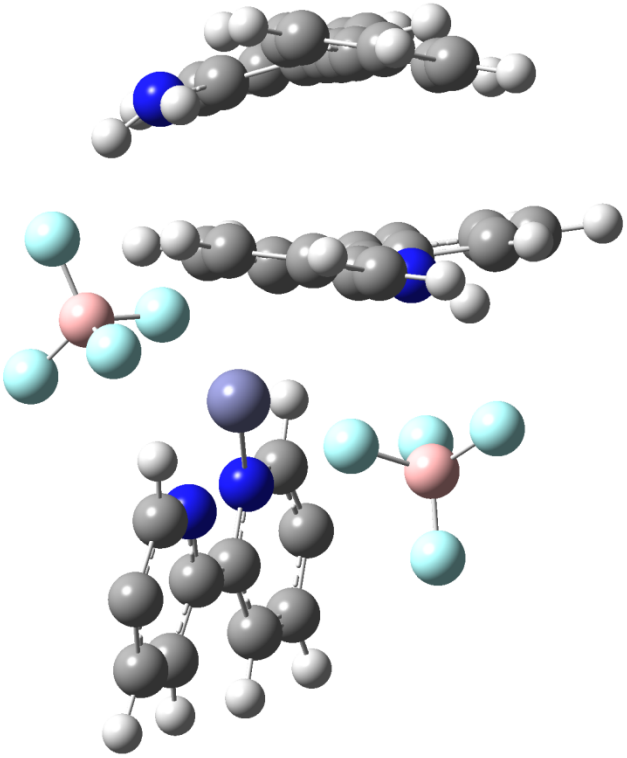
ONIOM: extrapolated energy = -3710.803635488984 a.u.

C	-8.11982700	4.21197200	2.88470900
C	-9.34870900	4.56120400	2.29038700
H	-9.98732100	5.33373800	2.72897300
C	-9.78918200	3.92822700	1.13566100
H	-10.74563300	4.20191700	0.69244200
C	-9.00106300	2.92572300	0.57284100
C	-7.33621400	3.28194800	2.19946800
H	-6.33020900	3.00743600	2.52096000
C	-10.17308600	0.44638900	-2.71094700
C	-8.88531200	0.47031900	-2.13644300
H	-8.09236500	-0.20185000	-2.46505500

C	-9.45807800	2.10329800	-0.58211300
C	-11.12250200	1.30782600	-2.15503600
H	-12.14551900	1.34299200	-2.53623500
C	-10.76446300	2.13509300	-1.08412500
H	-11.51025300	2.78938700	-0.63351300
N	-8.54687400	1.27273000	-1.12215400
N	-7.78337700	2.65762800	1.09034100
Zn	-6.72470100	1.28163700	-0.03252100
F	-4.63504200	4.47242400	-0.55456200
F	-3.45558300	2.56860600	-1.09038800
F	-4.80392800	2.60720900	0.77692500
F	-5.75733600	2.58184500	-1.28896700
F	-8.76951000	-1.42985200	0.27613200
F	-9.73651900	-3.07363400	-1.00038200
F	-7.81126600	-3.53361800	0.19797800
F	-7.73220100	-2.15821100	-1.63204800
B	-8.56399700	-2.52624100	-0.56058700
B	-4.57912700	3.11117300	-0.52899700
C	-6.85647800	-1.15707600	4.25363600
C	-6.74568800	-0.38310100	3.09348900
C	-6.22989100	-0.97319100	1.93382100
C	-5.86283300	-2.32416100	1.99138000
C	-5.98219800	-3.12394400	3.11167100
C	-6.47796500	-2.50672900	4.27038900
H	-7.24888900	-0.70008700	5.16454100
H	-7.05397000	0.66225800	3.09447100
H	-5.71321100	-4.18295100	3.09753100
H	-6.57469100	-3.08855400	5.18998000
N	-5.45845000	-2.71799400	0.64969800
H	-6.33244700	-3.23545400	0.27161900
H	-4.63476300	-3.32559400	0.60870400

C	-5.95106200	-0.43561600	0.59416700
C	-5.37127300	-1.43180400	-0.12327900
C	-4.73182200	-1.47960700	-1.43386200
C	-4.16214400	-2.66113600	-1.94827200
C	-4.59503400	-0.30196900	-2.19868300
C	-3.50175800	-2.67091600	-3.17861800
H	-4.22570700	-3.60137000	-1.39749100
C	-3.93406900	-0.31217800	-3.42209800
H	-4.96975900	0.64707900	-1.82801200
C	-3.38330900	-1.49667300	-3.92409800
H	-3.07226800	-3.60881900	-3.54362400
H	-3.82964200	0.62536500	-3.97250800
H	-2.84798400	-1.48927400	-4.87824200

Geometrical structure of QM region, energy and coordinates of QM region in intermediate 4



Thermal correction to Gibbs Free Energy= 0.525850 a.u.

ONIOM: gridpoint 1 method: low system: model energy: 0.498477825011 a.u.

ONIOM: gridpoint 2 method: high system: model energy: -4314.823094087847 a.u.

ONIOM: gridpoint 3 method: low system: real energy: 9.328742324564 a.u.

ONIOM: extrapolated energy = -4305.992829588294 a.u.

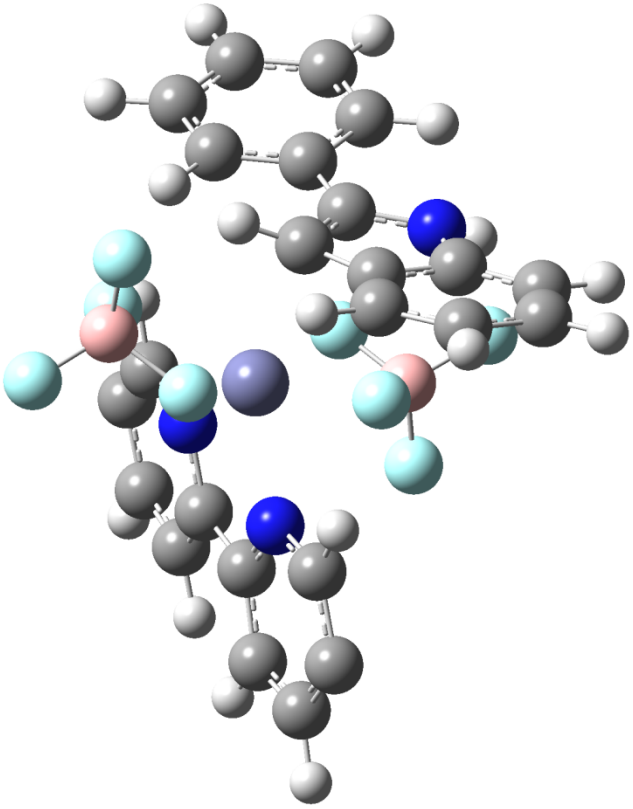
C	8.74447500	3.57710400	-0.37795500
C	9.99885900	3.23739000	0.15327700
H	10.73248800	4.01163500	0.39620800
C	10.33192300	1.90682000	0.38661500
H	11.30495600	1.65793500	0.80670500
C	9.39093400	0.91179500	0.12776900
C	7.87064100	2.52192500	-0.65128000
H	6.87798800	2.69375200	-1.05998400
C	9.99342300	-3.23297300	1.05795100

