Electronic Supplementary Information

PIO and IBO Analysis to Unravel the Hidden Details of CO_2 Sequestration Mechanism by Aromatically Tempered N/B based IFLPs

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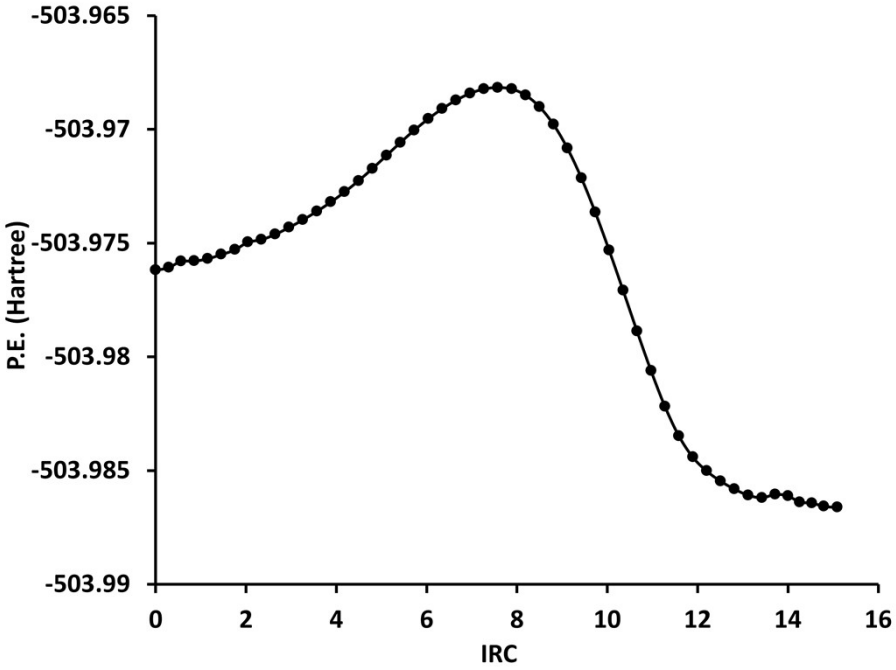


Figure S1. The IRC plot for the reaction of CO_2 with 1 in gas phase.

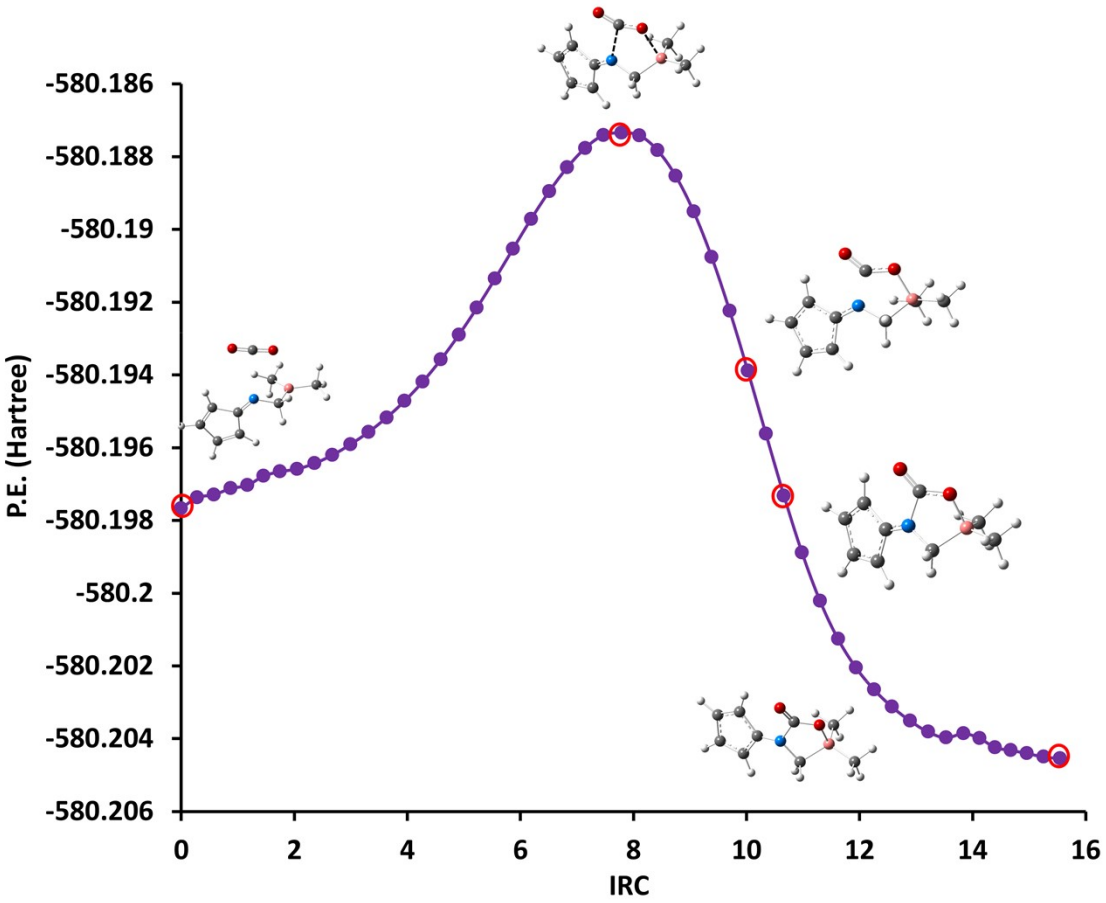


Figure S2. The IRC plot for the reaction of CO_2 with 3 in gas phase along with expected asynchronous stages observed in the reaction highlighted be red circles on the curve.