C	8.77417700	-2.67112800	0.62388000
H	7.86548400	-3.27177400	0.51547200
C	9.65740000	-0.52637800	0.42347300
C	11.08520400	-2.35987100	1.12926500
H	12.07008600	-2.71280500	1.44357000
C	10.91554000	-1.00980600	0.81073100
H	11.76641800	-0.33258800	0.87050700
N	8.61884800	-1.37742300	0.31847400
N	8.18196600	1.24036100	-0.37918200
Zn	6.83703400	-0.30900300	-0.19761600
F	7.90826400	1.14593900	3.37291400
F	5.62283300	0.91465400	3.62717700
F	6.47313300	2.10336000	1.86187900
F	6.73012800	-0.17863000	1.91740300
F	6.27777100	0.79913400	-2.67766500
F	7.91421600	-0.31981600	-3.83406300
F	5.71417500	-0.96610700	-4.03538800
F	6.85129400	-1.32456300	-2.05203900
B	6.70720100	-0.43336400	-3.21665300
B	6.69723700	1.05172600	2.74398700
C	4.03166500	-1.48215800	1.61151700
C	4.44812000	-1.74824900	0.28122900
C	4.57298000	-3.08008800	-0.14724300
C	4.25739900	-4.09386300	0.75942000
C	3.85674300	-3.80567300	2.07607800
C	3.75470100	-2.49368000	2.53105300
C	4.62533600	-0.44918500	-0.36184900
H	4.89334400	-3.30638400	-1.16674000
H	4.30496300	-5.13942600	0.45462000
H	3.59645900	-4.62658100	2.74718500
H	3.43945400	-2.26547600	3.55059200

C	4.17390400	0.51895600	0.56697600
C	3.93425200	1.94530700	0.38273000
C	3.23737500	2.68051800	1.35752000
C	4.36556400	2.59780400	-0.78469600
C	2.99736700	4.03968600	1.17632500
H	2.87288100	2.18780100	2.26070300
C	4.15023300	3.96364500	-0.94936600
H	4.87011600	2.02886700	-1.56471700
C	3.46385700	4.68755100	0.02895500
H	2.45749600	4.59951100	1.94455600
H	4.52322300	4.47634500	-1.83595500
H	3.30826600	5.75990100	-0.09431000
H	4.60228700	-0.29060300	-1.43413600
H	3.94838000	0.36053600	2.64054300
N	3.88655300	-0.11083500	1.73895500
C	1.42855800	2.88024500	-2.58043400
C	1.09151900	1.86284300	-1.70006700
C	1.59909500	0.55653500	-1.86476100
C	2.48221700	0.27153800	-2.95044700
C	2.83696000	1.32970500	-3.81543000
C	2.31025100	2.60230500	-3.63713300
H	1.04265400	3.88983400	-2.43100100
H	0.43808600	2.05816000	-0.84758700
H	3.54900600	1.12574800	-4.61716200
H	2.60009100	3.40129200	-4.32247400
N	2.97229900	-0.99098600	-3.15264600
H	2.83393600	-1.66015000	-2.40400800
H	3.85191200	-1.08480300	-3.65750100
C	1.27816600	-0.47785500	-0.94745900
C	1.05133100	-1.40880500	-0.19007900
C	0.77837800	-2.51108900	0.66636800

C	0.87640500	-3.83182300	0.17914100
C	0.40655800	-2.31839900	2.01466000
C	0.60177500	-4.91558800	1.00907800
H	1.17543100	-3.99241300	-0.85761900
C	0.14021500	-3.40813900	2.84034000
H	0.34660400	-1.30078000	2.40434100
C	0.23415600	-4.71274300	2.34320000
H	0.67961200	-5.92692900	0.60154700
H	-0.13403000	-3.23973100	3.88501900
H	0.02651800	-5.56297100	2.99879500

Geometrical structure of QM region, energy and coordinates of QM region in intermediate 5



Thermal correction to Gibbs Free Energy= 0.330576 a.u.

ONIOM: gridpoint 1 method: low system: model energy: 0.262585043457 a.u.

ONIOM: gridpoint 2 method: high system: model energy: -3719.688027054568 a.u.

ONIOM: gridpoint 3 method: low system: real energy: 9.095768832649 a.u.

ONIOM: extrapolated energy = -3710.854843265377 a.u.

C	8.70065900	-2.80653500	2.45242800
C	9.94624600	-2.82819500	1.80294400
H	10.65756500	-3.64033700	1.97960700
C	10.30282100	-1.81679700	0.91879100
H	11.26831100	-1.85131700	0.41721800
C	9.39642500	-0.79290900	0.65192300
C	7.86106800	-1.72757100	2.15969000
H	6.87601800	-1.63088200	2.61205200
C	10.10459700	2.32351200	-2.20500400

C	8.88725800	2.11385000	-1.52377500
H	8.00978000	2.74468200	-1.69706800
C	9.70059400	0.29520500	-0.32135100
C	11.16166000	1.47319100	-1.86065400
H	12.14285500	1.57430300	-2.33024200
C	10.95875700	0.46228200	-0.91772900
H	11.78164100	-0.20099200	-0.65491700
N	8.70025300	1.14273500	-0.62300900
N	8.19541100	-0.77384500	1.26897600
Zn	6.88060300	0.55622900	0.36136000
F	8.13059900	-2.49665300	-1.95134500
F	5.86674400	-2.50122000	-2.42779800
F	6.58994400	-2.68239900	-0.26225500
F	6.84167600	-0.68962100	-1.38194500
F	6.39450400	0.98663000	2.67732100
F	7.28833200	3.02384900	3.28889700
F	5.10031900	2.88338200	2.57853700
F	6.81741200	2.53635400	1.07598500
B	6.38678100	2.40951400	2.47942400
B	6.87549200	-2.16147100	-1.51724000
C	4.17261500	0.56100100	-1.99494500
C	4.45516500	1.50600000	-0.97434300
C	4.51763700	2.87279400	-1.29136400
C	4.27460600	3.24990000	-2.61216300
C	4.00611700	2.29555700	-3.61217600
C	3.96914800	0.93208100	-3.32576200
C	4.57553700	0.75193200	0.26592700
H	4.72716000	3.60670000	-0.51101200
H	4.28002700	4.30466400	-2.89139300
H	3.81303800	2.63484500	-4.63300400
H	3.76561800	0.18814700	-4.09863700

C	4.24842500	-0.58458200	-0.04850000
C	4.02021800	-1.71906400	0.84175000
C	3.44175500	-2.90169900	0.34971100
C	4.33891600	-1.63305200	2.20987500
C	3.19557600	-3.97497300	1.20103600
H	3.17647400	-2.98398400	-0.70551500
C	4.11951900	-2.72197300	3.05159800
H	4.78186200	-0.71509100	2.60163400
C	3.54395400	-3.89360700	2.55165100
H	2.74280200	-4.88605900	0.80137000
H	4.41166300	-2.67871100	4.09988700
H	3.39041700	-4.74823800	3.21109400
H	4.46533800	1.19466700	1.25281600
H	4.24113600	-1.54613600	-1.91188000
N	4.06084000	-0.68290700	-1.39716400

Energy and coordinates of intermediate 6

Thermal correction to Gibbs Free Energy= 0.332732 a.u.

SCF Done: E(B3LYP) = -3719.61637576 a.u.