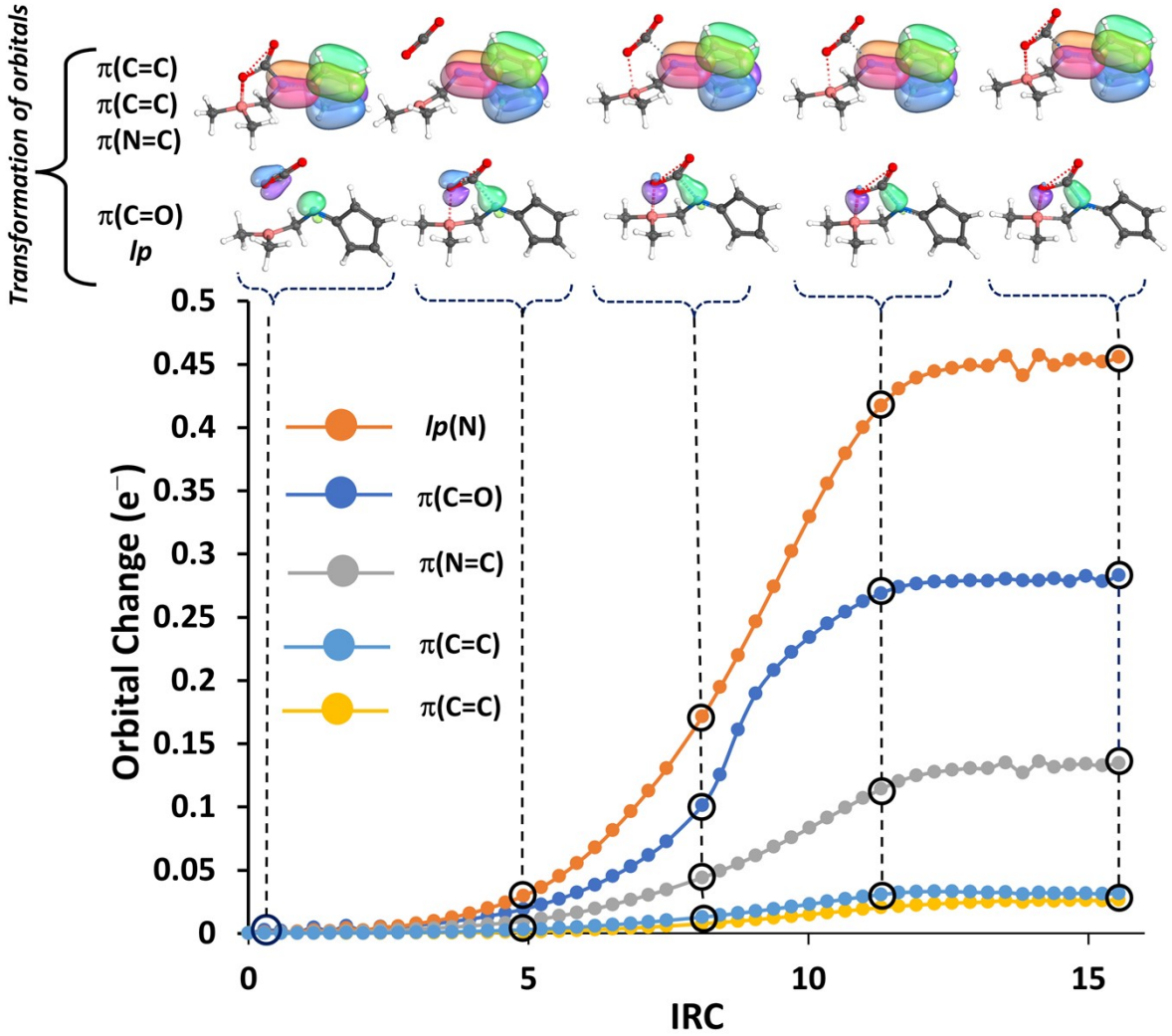


Figure S3. The orbital change plot for the reaction of CO2 with 3. The images of transformation of important orbitals are also given and indicated on the curves at respective the points.

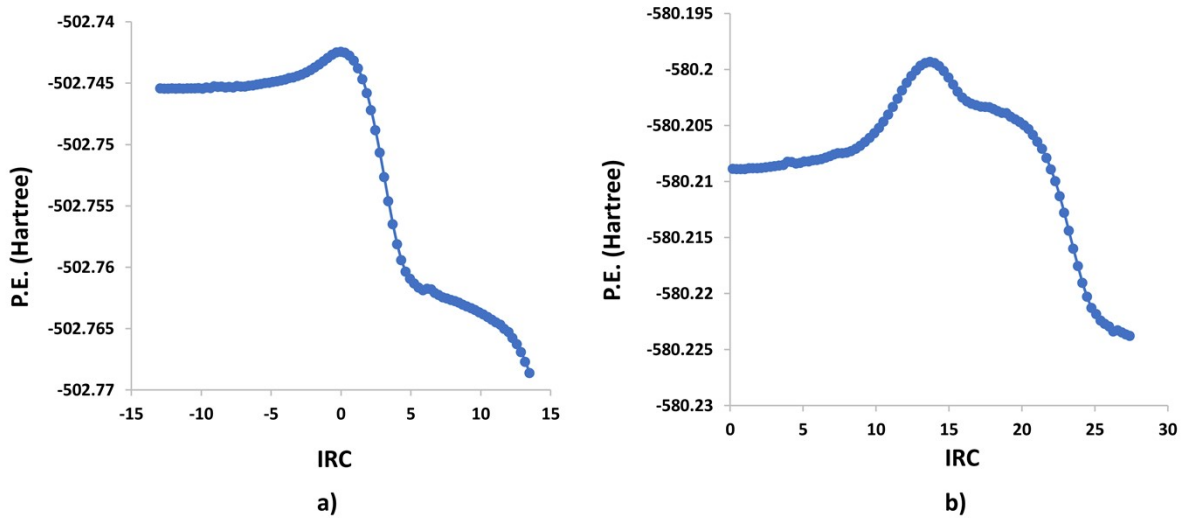


Figure S4. The IRC plot for the reaction of CO_2 with 2 and 3 in acetonitrile solvent.

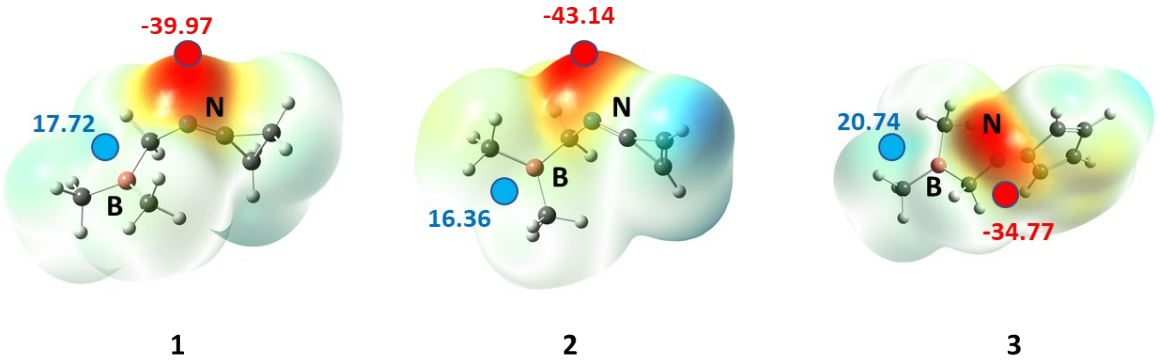


Figure S5. MESP surface of 1, 2 and 3 plotted at 0.01 a.u. iso value. Number in red shows the minima associated to the N atoms while the Numbers in blue shows the maxima associated to the B atoms. All the values are given in kcal/mol.

It can be seen from the Figure S5 that the minima at N is most negative in case of **2** which hints toward the increased basicity due to the aromaticity in the system. In case of 3 the minima associated with N was found to be -34.77 kcal/mol which least among the considered systems. This observation point towards the decreased reactivity of N atom in 3 because of the antiaromaticity in the system. Thus, MESP analysis also provides some insights regarding the effect of aromaticity on the catalytic activity of the FLPs.

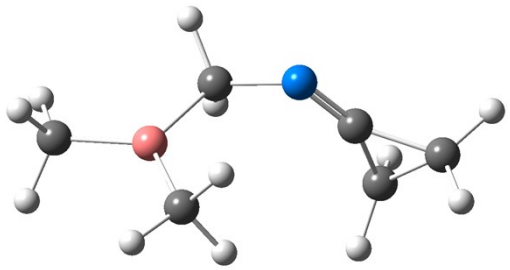
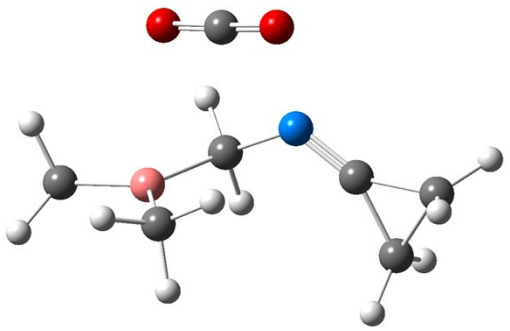
Table S1. Relative free energies of the structures obtained in the reaction of CO_2 with 2 and 3 in gas, acetonitrile and toluene solvents. All the values are given in kcal/mol.