C	-0.59566400	2.42969100	-1.25908700
C	-2.67021800	1.39552100	-0.96028900
C	-3.34839600	2.60270400	-1.11146100
C	-2.59970900	3.75724100	-1.34758100
C	-1.21106400	3.67321500	-1.42687000
C	0.87933700	2.22634600	-1.30924000
C	2.61092000	0.66631200	-1.17380800
C	3.57818100	1.65606500	-1.33534400
C	3.15706600	2.97632400	-1.48211000
C	1.79353600	3.26774500	-1.47673300
H	-3.19203900	0.45363300	-0.77822900
H	-4.43635800	2.63112100	-1.04115700
H	-3.09457100	4.72353100	-1.46563100
H	-0.61696300	4.56831700	-1.60089900
H	2.87970100	-0.38434600	-1.04666800
H	4.63537600	1.38890600	-1.32904100
H	3.88557100	3.78206800	-1.59353800
H	1.45255200	4.29664200	-1.57548900
N	-1.33836100	1.33062900	-1.03220600
N	1.30924700	0.95808600	-1.15892600
Zn	-0.19636400	-0.31407500	-0.53898800
F	-0.86135600	-3.57536000	-1.61123100
F	-1.06971900	-2.43166800	-3.59751700
F	-1.75137500	-1.44892200	-1.61685400
F	0.44627300	-1.71409900	-1.99951300
F	0.04206500	0.92444300	1.32502900
F	2.01778200	2.09800200	1.53094200

F	0.02466700	3.22646800	1.43243000
F	0.54751700	1.95377700	3.28953200
B	0.68229900	2.11301500	1.92538300
B	-0.83620900	-2.37315400	-2.26548400
C	3.74041700	-3.00551000	-0.28520100
C	2.36965500	-2.94997200	-0.08045400
C	1.82395000	-2.11456100	0.92070700
C	2.67831200	-1.33186500	1.76110600
C	4.07054400	-1.40294600	1.51851800
C	4.58399800	-2.21846900	0.51996200
H	4.15535200	-3.64752700	-1.06369700
H	1.68015100	-3.51912000	-0.70366200
H	4.73941200	-0.80359000	2.14046500
H	5.66533100	-2.24791200	0.36223700
N	2.18007500	-0.57791900	2.77881700
H	1.19369900	-0.34092900	2.75184200
H	2.74280800	0.20646900	3.08772200
C	0.41511200	-1.97557300	1.05214100
C	-0.78717400	-1.76891300	1.20106500
C	-2.17998700	-1.52633400	1.42867800
C	-2.57872200	-0.43129900	2.22478000
C	-3.15057200	-2.34524800	0.81710400
C	-3.93597100	-0.17165500	2.40715100
H	-1.81830200	0.21502600	2.66380500
C	-4.50282600	-2.07089900	1.00952600
H	-2.82422900	-3.16673100	0.17911500
C	-4.89877200	-0.98730200	1.80240200
H	-4.24265100	0.67677200	3.02298100
H	-5.25419900	-2.70462100	0.53318200
H	-5.96129300	-0.77780500	1.94785600

Energy and coordinates of 7-ts

Thermal correction to Gibbs Free Energy= 0.336651 a.u.

SCF Done: E(UB3LYP) = -3719.58459685 a.u.

Imaginary frequency: 316.36*i*

C	-3.38840300	-0.05592200	0.17432200
C	-2.89848300	-2.26112100	-0.39226100
C	-4.21820200	-2.65940600	-0.18021500
C	-5.14683100	-1.70251500	0.22514400
C	-4.73010500	-0.38398500	0.40205300
C	-2.85954100	1.32489100	0.32705700
C	-1.05722300	2.74514500	-0.00686100
C	-1.72338900	3.81655800	0.58463500
C	-3.01205700	3.60991000	1.06806100
C	-3.58824400	2.34774600	0.94103700
H	-2.13400300	-2.96383400	-0.72195900
H	-4.50084300	-3.70101600	-0.33786200
H	-6.19070000	-1.97468600	0.39597700
H	-5.44545800	0.38114800	0.69965300
H	-0.03654800	2.85073800	-0.36994400
H	-1.22342700	4.78120000	0.67860100
H	-3.56161100	4.41667300	1.55753900
H	-4.58250700	2.15816500	1.34250700
N	-2.50527800	-0.99486200	-0.21401000
N	-1.61771600	1.54170400	-0.14383300
Zn	-0.52305100	-0.29729400	-0.51096700
F	1.11128800	-2.41260200	-2.93277100
F	-1.01428400	-3.29479300	-2.80887900
F	-0.04049700	-2.39261200	-0.93468300
F	-0.71064800	-1.01722000	-2.61644200
F	-0.28566300	-0.27185500	1.64137400

F	1.03375800	1.62046700	1.92711400
F	-1.08865600	1.54415200	2.79660800
F	0.58487800	0.24938700	3.70451900
B	0.05585100	0.80750200	2.56596500
B	-0.14111200	-2.32481700	-2.39204700
C	1.87307000	3.48189700	-2.86750300
C	1.31357800	2.26306700	-2.46934900
C	1.85092700	1.58367400	-1.37293600
C	2.95331700	2.13687000	-0.67722400
C	3.50210600	3.35494700	-1.06563500
C	2.95747200	4.02442400	-2.17121300
H	1.46553000	4.00883200	-3.73311700
H	0.47613700	1.81794600	-3.01031800
H	4.34223400	3.78551400	-0.51597400
H	3.38813300	4.97699100	-2.48778700
N	3.40526100	1.31732400	0.39421200
H	2.86554900	1.50010500	1.25238000
H	4.40930600	1.32249100	0.56897100
C	1.42623800	0.29788600	-0.83826600
C	2.20219300	-0.29400000	0.00547800
C	2.60977900	-1.43059000	0.77050100
C	2.79172300	-1.37303200	2.16731000
C	2.79588700	-2.65037200	0.08458100
C	3.17135800	-2.51833000	2.86033200
H	2.58842700	-0.44975900	2.70834000
C	3.16485200	-3.79156100	0.79401000
H	2.61593100	-2.68602200	-0.99048200
C	3.36096800	-3.72580300	2.17688400
H	3.29798300	-2.47482000	3.94418800
H	3.29769100	-4.73722300	0.26390700
H	3.65260300	-4.62279100	2.72898200

Energy and coordinates of intermediate 8

Thermal correction to Gibbs Free Energy= 0.338782 a.u.

SCF Done: E(RB3LYP) = -3719.62320571 a.u.

C	0.04774600	-0.57821100	2.14024300
C	-1.09362400	-2.42496200	1.29310900
C	-0.20789300	-3.31189700	1.90339500
C	0.85659900	-2.78563500	2.63417700
C	0.97815500	-1.40410500	2.77245500
C	0.05867600	0.90476400	2.24037500
C	-1.03128800	2.86879000	1.62669900
C	-0.16526200	3.64927500	2.38838800
C	0.87041500	3.00894700	3.07424000
C	0.98478400	1.62286000	3.00515400
H	-1.93494800	-2.76813900	0.69043100
H	-0.34168700	-4.38659800	1.77908100
H	1.59953400	-3.44217700	3.09032000
H	1.81329000	-0.98347000	3.32710800
H	-1.85395500	3.30698900	1.05620800
H	-0.29336600	4.73181700	2.43028800
H	1.58899900	3.58668800	3.65923000
H	1.79535100	1.11022000	3.51961200
N	-0.94688600	-1.10222700	1.39542800
N	-0.90712400	1.54130200	1.55266100
Zn	-1.69334900	0.29004700	0.00422700
F	-4.95262400	0.34234100	-1.54829700
F	-5.23273600	0.02172000	0.71239600
F	-3.40361300	-0.90095500	-0.36199000
F	-3.48981000	1.33705700	-0.05467300
F	2.31058700	0.42377100	0.55359800
F	3.95370900	-0.42137100	-0.77876500