	Gas	Acetonitrile	Toluene
2			
CM_2	1.50	2.94	2.02

TS_2	6.96	4.87	5.33
AD_2	-5.86	-18.38	-12.33
3			
CM_3	3.55	2.92	4.23
TS_3	14.69	11.20	14.81
AD_3	7.11	-0.56	3.83

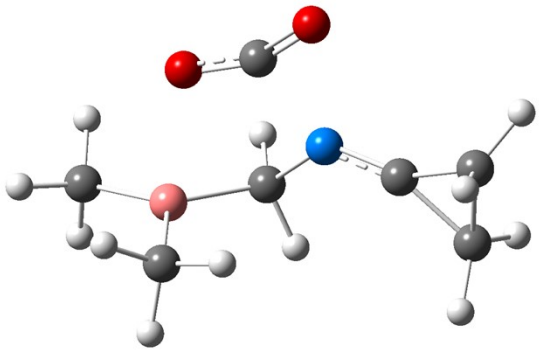
Cartesian Coordinates of the optimized geometries obtained in the reaction of IFLPs with CO_2 in gas phase

1

1			
	C	-0.58557500	0.93740100	0.41278400
	H	-0.34806700	1.50097400	-0.50644500
	H	-0.98742000	1.67099300	1.12000000
	B	-1.74001400	-0.06666400	0.02098400
	N	0.59146800	0.32114000	0.99817600
	C	1.57984400	0.14139400	0.25771800
	C	2.92872100	-0.38428300	0.13691100
	C	2.20861100	0.28192300	-1.06152000
	H	3.06777400	-1.45733500	0.09956600
	H	3.74356400	0.16640300	0.58936900
	H	2.56357700	1.25644400	-1.37282000
	H	1.88553000	-0.36391200	-1.86870200
	C	-1.47032300	-1.60728900	0.03800800
	H	-1.02343900	-1.90849500	0.98958200
	H	-2.33911100	-2.22911500	-0.17584500
	H	-0.69975200	-1.82812200	-0.71183700
	C	-3.12748200	0.52370800	-0.41124700
	H	-3.14812600	1.60563000	-0.54688500
	H	-3.50474900	0.04175700	-1.31685400
	H	-3.85276800	0.27299100	0.37279600
Zero-point correction= 0.169470 (Hartree/Particle) Thermal correction to Energy= 0.179928 Thermal correction to Enthalpy= 0.180872 Thermal correction to Gibbs Free Energy= 0.132817 Sum of electronic and zero-point Energies= -315.202828 Sum of electronic and thermal Energies= -315.192369 Sum of electronic and thermal Enthalpies= -315.191425 Sum of electronic and thermal Free Energies= -315.239480				
CM_1				
	C	-0.24443000	-1.01646300	-0.94408800
	H	0.23985200	-2.00591900	-1.01600700
	H	-0.72446300	-0.83028700	-1.90881000
	B	-1.35811500	-1.15849500	0.17275100
	N	0.71569100	0.04396500	-0.69593000
	C	1.84961300	-0.26102300	-0.27267200
	C	3.13946900	0.21782100	0.19151700
	C	2.80812300	-1.29389200	0.13235000
	H	3.20007600	0.67848800	1.16933800
	H	3.84518400	0.59611500	-0.53687800
	H	3.30252300	-1.87959400	-0.63241200
	H	2.65476500	-1.80727500	1.07348700
	C	-0.94004800	2.16897100	-0.12298900
	O	-1.81569800	1.54300400	-0.55103100
	O	-0.11717000	2.84075600	0.32514100
	C	-2.69168500	-1.88932700	-0.20462300
	H	-2.61621500	-2.54941900	-1.07022300
	H	-3.15014500	-2.42738700	0.62638600
	H	-3.39409100	-1.09103100	-0.48036500
	C	-1.09753900	-0.67105900	1.63918100
	H	-2.01293800	-0.41242800	2.17399800
	H	-0.66651000	-1.52885300	2.17489600
	H	-0.37537800	0.14205100	1.72942100
Zero-point correction= 0.182761 (Hartree/Particle)				

Thermal correction to Energy= 0.197090
Thermal correction to Enthalpy= 0.198034
Thermal correction to Gibbs Free Energy= 0.139403
Sum of electronic and zero-point Energies= -503.795607
Sum of electronic and thermal Energies= -503.781278
Sum of electronic and thermal Enthalpies= -503.780333
Sum of electronic and thermal Free Energies= -503.838964

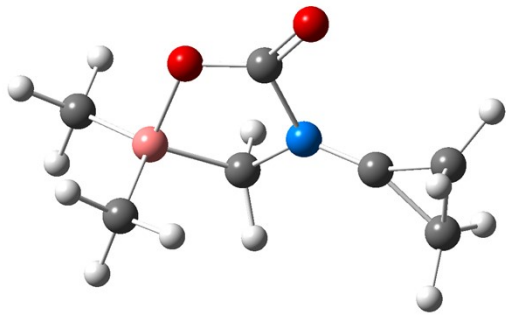
TS_1



C	-0.53425900	-0.95691900	-0.86712400
H	-0.24286100	-2.01119700	-0.79136100
H	-0.77598100	-0.74024600	-1.91054800
B	-1.78953700	-0.64102100	0.08545700
N	0.56432200	-0.09111400	-0.48698800
C	1.71218200	-0.47723600	-0.19231500
C	3.02629600	-0.08121300	0.27274300
C	2.68494400	-1.55481600	-0.03814100
H	3.13321100	0.20478000	1.31095000
H	3.67334000	0.44332200	-0.41783300
H	3.11085600	-1.99348700	-0.93126600
H	2.56880000	-2.23162400	0.79872700
C	-0.07827100	1.71385100	-0.07667800
O	-1.25379700	1.52830500	-0.11636200
O	0.87498100	2.37559800	0.08600300
C	-3.22804100	-0.66377600	-0.54376500
H	-3.48913400	-1.70575400	-0.76757400
H	-4.00004800	-0.27708700	0.12188200
H	-3.27544800	-0.12198700	-1.48989000
C	-1.58447000	-0.74115700	1.64269700
H	-2.24740700	-0.06499200	2.18449500
H	-1.85744700	-1.75717200	1.95343900
H	-0.56020400	-0.56528400	1.97897500

Zero-point correction= 0.183609 (Hartree/Particle)
Thermal correction to Energy= 0.196507
Thermal correction to Enthalpy= 0.197452
Thermal correction to Gibbs Free Energy= 0.143982
Sum of electronic and zero-point Energies= -503.784547
Sum of electronic and thermal Energies= -503.771649
Sum of electronic and thermal Enthalpies= -503.770704
Sum of electronic and thermal Free Energies= -503.824174

AD_1

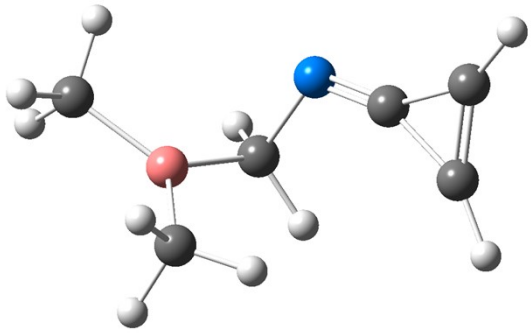


C	-0.51965900	-1.03716300	-0.71603400
H	-0.26170400	-2.04984100	-0.41123600
H	-0.62784100	-0.99103000	-1.80298500
B	-1.79885900	-0.31181100	0.05277400
N	0.56862500	-0.13005300	-0.35479200
C	1.77764000	-0.38937600	-0.13299300
C	3.05885200	0.10815300	0.29809400
C	2.84844400	-1.36383600	-0.10701500
H	3.17698900	0.33906600	1.34922200
H	3.59085600	0.76154200	-0.38101200
H	3.24853500	-1.69796800	-1.05606400
H	2.82806900	-2.11022000	0.67716400
C	0.02159800	1.28122100	-0.07681100
O	-1.23356200	1.18415200	-0.00055400
O	0.80046000	2.17861600	0.01735400
C	-3.17046100	-0.36510900	-0.76552800
H	-3.53851300	-1.39309600	-0.83980900
H	-3.95453600	0.21572100	-0.27330200
H	-3.06992300	0.01824200	-1.78529100

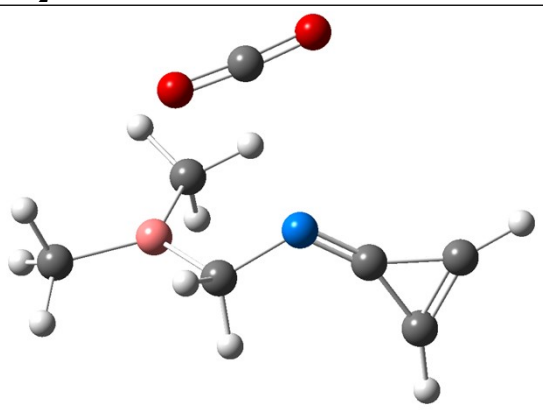
	C	-1.88040700	-0.73285000	1.60394100
	H	-2.57562700	-0.09437900	2.15466800
	H	-2.23811100	-1.76157900	1.70845100
	H	-0.91549900	-0.67540800	2.12354200

Zero-point correction= 0.186958 (Hartree/Particle)
Thermal correction to Energy= 0.198804
Thermal correction to Enthalpy= 0.199748
Thermal correction to Gibbs Free Energy= 0.149633
Sum of electronic and zero-point Energies= -503.800059
Sum of electronic and thermal Energies= -503.788213
Sum of electronic and thermal Enthalpies= -503.787269
Sum of electronic and thermal Free Energies= -503.837384

2

2				
	C	-0.54093300	-0.68084600	1.02461700
	H	-0.05558700	-0.11670400	1.82994600
	H	-0.97828000	-1.59059200	1.43822600
	B	-1.52912200	0.16821400	0.12435800
	N	0.41136400	-1.06817900	-0.03248700
	C	1.47304300	-0.39856200	-0.10712600
	C	2.71881700	-0.12376800	-0.72987900
	C	2.40059700	0.60554800	0.32925100
	H	3.44850400	-0.31729800	-1.49957200
	H	2.70691400	1.40262900	0.98737900
	C	-1.26522300	1.70671400	-0.05351600
	H	-0.25571500	2.02109600	0.21795600
	H	-1.50482400	2.08041000	-1.05040300
	H	-1.94849100	2.22130600	0.63607000
	C	-2.71708900	-0.56479600	-0.58848400
	H	-3.20635100	0.00344300	-1.37961300
	H	-2.38106200	-1.52437500	-0.99015600
	H	-3.47432100	-0.80947100	0.16660000

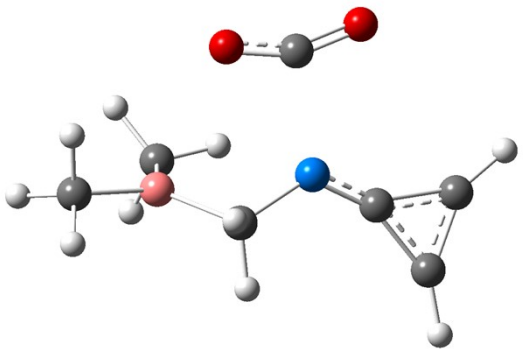
Zero-point correction= 0.146108 (Hartree/Particle)
Thermal correction to Energy= 0.156273
Thermal correction to Enthalpy= 0.157217
Thermal correction to Gibbs Free Energy= 0.109963
Sum of electronic and zero-point Energies= -313.978206
Sum of electronic and thermal Energies= -313.968042
Sum of electronic and thermal Enthalpies= -313.967098
Sum of electronic and thermal Free Energies= -314.014352

CM_2				
	C	0.23214700	-1.03696200	-0.88299900
	H	0.65925100	-0.86342800	-1.87627900
	H	-0.19607500	-2.05574800	-0.91974400
	B	1.40147700	-1.09756500	0.17902000
	N	-0.77997500	-0.02197100	-0.62822900
	C	-1.91224300	-0.39104600	-0.23655000
	C	-3.23091800	-0.08598200	0.19328300
	C	-2.90087600	-1.36668200	0.12721800
	H	-3.99938500	0.63249100	0.42836000
	H	-3.23372600	-2.38110900	0.27660000
	C	1.19575600	-0.58403200	1.64630600
	H	0.92717400	-1.45876800	2.25437600
	H	2.11365500	-0.18838900	2.08604700
	H	0.38958900	0.14195100	1.76141600

	C	2.75705400	-1.76089400	-0.24872300
	H	2.67433400	-2.45225800	-1.08930100
	H	3.39212800	-0.93187400	-0.58957000
	H	3.29417900	-2.24324100	0.56930000
	C	0.68713000	2.19379500	-0.14278400
	O	1.60969200	1.64077100	-0.57211700
	O	-0.17681500	2.81333000	0.30546700

Zero-point correction= 0.159001 (Hartree/Particle)
Thermal correction to Energy= 0.172928
Thermal correction to Enthalpy= 0.173872
Thermal correction to Gibbs Free Energy= 0.116196
Sum of electronic and zero-point Energies= -502.574799
Sum of electronic and thermal Energies= -502.560872
Sum of electronic and thermal Enthalpies= -502.559928
Sum of electronic and thermal Free Energies= -502.617604

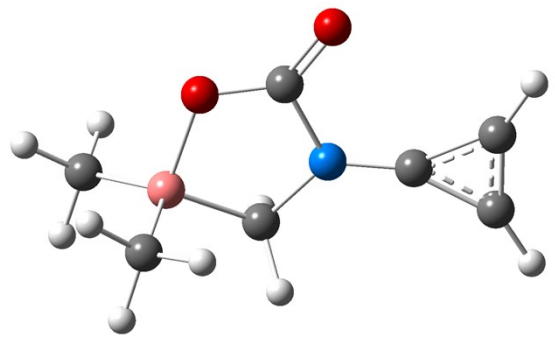
TS_2



C	0.57564200	-0.98066100	-0.80352100
H	0.82806600	-0.79005600	-1.85054200
H	0.35588100	-2.05609700	-0.72093300
B	1.82189200	-0.66780900	0.13516800
N	-0.58235600	-0.17730500	-0.45756400
C	-1.70960600	-0.65067000	-0.17114800
C	-3.04265200	-0.42460200	0.23614000
C	-2.67183400	-1.67937100	0.02901500
H	-3.82021500	0.26553400	0.51712400
H	-2.95480000	-2.71900000	0.02861700
C	1.62059200	-0.44276400	1.67344600
H	1.88674800	-1.37738700	2.18385300
H	2.30690800	0.31407400	2.05871900
H	0.60424600	-0.17967500	1.96944900
C	3.25756000	-0.72969900	-0.48904300
H	3.34291600	-1.41800300	-1.33274400
H	3.43978300	0.27416800	-0.89447600
H	4.05316500	-0.93331200	0.22811600
C	-0.19058000	1.76416200	-0.14445600
O	0.97541900	1.78612500	-0.32839100
O	-1.23921800	2.22157100	0.12305600