F	4.49027900	0.53964200	1.26243300
F	3.41327300	-1.48796400	1.18956600
B	3.55900700	-0.23107900	0.62337700
B	-4.38423800	0.19564000	-0.32844900
C	0.73645700	4.13681300	-2.09447200
C	-0.11581300	3.10189600	-1.69320700
C	0.34189400	1.78258200	-1.77077900
C	1.63546400	1.55704800	-2.26453700
C	2.50805500	2.55677900	-2.65104900
C	2.03192100	3.87400300	-2.56080600
H	0.38832200	5.17101700	-2.04285300
H	-1.12670400	3.30936800	-1.33791000
H	3.52019000	2.34015800	-2.99782400
H	2.68106500	4.70035700	-2.85681100
N	1.87738900	0.11860600	-2.24103600
H	2.70273900	-0.10486600	-1.59361700
H	2.12443500	-0.25903700	-3.16422600
C	-0.28479500	0.50707500	-1.40233000
C	0.59731300	-0.47167300	-1.71951100
C	0.51580900	-1.92838100	-1.62701600
C	1.63128900	-2.72115100	-1.29365600
C	-0.72426900	-2.55631700	-1.85949400
C	1.50029000	-4.10690700	-1.19515000
H	2.59282200	-2.26000300	-1.06888400
C	-0.84485700	-3.94146900	-1.76088400
H	-1.59287300	-1.94625000	-2.11389600
C	0.26727900	-4.72248200	-1.42993500
H	2.37123900	-4.70670300	-0.92153700
H	-1.81255700	-4.41264600	-1.94862500
H	0.17344000	-5.80871000	-1.35777300

Energy and coordinates of intermediate 9

Thermal correction to Gibbs Free Energy= 0.529371 a.u.

SCF Done: E(RB3LYP) = -4314.77669461 a.u.

C	-3.43917900	-1.17217200	0.93868000
C	-3.96519900	-1.09847100	-1.33171700
C	-5.31801800	-0.90733000	-1.06092700
C	-5.72495000	-0.84075300	0.27158300
C	-4.77898000	-0.98186600	1.28483200
C	-2.35615000	-1.34448700	1.94219500
C	-0.07424900	-1.67661800	2.25586600
C	-0.20676000	-1.66627600	3.64211900
C	-1.48340500	-1.48379900	4.17908600
C	-2.57156200	-1.33032100	3.32571600
H	-3.58033400	-1.18278500	-2.34900300
H	-6.03036300	-0.81528700	-1.88170200
H	-6.77505800	-0.68105900	0.52483100
H	-5.07677000	-0.91322300	2.32791800
H	0.89564300	-1.82245900	1.76896200
H	0.66792000	-1.79627000	4.28149700
H	-1.63106000	-1.45359100	5.26032700
H	-3.56477700	-1.15711700	3.73159200
N	-3.06171600	-1.21086300	-0.35350200
N	-1.12130300	-1.51687200	1.44353300
Zn	-1.02879800	-1.41136600	-0.71650300
C	2.82436400	-0.27957600	-1.90724200
C	1.86232500	-1.09598100	-1.24444500
C	2.26659700	-2.35469000	-0.75627700
C	3.59364700	-2.74563300	-0.90699800
C	4.53232600	-1.90658300	-1.54308900
C	4.16142900	-0.66587200	-2.05579100

C	0.58427500	-0.40923100	-1.26442500
H	1.53258600	-3.03060700	-0.31064100
H	3.91671800	-3.71981000	-0.53435600
H	5.56907100	-2.23638600	-1.63595800
H	4.88855900	-0.02172200	-2.55572100
C	0.81977100	0.77760500	-1.96518000
C	-0.10334700	1.86845400	-2.29824100
C	0.30516100	2.99099000	-3.04435400
C	-1.43422000	1.83928500	-1.83892800
C	-0.57377500	4.04259700	-3.30264900
H	1.32296800	3.05987000	-3.43315400
C	-2.30942900	2.89156300	-2.08721100
H	-1.78130900	1.00716900	-1.23263600
C	-1.88535500	4.00279500	-2.82258300
H	-0.22762700	4.90284500	-3.88051700
H	-3.32202900	2.84523300	-1.68148300
H	-2.56987100	4.83139700	-3.01773300
H	0.29601000	0.78034400	0.33378400
H	2.60084000	1.63412200	-2.78606300
N	2.16120900	0.84909000	-2.32815700
C	1.52844300	5.23684500	-0.32714000
C	2.50963300	4.27356700	-0.10474700
C	2.16203100	3.01258500	0.41815800
C	0.80160300	2.76725700	0.69840100
C	-0.18096300	3.72755200	0.49608800
C	0.19077500	4.97004700	-0.02083500
H	1.81077700	6.20883800	-0.73727900
H	3.55800500	4.48137800	-0.32387600
H	-1.22138800	3.51038500	0.73013600
H	-0.57694600	5.72600600	-0.19083400
N	0.43591100	1.43358000	1.15883100

H	1.21866200	1.02216800	1.68153900
H	-0.40859300	1.43473100	1.78538700
C	3.12419300	2.00075200	0.68884400
C	3.87495000	1.07922100	0.96226400
C	4.75720200	0.00531600	1.27298000
C	4.28016600	-1.13596900	1.94655100
C	6.11413200	0.05986500	0.89499900
C	5.13730100	-2.19625200	2.22995700
H	3.22816800	-1.18730400	2.22996300
C	6.96452000	-1.00494300	1.18037600
H	6.48468900	0.94022100	0.36747000
C	6.47983500	-2.13596500	1.84658300
H	4.75344400	-3.08041900	2.74347800
H	8.01328200	-0.95562000	0.87886000
H	7.14928200	-2.97087000	2.06543500
B	-1.61935500	-3.76861600	-2.00857100
F	-1.66169700	-2.44853300	-2.60017300
F	-0.89954700	-4.62672600	-2.76961500
F	-2.89106500	-4.17259200	-1.70800800
F	-0.90426300	-3.49987300	-0.74332400
B	-2.69734700	1.95042900	2.32222200
F	-2.77568200	3.32471500	2.35972400
F	-2.52999700	1.51604600	0.97997500
F	-1.48598400	1.52278300	2.99546600
F	-3.78583300	1.32930800	2.90447200

Energy and coordinates of 10-ts

Thermal correction to Gibbs Free Energy= 0.529343 a.u.

SCF Done: E(UB3LYP) = -4314.76869864 a.u.