Zero-point correction= 0.159393 (Hartree/Particle)
Thermal correction to Energy= 0.172141
Thermal correction to Enthalpy= 0.173085
Thermal correction to Gibbs Free Energy= 0.119566
Sum of electronic and zero-point Energies= -502.569078
Sum of electronic and thermal Energies= -502.556331
Sum of electronic and thermal Enthalpies= -502.555387
Sum of electronic and thermal Free Energies= -502.608905

AD_2

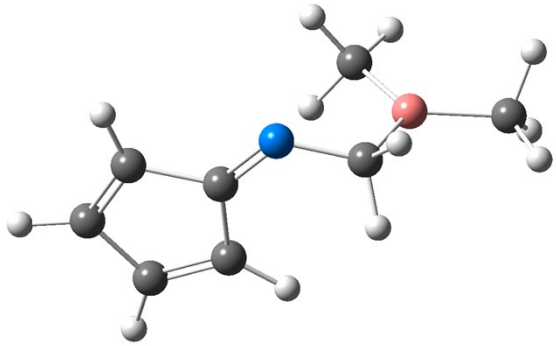


C	-0.45332100	-1.19396700	-0.36102600
H	-0.29741500	-2.05030200	0.29552800
H	-0.43541300	-1.52515600	-1.40194400
B	-1.77790000	-0.26712600	0.02863200
N	0.64108900	-0.23094000	-0.16783400
C	1.89201100	-0.45616900	-0.06002200
C	3.18345700	0.02675700	0.13132700
C	3.01502300	-1.28401400	-0.01980000
H	3.82424500	0.87757300	0.28610000
H	3.44101900	-2.27158400	-0.07414400
C	-2.19971200	-0.45248500	1.57167900
H	-1.35039800	-0.36602700	2.26060800
H	-2.93894700	0.29136600	1.87984500

	H	-2.64679400	-1.43787300	1.73717600
	C	-2.97198700	-0.36457600	-1.03500200
	H	-3.78361100	0.32781600	-0.79701100
	H	-2.64573800	-0.14771300	-2.05707500
	H	-3.40486400	-1.37015200	-1.04038300
	C	0.15773700	1.18180700	-0.08082200
	O	-1.10601600	1.17021600	-0.09880600
	O	0.96858500	2.06480400	-0.01807300

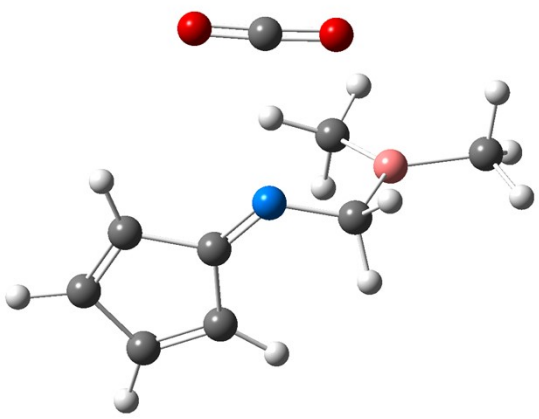
Zero-point correction= 0.163965 (Hartree/Particle)
Thermal correction to Energy= 0.175339
Thermal correction to Enthalpy= 0.176283
Thermal correction to Gibbs Free Energy= 0.126872
Sum of electronic and zero-point Energies= -502.592230
Sum of electronic and thermal Energies= -502.580856
Sum of electronic and thermal Enthalpies= -502.579912
Sum of electronic and thermal Free Energies= -502.629323

3

3				
	C	-2.25172000	-0.86514700	0.57072900
	C	-3.13206000	0.11692600	0.35209500
	C	-2.50082000	1.14630300	-0.50674000
	C	-1.24715200	0.78261700	-0.80705500
	H	-2.37212900	-1.76692900	1.14956500
	H	-4.14322300	0.17663000	0.72578700
	H	-2.99724500	2.04932200	-0.83215000
	H	-0.54454200	1.33065400	-1.41394000
	C	-0.99378400	-0.52153600	-0.13603200
	N	0.04436800	-1.24886000	-0.09275600
	C	1.25403500	-0.82604400	-0.74607500
	H	1.80986400	-1.71232100	-1.06803700
	H	1.07599800	-0.23547600	-1.65896400
	B	2.21925400	0.06383800	0.14482300
	C	3.66020100	0.35371800	-0.39963600
	H	4.37180400	-0.17055000	0.25010100
	H	3.84419700	0.02731800	-1.42366600
	H	3.91507800	1.41274800	-0.30929500
	C	1.71315600	0.64216900	1.50461800
	H	1.32925700	-0.16387500	2.13781100
	H	2.45194700	1.21987700	2.05879100
	H	0.84100400	1.28139000	1.31775800

Zero-point correction= 0.182591 (Hartree/Particle)
Thermal correction to Energy= 0.193736
Thermal correction to Enthalpy= 0.194681
Thermal correction to Gibbs Free Energy= 0.144937
Sum of electronic and zero-point Energies= -391.411231
Sum of electronic and thermal Energies= -391.400086
Sum of electronic and thermal Enthalpies= -391.399142
Sum of electronic and thermal Free Energies= -391.448885

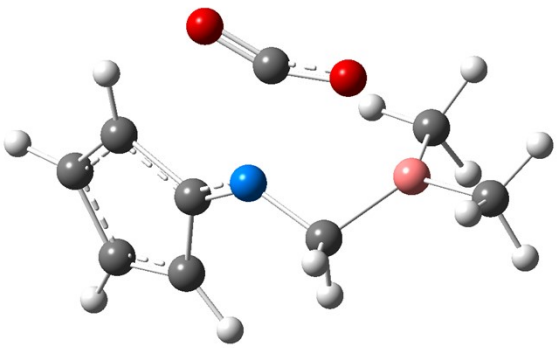
CM_3				
	C	2.31108700	0.96984700	-0.11035100
	C	3.44332700	0.38926200	0.29881400
	C	3.27600100	-1.08312100	0.24860500



C	2.04842000	-1.38777800	-0.19120400
H	2.07590900	2.01898600	-0.19402900
H	4.34694000	0.88549000	0.61952800
H	4.04479600	-1.78864200	0.52945200
H	1.63909200	-2.37479500	-0.33228700
C	1.34282600	-0.10324900	-0.44519700
N	0.16001500	0.13435100	-0.83658300
C	-0.77927900	-0.92882200	-1.06832800
H	-1.41489100	-0.65463800	-1.91439000
H	-0.30484800	-1.88847500	-1.32788200
B	-1.71256900	-1.24206100	0.18098000
C	-3.05210600	-2.00695000	-0.08588100
H	-3.34067600	-2.67504300	0.72701000
H	-3.82800400	-1.23089400	-0.13428700
H	-3.08844900	-2.54624000	-1.03351900
C	-1.25073600	-0.88259300	1.63152400
H	-0.65067500	0.02634800	1.70334900
H	-2.06696200	-0.84548700	2.35362000
H	-0.58653600	-1.69889200	1.95134700
C	-1.50192000	2.17822000	0.00580000
O	-0.65401100	2.90225200	0.29991600
O	-2.39707200	1.49440300	-0.26234400