Imaginary frequency: 1341.60*i*

C	-3.55031800	-1.45343400	0.64590600
C	-3.71303100	-1.25031800	-1.67345200
C	-5.10378200	-1.19701100	-1.61843100
C	-5.72157300	-1.26490000	-0.36958400
C	-4.93990300	-1.40100700	0.77601500
C	-2.62947800	-1.60600100	1.80276000
C	-0.41044700	-1.73198000	2.48737000
C	-0.77041500	-1.82889300	3.82810400
C	-2.12923100	-1.81356300	4.14640400
C	-3.06966900	-1.70707000	3.12699400
H	-3.16227100	-1.21620100	-2.61433200
H	-5.68214900	-1.10207900	-2.53820300
H	-6.80895700	-1.21257700	-0.28405400
H	-5.40600200	-1.43824300	1.75744600
H	0.63810100	-1.73829500	2.17535900
H	-0.00377700	-1.90632700	4.60035900
H	-2.45646800	-1.87183600	5.18623900
H	-4.12923000	-1.66012400	3.36420800
N	-2.97197300	-1.36204800	-0.56683800
N	-1.31705900	-1.63010900	1.51302000
Zn	-0.90841900	-1.31185300	-0.55660200
C	2.78738200	-0.27511100	-1.84449600
C	1.94683300	-0.88449500	-0.87481800
C	2.40646000	-2.04567800	-0.23218400
C	3.66989100	-2.54269100	-0.54230000
C	4.48961500	-1.90432500	-1.49142500

C	4.05693400	-0.76229100	-2.16351800
C	0.69652000	-0.12595800	-0.80699400
H	1.76588700	-2.58271100	0.47049300
H	4.03249600	-3.44397500	-0.04497100
H	5.47787900	-2.31393900	-1.70839600
H	4.68433400	-0.27398600	-2.91258300
C	0.84517300	0.88846000	-1.78032000
C	-0.08482000	1.96134300	-2.14304600
C	0.35177300	3.12455500	-2.80536100
C	-1.44296100	1.86795000	-1.79027700
C	-0.54177500	4.15072000	-3.10809100
H	1.40751200	3.25759800	-3.05067600
C	-2.33083300	2.90051700	-2.07337500
H	-1.80653300	1.00150800	-1.24624500
C	-1.88642100	4.04518500	-2.74213500
H	-0.17994600	5.04902700	-3.61349000
H	-3.37059800	2.80944500	-1.75355000
H	-2.58223300	4.85654500	-2.96790800
H	0.39241000	0.59604100	0.42261800
H	2.41405600	1.39538700	-3.10853800
N	2.08463900	0.80065700	-2.35997100
C	1.26258300	5.20830300	-0.10215500
C	2.27773900	4.27856200	0.09913100
C	1.98950300	3.01200300	0.64663400
C	0.64924600	2.71141100	0.98394900
C	-0.36626300	3.64787300	0.79118000
C	-0.05439800	4.89497100	0.25113000
H	1.49804700	6.18442200	-0.53160800
H	3.31165100	4.51427800	-0.15842700
H	-1.39390400	3.40461300	1.05901500
H	-0.85348800	5.62229200	0.09848100

N	0.34282600	1.38679200	1.43357800
H	1.07935600	1.02804200	2.04646700
H	-0.56837300	1.31586000	1.92260400
C	3.00989600	2.04742400	0.87780400
C	3.84138800	1.18452900	1.10348200
C	4.81588900	0.17435100	1.34730500
C	4.55741200	-0.86446100	2.26430000
C	6.04520600	0.18431900	0.65856200
C	5.49972100	-1.86661500	2.47951400
H	3.60521000	-0.87866300	2.79747400
C	6.98360700	-0.82136900	0.87922700
H	6.24471700	0.98196200	-0.05845100
C	6.71434200	-1.85083500	1.78631500
H	5.28513500	-2.66933800	3.18876100
H	7.93082000	-0.80606100	0.33513700
H	7.45088800	-2.63987200	1.95440300
B	-0.89735000	-3.39551700	-2.35409600
F	-1.03124000	-1.99666400	-2.70113300
F	0.08832300	-3.98620400	-3.06994200
F	-2.12187000	-3.99877000	-2.42569600
F	-0.50120900	-3.31085800	-0.93077100
B	-3.03371100	1.59961900	2.17486400
F	-3.18463200	2.97212100	2.23401100
F	-2.65870800	1.22058600	0.85617800
F	-1.93818400	1.19790300	3.01049900
F	-4.18431300	0.92393400	2.55433400

Energy and coordinates of intermediate 11

Thermal correction to Gibbs Free Energy= 0.533385 a.u.

SCF Done: E(RB3LYP) = -4314.79842748 a.u.

C	-2.67454700	-1.59423000	1.13184700
C	-2.40445000	-2.91006100	-0.78453400
C	-3.77553500	-2.92802900	-1.01827300
C	-4.60794600	-2.22772400	-0.14280600
C	-4.05960400	-1.55038400	0.94489100
C	-1.97514400	-0.91174000	2.25464000
C	0.09151200	-0.44661900	3.23845800
C	-0.50159400	0.31830500	4.23962300
C	-1.88930200	0.46616500	4.22255400
C	-2.63814100	-0.16837100	3.23366400
H	-1.69013400	-3.40988800	-1.44044400
H	-4.17329700	-3.46120600	-1.88232700
H	-5.68588700	-2.19063400	-0.31288300
H	-4.68862200	-0.94317600	1.59273600
H	1.17332700	-0.59430400	3.19317900
H	0.11567600	0.79305300	5.00364900
H	-2.39592700	1.08641000	4.96367300
H	-3.71465300	-0.02202400	3.18994900
N	-1.88440600	-2.25811800	0.26257500
N	-0.62928400	-1.03231900	2.27672800
Zn	0.10695900	-1.87494600	0.52909300
C	2.83488200	-1.04883100	-1.38330900
C	2.37759800	-0.43755800	-0.18905800
C	3.25702600	-0.31983600	0.89853800
C	4.54903800	-0.81521400	0.76916500
C	4.97832200	-1.42990500	-0.42434900
C	4.12903900	-1.55609400	-1.51915700

C	0.97031700	-0.11727400	-0.39783000
H	2.94100000	0.17168600	1.81937400
H	5.24864100	-0.71370300	1.59999200
H	5.99668100	-1.81801300	-0.48962600
H	4.45386000	-2.04998700	-2.43640100
C	0.66363400	-0.48297400	-1.73533000
C	-0.62008100	-0.37630000	-2.42620600
C	-0.82122600	-0.90863500	-3.71414500
C	-1.70521000	0.22930600	-1.76709500
C	-2.07429700	-0.83515600	-4.32018700
H	-0.00289100	-1.38806600	-4.25660900
C	-2.95599200	0.30192600	-2.37325100
H	-1.59266900	0.64631300	-0.76900900
C	-3.14479700	-0.23036700	-3.65138000
H	-2.21552700	-1.25038900	-5.32059200
H	-3.76761300	0.77638800	-1.82117500
H	-4.12520200	-0.17415100	-4.13031800
H	0.40137300	0.63568500	0.15418400
H	1.79161800	-1.52663300	-3.17038700
N	1.77801100	-1.03629900	-2.28538600
C	-1.01357100	4.05453300	-3.23378300
C	0.22596100	3.81316800	-2.65535100
C	0.33452600	3.39003000	-1.31302800
C	-0.84635100	3.19171200	-0.54109000
C	-2.09300300	3.47228000	-1.13362600
C	-2.16946200	3.89168900	-2.45710100
H	-1.08245500	4.38009800	-4.27364700
H	1.14495300	3.95374300	-3.22800200
H	-3.00428600	3.34638100	-0.55034700
H	-3.15219400	4.09472200	-2.88977500
N	-0.76778500	2.65722900	0.73448100

H	0.08338800	2.87347200	1.24332500
H	-1.61880900	2.69166000	1.29779800
C	1.61462500	3.17266600	-0.73266600
C	2.71327000	2.99475000	-0.23095400
C	4.00651100	2.74720000	0.31246400
C	4.23919300	2.82975700	1.70185100
C	5.07531500	2.37936500	-0.53125100
C	5.49565900	2.53551700	2.22787500
H	3.41927300	3.12386300	2.36034800
C	6.32849700	2.08879700	0.00212000
H	4.89960100	2.30480900	-1.60547700
C	6.54496600	2.16107900	1.38206200
H	5.66002800	2.60167300	3.30623000
H	7.14307500	1.79466700	-0.66387800
H	7.52880300	1.92995900	1.79686000
B	1.48419200	-4.15868600	-0.04855100
F	0.62348000	-3.39940700	-0.95459700
F	2.75152200	-4.18844600	-0.52271700
F	0.91867700	-5.35405300	0.23521200
F	1.41744300	-3.28851900	1.15557000
B	-4.20369600	1.98850900	1.42886900
F	-4.87145400	2.96109500	0.71501600
F	-3.46737700	1.16244800	0.53419000
F	-3.26900200	2.56712000	2.32240600
F	-5.09617500	1.16929000	2.15075100

Energy and coordinates of intermediate 12

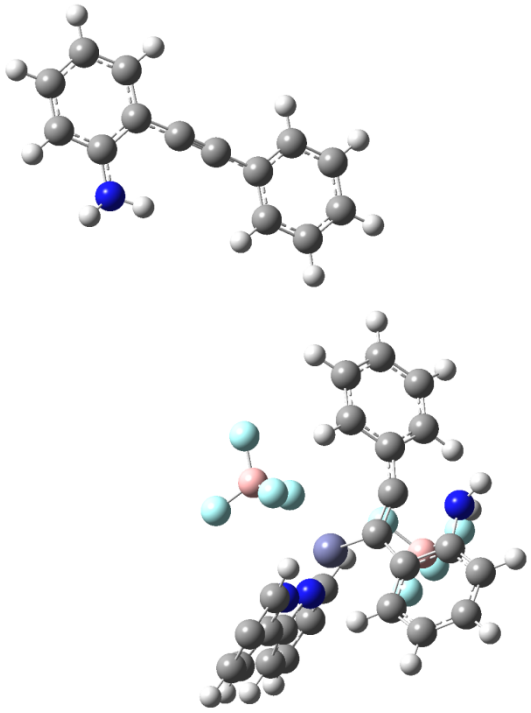
Thermal correction to Gibbs Free Energy= 0.337723 a.u.

SCF Done: E(RB3LYP) = -3719.65462811 a.u.

C	2.30535100	-0.62745100	1.27393200
C	1.60710000	1.56370200	1.68232700
C	2.89520400	1.95443600	2.03627400
C	3.91210900	1.00259600	2.00012900
C	3.61601200	-0.30629300	1.62646200
C	1.88164600	-1.98673400	0.84745200
C	0.06455500	-3.36542700	0.33881500
C	0.89282300	-4.46591800	0.13940400
C	2.27209900	-4.28886100	0.27674400
C	2.77487900	-3.04124200	0.63704400
H	0.76597200	2.25701300	1.69225300
H	3.09009200	2.98947700	2.31890600
H	4.93784100	1.27632500	2.25441000
H	4.40233700	-1.05477300	1.57727400
H	-1.01980800	-3.42851200	0.22390400
H	0.46507500	-5.43156700	-0.13317100
H	2.95719600	-5.11979000	0.09630500
H	3.84646100	-2.87466200	0.70705900
N	1.33512000	0.30789700	1.31417200
N	0.55678300	-2.16724400	0.67369900
Zn	-0.43863800	-0.36203300	0.55759600
C	-3.35182900	-0.17769900	-1.15095900
C	-2.23381700	-0.94143700	-1.57066500
C	-2.40661200	-2.29860500	-1.88770900
C	-3.67224200	-2.85977700	-1.73397600
C	-4.75973800	-2.09287300	-1.26491800
C	-4.61671700	-0.73995400	-0.96691000

C	-1.08241400	-0.05255000	-1.52786500
H	-1.56558100	-2.89229900	-2.25174800
H	-3.83004000	-3.91230900	-1.98010300
H	-5.73433000	-2.56878200	-1.13727200
H	-5.45207200	-0.14478700	-0.59563300
C	-1.57820100	1.23344600	-1.19118900
C	-0.82997400	2.48570500	-1.08571900
C	-1.46477300	3.70954600	-0.80779700
C	0.56759200	2.46067900	-1.24646400
C	-0.71520600	4.87921200	-0.69284100
H	-2.54887800	3.75956900	-0.68631400
C	1.31336600	3.63101400	-1.12914800
H	1.09744000	1.52674100	-1.42653400
C	0.67508900	4.84404200	-0.85346800
H	-1.21877300	5.82436400	-0.47811100
H	2.39635900	3.56627000	-1.24774500
H	1.25731400	5.76421500	-0.76276200
H	-0.11012600	-0.23769900	-1.98805200
H	-3.45186100	1.80391700	-0.42560300
N	-2.91805800	1.12683000	-0.95919800
B	-2.48138800	0.47706400	2.23965000
F	-1.41174400	1.30148600	1.72222100
F	-3.68408000	0.91807100	1.75265800
F	-2.40851100	0.36335500	3.58385600
F	-2.14659400	-0.82020900	1.61180100
B	3.22528600	-0.15175200	-1.76908200
F	3.29897200	1.09197000	-1.10630400
F	1.86314500	-0.61580500	-1.63257900
F	3.53975900	-0.03334400	-3.09899600
F	4.05353200	-1.07863600	-1.11401400

Geometrical structure of QM region, energy and coordinates of QM region in transition state 2'-ts



Thermal correction to Gibbs Free Energy= 0.514040 a.u.

ONIOM: gridpoint 1 method: low system: model energy: 0.768715990882 a.u.

ONIOM: gridpoint 2 method: high system: model energy: -4314.705218415242 a.u.

ONIOM: gridpoint 3 method: low system: real energy: 9.543295609363 a.u.

ONIOM: extrapolated energy = -4305.930638796761 a.u.

Imaginary frequency: 308.68*i*

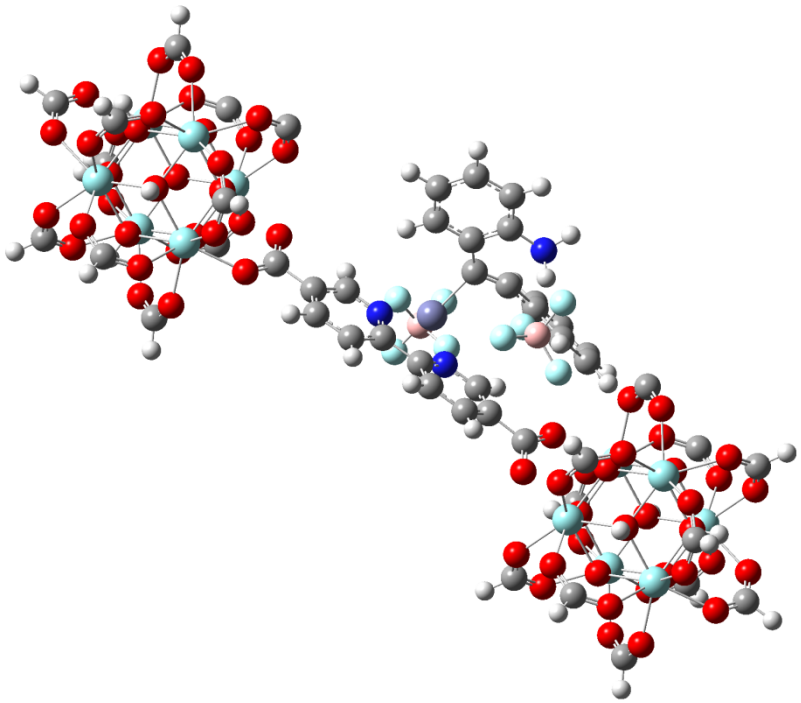
C	-8.20415300	4.40196500	2.00930500
C	-8.99853200	5.24490900	1.21162900
H	-9.49275300	6.11981500	1.64502900
C	-9.19187100	4.97189000	-0.13710800
H	-9.81466400	5.62991300	-0.74133300
C	-8.62384200	3.81852200	-0.68019400
C	-7.57150800	3.33465600	1.36096500
H	-6.87874300	2.66166400	1.86945600
C	-9.23527600	2.47739100	-4.69413200