Zero-point correction= 0.195805 (Hartree/Particle)
Thermal correction to Energy= 0.210891
Thermal correction to Enthalpy= 0.211836
Thermal correction to Gibbs Free Energy= 0.151046
Sum of electronic and zero-point Energies= -580.004101
Sum of electronic and thermal Energies= -579.989015
Sum of electronic and thermal Enthalpies= -579.988071
Sum of electronic and thermal Free Energies= -580.048861

TS_3

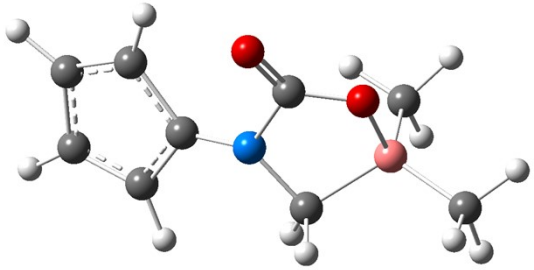


C	2.32218200	0.86253600	0.17534400
C	3.48858800	0.24195100	0.36868600
C	3.33831700	-1.20094600	0.05014800
C	2.08304500	-1.45213600	-0.33420800
H	2.07962200	1.90321200	0.30731400
H	4.41012900	0.69506500	0.70181200
H	4.13816600	-1.92325900	0.12336000
H	1.66718700	-2.39927200	-0.63344800
C	1.34668200	-0.16203700	-0.28186500
N	0.13423000	0.08326200	-0.55937800
C	-0.85473000	-0.89842200	-0.91510800
H	-1.20850000	-0.65626400	-1.92133200
H	-0.45697900	-1.91707000	-0.92008400
B	-2.07937300	-0.76590200	0.13330300
C	-3.53411900	-1.05870100	-0.39756300
H	-4.30904700	-0.72649500	0.29503800
H	-3.73141000	-0.61797200	-1.37639300
H	-3.65304400	-2.14299900	-0.50605800
C	-1.74261900	-0.96249800	1.66413900
H	-0.75197700	-0.60620700	1.95756300
H	-2.48297300	-0.49075900	2.31255900
H	-1.77363900	-2.03565700	1.88536400
C	-0.93761500	1.77317500	-0.08627600
O	-0.19115200	2.66566300	-0.06677900
O	-1.99993200	1.24769000	0.01223600

Zero-point correction= 0.196858 (Hartree/Particle)
Thermal correction to Energy= 0.210360
Thermal correction to Enthalpy= 0.211304
Thermal correction to Gibbs Free Energy= 0.156233

Sum of electronic and zero-point Energies= -579.990491
Sum of electronic and thermal Energies= -579.976989
Sum of electronic and thermal Enthalpies= -579.976045
Sum of electronic and thermal Free Energies= -580.031116

AD_3



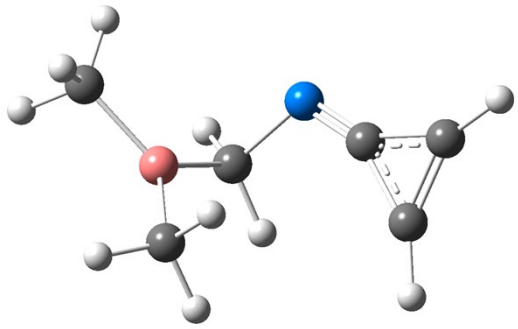
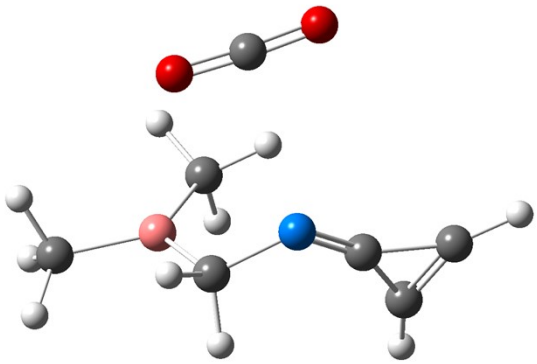
C	2.29390000	0.85287100	0.35178800
C	3.46669100	0.22450200	0.45179600
C	3.33430700	-1.17454100	-0.04571600
C	2.07643200	-1.39419300	-0.43417400
H	2.04074400	1.86371000	0.61393600
H	4.38426000	0.64718500	0.83198300
H	4.14583600	-1.88581800	-0.08231700
H	1.65501400	-2.29128600	-0.85336400
C	1.33803800	-0.13256000	-0.21300200
N	0.09405000	0.04583300	-0.45814100
C	-0.90128200	-0.95250000	-0.79347400
H	-1.16302900	-0.82062700	-1.84711900
H	-0.52513600	-1.95379800	-0.60851400
B	-2.17660600	-0.43130400	0.15065300
C	-3.60861300	-0.69529100	-0.50511800
H	-4.40697400	-0.24503700	0.09034300
H	-3.69113800	-0.29471900	-1.51958300
H	-3.82185000	-1.76714000	-0.55866800
C	-1.99978000	-0.87329700	1.68622100
H	-0.99689100	-0.68311100	2.08790000
H	-2.70562900	-0.34370100	2.33111500
H	-2.19609700	-1.94237100	1.80875000
C	-0.62514100	1.38346100	-0.19133700
O	-0.00559500	2.39958900	-0.25035400
O	-1.83712300	1.11562200	0.04002300

Zero-point correction= 0.200094 (Hartree/Particle)
Thermal correction to Energy= 0.212657
Thermal correction to Enthalpy= 0.213601
Thermal correction to Gibbs Free Energy= 0.161558
Sum of electronic and zero-point Energies= -580.004657
Sum of electronic and thermal Energies= -579.992094
Sum of electronic and thermal Enthalpies= -579.991150
Sum of electronic and thermal Free Energies= -580.043193

Cartesian Coordinates of the optimized geometries obtained in the reaction of IFLPs with CO_2 in Solvent phase