C	-8.42862800	1.82168900	-3.74369000
H	-7.88900700	0.90134100	-3.97438200
C	-8.90150300	3.37343300	-2.07537800
C	-9.93924100	3.60231400	-4.25529300
H	-10.60047800	4.15318600	-4.92831700
C	-9.76848900	4.05200100	-2.94227900
H	-10.30298600	4.93793500	-2.60172600
N	-8.27835400	2.25307500	-2.48513200
N	-7.81178800	3.04753500	0.06704900
Zn	-7.16852600	1.27823400	-0.93315000
F	-4.84374200	3.91957100	-0.86848100
F	-3.15338200	2.34916900	-0.89984100
F	-4.81459000	2.23500000	0.67964400
F	-5.29981000	1.75655900	-1.51822500
F	-9.15179200	-0.35557000	-1.31892200
F	-8.98072600	-1.37851600	-3.37335000
F	-8.10669700	-2.40631600	-1.50603800
F	-7.13774100	-0.46792800	-2.35698600
B	-8.38516400	-1.18518600	-2.15848700
B	-4.47104900	2.62262700	-0.62423200
C	-9.88286000	-0.19748100	3.20254900
C	-9.01540500	0.33681600	2.24434400
C	-8.09784200	-0.49042100	1.59098200
C	-8.09074200	-1.87697000	1.88735000
C	-8.96828400	-2.41438300	2.82339200
C	-9.85930400	-1.56377400	3.49189300
H	-10.57427200	0.46251700	3.73018800
H	-9.04026300	1.40206900	2.02466600
H	-8.96070700	-3.48803200	3.03130200
H	-10.54169800	-1.97659000	4.23940500
N	-7.11577000	-2.61154700	1.16047200

H	-7.46901200	-2.88251300	0.23116200
H	-6.70172600	-3.40386200	1.64962400
C	-7.05320000	-0.10953000	0.64272900
C	-6.16447700	-0.98053000	0.31667800
C	-4.96601900	-1.41173900	-0.34161900
C	-4.94302700	-2.53080000	-1.19990000
C	-3.79463400	-0.65335000	-0.14830600
C	-3.75403100	-2.90345000	-1.81884000
H	-5.86390500	-3.07479500	-1.40566400
C	-2.61692800	-1.01769400	-0.80047800
H	-3.83185100	0.23110000	0.48581700
C	-2.59021300	-2.14996600	-1.61786200
H	-3.74231300	-3.77274200	-2.47998300
H	-1.72500300	-0.40127600	-0.66746600
H	-1.66164300	-2.44898700	-2.11290200
C	8.79982800	2.49071900	-1.74059400
C	7.82898400	1.53557600	-2.02100800
C	6.46006800	1.79346100	-1.80673700
C	6.05845500	3.06014700	-1.28138300
C	7.05929400	4.01356200	-0.99922900
C	8.40172000	3.73411100	-1.22890000
H	9.85519600	2.27407800	-1.91818400
H	8.11046300	0.55908300	-2.42075500
H	6.76445600	4.98990200	-0.60788800
H	9.15011300	4.49894700	-1.00545900
N	4.73315800	3.34963000	-1.09988500
H	4.07373500	2.58124800	-1.11820800
H	4.48948200	4.12949100	-0.50457000
C	5.47315300	0.82170700	-2.13060400
C	4.60370800	0.01844800	-2.43013000
C	3.58561000	-0.90786400	-2.80167100

C	2.22730900	-0.61621500	-2.55078700
C	3.90946300	-2.12896500	-3.43427700
C	1.22759300	-1.51514400	-2.91756800
H	1.96402700	0.32588400	-2.06706400
C	2.90248300	-3.02348600	-3.79415200
H	4.95763700	-2.36363500	-3.63473100
C	1.55974100	-2.72349600	-3.53864000
H	0.18300600	-1.27018400	-2.71567800
H	3.16504900	-3.96400100	-4.28502400
H	0.77491300	-3.42950300	-3.81952300

Geometrical structure of QM region, energy and coordinates of QM region in transition state 2''-ts



Thermal correction to Gibbs Free Energy= 0.514040 a.u.

ONIOM: gridpoint 1 method: low system: model energy: 2.682406783074 a.u.

ONIOM: gridpoint 2 method: high system: model energy: -10037.190540054400 a.u.

ONIOM: gridpoint 3 method: low system: real energy: 7.557172846578 a.u.

ONIOM: extrapolated energy = -10032.315773990942 a.u.

Imaginary frequency: 251.27*i*

O	-8.58009700	-6.95436700	-8.47398800
C	-9.04952500	-7.66437600	-7.50880000
O	-9.85199500	-7.28741400	-6.57606000
Zr	-10.80679100	-5.32931000	-6.14691100
Zr	-8.87807200	-4.82427500	-9.02495100
O	-8.72858300	10.03938500	4.31308200
C	-9.75636600	9.40477400	3.86924400
O	-10.30239700	8.35088100	4.36646000
O	-12.12982400	0.14670800	-6.79812900

C	-11.66033200	0.85677000	-7.76315300
O	-10.85789200	0.47979600	-8.69591100
Zr	-7.41617600	9.68680200	6.06879200
Zr	-9.80264100	7.12650800	6.14998000
Zr	-9.90327800	-1.47824800	-9.12483800
Zr	-11.83206600	-1.98224700	-6.24547100
O	-5.70595900	11.03116600	6.51272900
C	-4.82932900	11.02143800	7.45479200
O	-4.72793800	10.17997100	8.42314700
Zr	-5.93338100	8.39610900	8.96576700
O	-7.87439200	-3.94611900	-10.80009400
C	-7.89918500	-2.76076700	-11.30047600
O	-8.55050000	-1.73947000	-10.86596200
O	-10.03007800	4.49144000	8.60298600
C	-10.90670900	4.50117000	7.66092500
O	-11.00809300	5.34263200	6.69257100
O	-12.83553600	-2.86157400	-4.47194400
C	-12.81070000	-4.04684900	-3.97149800
O	-12.15938500	-5.06814500	-4.40600600
Zr	-8.31958800	5.83547800	9.04671600
O	-7.00745300	5.48322200	10.80263100
C	-5.97966500	6.11782900	11.24646900
O	-5.43364100	7.17172500	10.74925300
O	-9.49437800	-5.68188900	-4.39121100
C	-8.46659200	-5.04728000	-3.94737600
O	-7.92056800	-3.99338900	-4.44459100
O	-6.09321700	4.21076400	6.71994600
C	-6.56256900	3.50074600	7.68506700
O	-7.36506800	3.87770000	8.61778200
Zr	-8.42029000	-2.76904700	-6.22813300
Zr	-6.39064000	6.33952700	6.16743000

O	-8.19288600	-0.13394700	-8.68111500
C	-7.31625200	-0.14367500	-7.73905100
O	-7.21486100	-0.98514000	-6.77069400
O	-5.38748100	7.21908300	4.39379200
C	-5.41224400	8.40434900	3.89338100
O	-6.06357500	9.42564200	4.32787900
O	-6.40843400	6.42465700	8.30158100
O	-9.77366700	7.19907100	8.28292400
Zr	-9.34489700	9.18177100	8.94682400
O	-7.41939100	9.72489400	8.20307300
O	-7.87115600	7.69731300	5.44414800
O	-8.31672700	5.79806000	6.91274200
O	-9.32804000	9.09863800	6.81408900
O	-7.86501100	7.82533200	9.67189500
O	-5.96269200	8.32346300	6.83320600
O	-10.34856800	8.30361600	10.72196100
O	-9.64286500	11.31186200	8.39585800
O	-7.37012700	5.18584700	4.38097500
O	-11.50702700	9.31184800	8.45908700
O	-8.48440200	10.30362800	10.65873600
O	-4.22901200	6.21084300	6.65666200
O	-9.67246200	6.09696500	10.78783700
O	-8.37096700	11.64490900	6.49793300
O	-9.56516900	5.72765400	4.45620800
C	-8.55647500	5.10522700	3.99762000
C	-8.85987300	4.15183200	2.85856500
C	-10.17634700	3.77613200	2.56108300
H	-10.98777400	4.19201600	3.16033800
C	-10.43204000	2.89208200	1.51393700
H	-11.45575000	2.60507000	1.27778800
C	-9.36339900	2.39851200	0.75454800

C	-7.84182100	3.60966100	2.06631200
H	-6.79545100	3.86853300	2.24503700
O	-8.71361000	-1.23561000	-4.55322200
C	-9.76814500	-0.77121000	-4.03643700
C	-9.67806800	-0.00711000	-2.74332100
C	-8.48415000	0.56787100	-2.29269300
H	-7.55513800	0.43527800	-2.84960300
C	-9.53218800	1.50268300	-0.42753100
O	-10.91821100	-0.82341900	-4.55831000
C	-10.81739600	0.15693700	-1.95273000
H	-11.74733400	-0.32193500	-2.25879500
C	-10.74595000	0.91210800	-0.78295900
H	-11.62659300	1.01866700	-0.15172600
O	-3.92709200	7.56621400	8.50117400
O	-6.23448600	9.78547900	10.67122600
O	-11.80893800	7.95638700	6.61455600
C	-3.52391600	6.76084600	7.58199700
O	-6.41402000	-3.59889900	-6.69267100
C	-6.01083200	-4.40424200	-7.61186400
O	-6.71593400	-4.95435300	-8.53721500
C	-7.28508500	10.37839400	11.11928200
C	-12.21212300	8.76174700	7.53373300
C	-9.17343800	12.02187100	7.43067300
C	-10.32377600	7.11826300	11.22234900
O	-9.90633700	-1.44042800	-6.99097800
O	-10.35795300	-3.46783700	-9.75002300
O	-11.21550800	-1.12572800	-10.88076000
C	-12.24329500	-1.76033200	-11.32459700
O	-12.78931600	-2.81422800	-10.82738100
O	-8.89493300	-4.74113500	-6.89223300
O	-12.25992400	-3.96606600	-6.91126500

Zr	-12.28959800	-4.03861100	-9.04389400
O	-11.81498000	-2.06671800	-8.37973000
O	-10.80357000	-5.36739900	-8.28120000
O	-8.44931300	-2.84157700	-8.36105300
O	-10.35187000	-3.33984100	-5.52220300
O	-13.99392400	-1.85325900	-6.73487800
O	-9.73855300	-5.94613400	-10.73686300
O	-12.51700200	-6.67366800	-6.59085900
C	-13.39363300	-6.66394300	-7.53292000
O	-13.49502400	-5.82247700	-8.50127600
O	-14.29586600	-3.20871800	-8.57930500
O	-11.98847400	-5.42798600	-10.74935300
C	-14.69905900	-2.40340800	-7.66008000
C	-10.93787700	-6.02090400	-11.19741100
H	-8.73619200	-8.68700900	-7.47827300
H	-13.40013800	-4.20118900	-3.09193300
H	-14.12298500	-7.44644500	-7.50818500
H	-15.74173600	-2.16324800	-7.66589600
H	-12.69653900	-1.36586300	-12.20994800
H	-11.97369100	1.87939200	-7.79370000
H	-7.30974600	-2.60642300	-12.18003800
H	-11.63606400	3.71866200	7.68566200
H	-13.25481200	9.00186400	7.52794700
H	-10.91321200	6.96391700	12.10190600
H	-7.14516800	11.00655900	11.97410700
H	-9.48676600	13.04450200	7.40014300
H	-4.09997200	11.80394400	7.43005600
H	-5.52641800	5.72335800	12.13182000
H	-10.20961600	9.79924900	2.98389800
H	-11.07779400	-6.64906400	-12.05223300
H	-10.67379400	6.94318300	8.63529100

H	-7.85449700	7.86829200	10.67089300
H	-10.02194500	9.73022800	6.46833600
H	-7.22850500	10.66633700	8.48105800
H	-7.55135200	-2.56982300	-8.70719400
H	-11.01736300	-6.28964900	-8.60317600
H	-9.69860300	-0.51238800	-6.68079500
H	-13.16184200	-4.23541600	-6.57179600
N	-8.42666700	1.30405800	-1.17957000
N	-8.09925000	2.77145600	1.05414000
Zn	-6.68080900	1.81490200	-0.12725600
F	-4.88559300	4.60582200	-1.76533100
F	-3.47990200	2.88674300	-1.15895700
F	-5.30150800	3.40519100	0.17061600
F	-5.64630600	2.42007400	-1.82478200
F	-8.16342000	-1.79088000	-0.79397100
F	-10.31523300	-2.07670900	-0.04456400
F	-8.83720100	-3.84897300	-0.08118500
F	-9.67433600	-2.98689800	-2.05067500
B	-9.28465800	-2.70498100	-0.73457200
B	-4.74302300	3.39288900	-1.18175200
C	-6.91092200	-0.63789400	4.25281400
C	-6.67956800	0.09464400	3.08580100
C	-6.33095700	-0.56846700	1.90533600
C	-6.24783200	-1.98522200	1.88891600
C	-6.46754800	-2.70741200	3.06236300
C	-6.79079000	-2.03035700	4.24369400
H	-7.17984700	-0.11717700	5.17451900
H	-6.74082600	1.18376800	3.09840400
H	-6.41158900	-3.79810700	3.04585300
H	-6.96201000	-2.59984700	5.16019900
N	-5.91802200	-2.55341300	0.64129300

H	-6.76004100	-2.61833500	0.04675200
H	-5.45490400	-3.45867300	0.70036700
C	-5.98300400	0.04990900	0.63315400
C	-5.50394000	-0.58929600	-0.36703000
C	-4.98338500	-0.80180000	-1.67270200
C	-5.70226600	-1.54473600	-2.63703100
C	-3.74112100	-0.21835300	-2.00972900
C	-5.15421800	-1.73963100	-3.90092100
H	-6.68435900	-1.94304700	-2.38324300
C	-3.22401900	-0.39206400	-3.29020500
H	-3.21831100	0.39485000	-1.27574200
C	-3.91791300	-1.16691600	-4.22535800
H	-5.69008500	-2.33907900	-4.63520400
H	-2.27450400	0.07662400	-3.55739800
H	-3.49660400	-1.31448100	-5.22308000