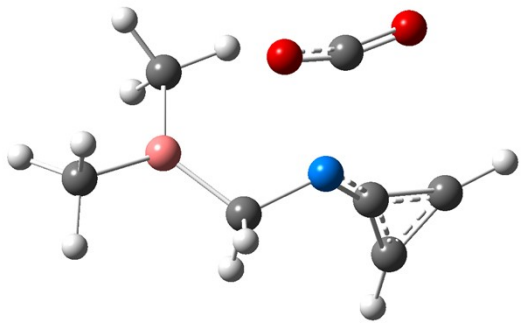
Acetonitrile

2

2			
	C	-0.57334800	-0.80035700	1.03584900
	H	-0.09004900	-0.32189800	1.89447600
	H	-1.09079300	-1.69768300	1.38065900
	B	-1.46946200	0.16664100	0.16193600
	N	0.42045900	-1.20590200	0.01187300
	C	1.42296400	-0.43740900	-0.10237900
	C	2.64351100	-0.08454900	-0.71856000
	C	2.20388100	0.69472100	0.26178500
	H	3.41381100	-0.26528100	-1.45246700
	H	2.37897300	1.57590200	0.85928000
	C	-1.13280900	1.70043500	0.08906600
	H	-0.43434100	1.84213800	-0.74807900
	H	-2.00857900	2.30985700	-0.15011600
	H	-0.64853700	2.10365800	0.98075900
	C	-2.61397300	-0.43777600	-0.72271800
	H	-2.82214300	0.12654600	-1.63476300
	H	-2.47000900	-1.49163200	-0.97136700
	H	-3.52559700	-0.38389400	-0.10944400
Zero-point correction= 0.145901 (Hartree/Particle) Thermal correction to Energy= 0.155860 Thermal correction to Enthalpy= 0.156804 Thermal correction to Gibbs Free Energy= 0.110656 Sum of electronic and zero-point Energies= -313.992104 Sum of electronic and thermal Energies= -313.982146 Sum of electronic and thermal Enthalpies= -313.981202 Sum of electronic and thermal Free Energies= -314.027349				
CM_2			
	C	0.44562400	-0.95274700	-1.11078500
	H	1.02585800	-0.69806700	-2.00330400
	H	0.16955500	-2.01512000	-1.24294900
	B	1.39022400	-0.95956000	0.15318500
	N	-0.73953400	-0.09501100	-1.05817700
	C	-1.71913700	-0.54665000	-0.39951700
	C	-3.02416500	-0.41307700	0.12849900
	C	-2.37290600	-1.53938500	0.38816600
	H	-3.93058000	0.15670600	0.26588200
	H	-2.39832000	-2.49967200	0.87938000
	C	2.85685400	-1.48825000	-0.02766600
	H	3.25669600	-1.98303900	0.86064800
	H	2.99466500	-2.13661700	-0.89621500
	H	3.48466600	-0.60160300	-0.19521500
	C	0.88841700	-0.53339500	1.57678100
	H	1.67668800	-0.06272500	2.17111700
	H	-0.00280400	0.09715400	1.59625800
	H	0.63069700	-1.46226500	2.10576000
	C	0.38994900	2.22784400	-0.01962600
	O	-0.59698800	2.64916300	0.40668000
	O	1.41332200	1.86859800	-0.42107400
Zero-point correction= 0.158619 (Hartree/Particle)				

Thermal correction to Energy= 0.172342
Thermal correction to Enthalpy= 0.173287
Thermal correction to Gibbs Free Energy= 0.117233
Sum of electronic and zero-point Energies= -502.587292
Sum of electronic and thermal Energies= -502.573569
Sum of electronic and thermal Enthalpies= -502.572625
Sum of electronic and thermal Free Energies= -502.628678

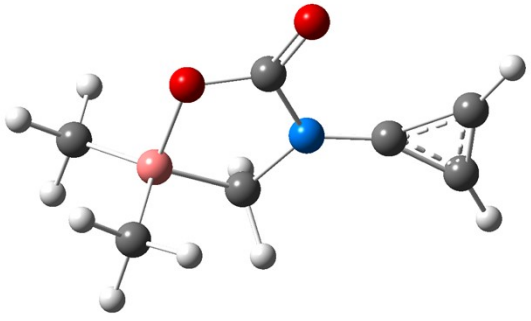
TS_2



C	0.56417400	-0.91443900	-0.81320800
H	0.86658800	-0.67173500	-1.83872100
H	0.35890600	-1.99850200	-0.81409700
B	1.79294900	-0.70916800	0.15792200
N	-0.62243300	-0.14208900	-0.47600100
C	-1.69626300	-0.72943000	-0.16462800
C	-3.04497400	-0.67908800	0.25055200
C	-2.50654800	-1.87485100	0.05525000
H	-3.92023000	-0.11457800	0.53232000
H	-2.64715400	-2.94417600	0.07057300
C	3.22463400	-1.04311600	-0.38861600
H	3.92513000	-1.37943800	0.37898700
H	3.23188300	-1.74902000	-1.22268900
H	3.62322900	-0.09548600	-0.77932500
C	1.60608100	-0.25807200	1.64636200
H	2.43251600	0.36432200	2.00015900
H	0.65985600	0.23980600	1.86546100
H	1.64008700	-1.17354800	2.25446200
C	-0.19721500	2.00769300	-0.17291000
O	-1.23043200	2.38438900	0.21553400
O	0.92069900	1.99194100	-0.51322700

Zero-point correction= 0.158013 (Hartree/Particle)
Thermal correction to Energy= 0.171082
Thermal correction to Enthalpy= 0.172027
Thermal correction to Gibbs Free Energy= 0.116886
Sum of electronic and zero-point Energies= -502.584466
Sum of electronic and thermal Energies= -502.571397
Sum of electronic and thermal Enthalpies= -502.570453
Sum of electronic and thermal Free Energies= -502.625594

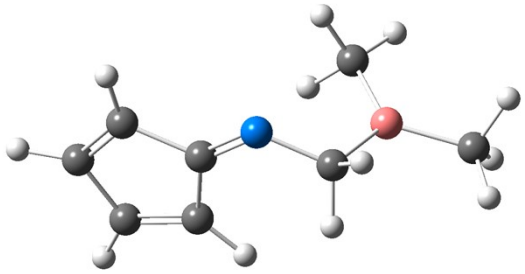
AD_2



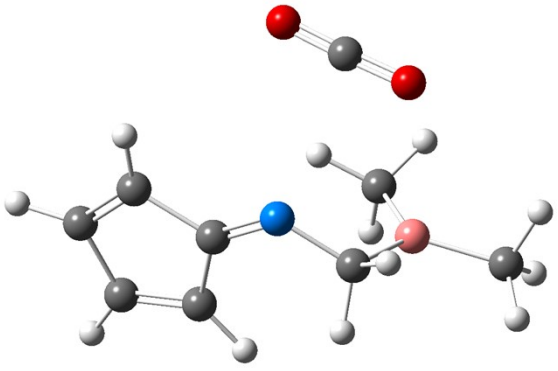
C	-0.41179200	-1.18909400	-0.25708100
H	-0.24978200	-1.98757300	0.46793800
H	-0.34275700	-1.60872700	-1.26364100
B	-1.76275900	-0.27744500	0.01638900
N	0.65518500	-0.18620300	-0.10434800
C	1.92560900	-0.42234400	-0.03425800
C	3.23283000	0.00230000	0.09178600
C	2.98773100	-1.30525500	-0.01788100
H	3.93711900	0.81123600	0.19985800
H	3.35031500	-2.31960900	-0.06219700
C	-2.31067700	-0.43185100	1.52894500
H	-1.51630000	-0.30457000	2.27501700
H	-3.09361100	0.29836000	1.76314300
H	-2.74263600	-1.42611200	1.69164600
C	-2.89464400	-0.42252500	-1.11967800
H	-3.73636700	0.26053800	-0.95890400
H	-2.50626600	-0.23012500	-2.12630400
H	-3.30951800	-1.43714500	-1.12775000
C	0.15780400	1.17291100	-0.06689600
O	-1.12181200	1.16183900	-0.09945700
O	0.91133000	2.11435200	-0.02053400

Zero-point correction=	0.163934 (Hartree/Particle)
Thermal correction to Energy=	0.175179
Thermal correction to Enthalpy=	0.176123
Thermal correction to Gibbs Free Energy=	0.127030
Sum of electronic and zero-point Energies=	-502.625742
Sum of electronic and thermal Energies=	-502.614497
Sum of electronic and thermal Enthalpies=	-502.613553
Sum of electronic and thermal Free Energies=	-502.662646

3

3			
	C	-2.25936100	-0.99817900	0.27953200
	C	-3.14605300	-0.00160900	0.37421100
	C	-2.52217100	1.24698300	-0.12276500
	C	-1.26614400	1.00209000	-0.51981300
	H	-2.37534900	-2.03602300	0.55132400
	H	-4.15778400	-0.06605600	0.74691900
	H	-3.02575200	2.20303300	-0.15189400
	H	-0.56547800	1.71419500	-0.92636500
	C	-1.00472300	-0.44393800	-0.28559100
	N	0.03959800	-1.14097700	-0.46890500
	C	1.24581200	-0.53380100	-0.96587100
	H	1.79435900	-1.27576200	-1.55638300
	H	1.06257700	0.31500300	-1.64219400
	B	2.23383100	0.00825900	0.15044700
	C	3.65266000	0.49282800	-0.30162100
	H	4.39313400	-0.19961700	0.11906900
	H	3.81092300	0.53341700	-1.38057000
	H	3.89349000	1.46901100	0.12993500
	C	1.77717000	0.07259700	1.64261300
	H	1.39499900	-0.89850100	1.97397300
	H	2.54602300	0.41196200	2.33760600
	H	0.91937900	0.75305200	1.72451700

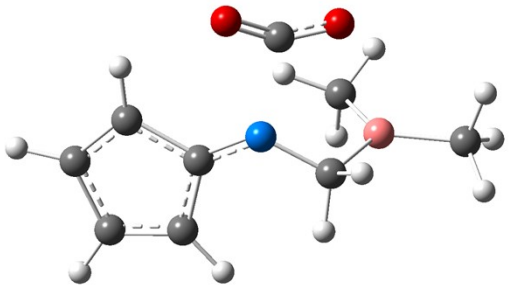
Zero-point correction=	0.182517 (Hartree/Particle)
Thermal correction to Energy=	0.193681
Thermal correction to Enthalpy=	0.194625
Thermal correction to Gibbs Free Energy=	0.144676
Sum of electronic and zero-point Energies=	-391.419826
Sum of electronic and thermal Energies=	-391.408663
Sum of electronic and thermal Enthalpies=	-391.407719
Sum of electronic and thermal Free Energies=	-391.457668

CM_3				
	C	2.36383800	0.92177300	-0.36588300
	C	3.42313600	0.36051100	0.22860600
	C	3.13886900	-1.07603600	0.46733600
	C	1.91568000	-1.37969700	0.01117500
	H	2.23118700	1.94635700	-0.67980600
	H	4.34819800	0.84709700	0.50276200
	H	3.83230400	-1.75578700	0.94287500
	H	1.42590000	-2.34048800	0.04669700
	C	1.33150700	-0.13018400	-0.54479800
	N	0.18916600	0.09316200	-1.05307700
	C	-0.79020100	-0.96049500	-1.13993500
	H	-1.45022100	-0.75938300	-1.98762100
	H	-0.34022700	-1.95001000	-1.31852400
	B	-1.67453300	-1.17903900	0.16149800
	C	-3.02364100	-1.95471100	-0.01432600

	H	-3.05807600	-2.59493900	-0.89858400
	H	-3.30650300	-2.53518600	0.86662700
	H	-3.80420900	-1.19263500	-0.14731300
	C	-1.20288800	-0.72255000	1.58162300
	H	-0.40838200	0.02598300	1.60977200
	H	-2.04042800	-0.38662300	2.19989600
	H	-0.81067600	-1.62072900	2.07950400
	C	-1.46569000	2.13449900	0.08493400
	O	-0.59381000	2.75125400	0.52163400
	O	-2.37044500	1.54883900	-0.33471300

Zero-point correction= 0.195220 (Hartree/Particle)
Thermal correction to Energy= 0.210253
Thermal correction to Enthalpy= 0.211197
Thermal correction to Gibbs Free Energy= 0.151026
Sum of electronic and zero-point Energies= -580.014832
Sum of electronic and thermal Energies= -579.999799
Sum of electronic and thermal Enthalpies= -579.998855
Sum of electronic and thermal Free Energies= -580.059026

TS_3

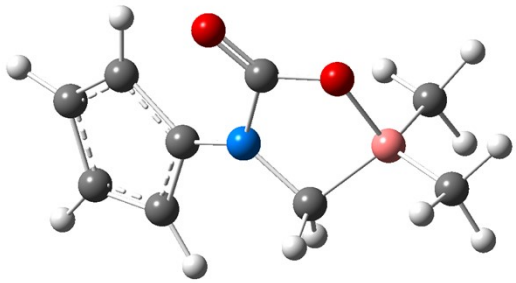


C	2.30459500	0.68509900	0.29225000
C	3.37204300	-0.10400700	0.44494200
C	3.05404000	-1.46893600	-0.04843400
C	1.79487600	-1.50568000	-0.49680700
H	2.19931400	1.72541000	0.54873100
H	4.32838600	0.17997800	0.85971300
H	3.75299700	-2.29321500	-0.03582700
H	1.27129300	-2.34921700	-0.91647800
C	1.22555200	-0.14520500	-0.30775600
N	0.04963900	0.26199500	-0.56048700
C	-1.01424200	-0.58450800	-1.03399400
H	-1.53413000	-0.05642900	-1.83713300
H	-0.64350900	-1.53091400	-1.44355100
B	-2.05207500	-0.95553600	0.11632200
C	-3.52206400	-1.27259700	-0.31685000
H	-3.61422000	-1.62108100	-1.34813500
H	-4.03287200	-1.96965200	0.35047000
H	-4.07045400	-0.32210000	-0.25902300
C	-1.58370000	-1.12993100	1.59709200
H	-0.68826600	-0.57089400	1.87420200
H	-2.37945000	-0.91129300	2.31334500
H	-1.35036400	-2.19765000	1.71972200
C	-0.68749200	1.99952000	-0.02297200
O	0.17971000	2.78942200	-0.14267600
O	-1.80314400	1.71285800	0.25154400

Zero-point correction= 0.195622 (Hartree/Particle)
Thermal correction to Energy= 0.209458
Thermal correction to Enthalpy= 0.210402
Thermal correction to Gibbs Free Energy= 0.153497
Sum of electronic and zero-point Energies= -580.003710
Sum of electronic and thermal Energies= -579.989874
Sum of electronic and thermal Enthalpies= -579.988930
Sum of electronic and thermal Free Energies= -580.045835

AD_3

C	2.34652700	0.86479100	0.32555100
C	3.52112600	0.23655200	0.39195800
C	3.36376500	-1.18204200	-0.05499000
C	2.08829500	-1.41193900	-0.36978800
H	2.11376700	1.88159600	0.58259000
H	4.45715300	0.66388400	0.72034100



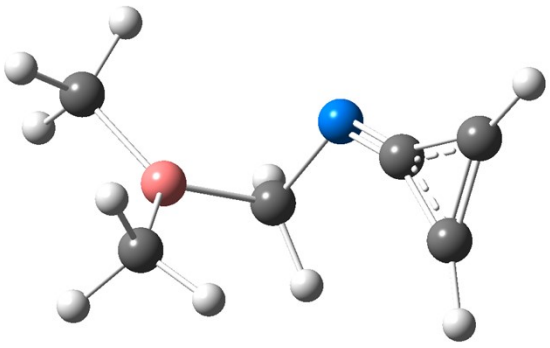
H	4.17692900	-1.89098200	-0.10960600
H	1.64085000	-2.31858800	-0.74070700
C	1.36709700	-0.13845100	-0.16067100
N	0.11031900	0.02522700	-0.36362600
C	-0.88187800	-1.00875000	-0.66272800
H	-1.02768100	-1.00786400	-1.74725000
H	-0.51616500	-1.97839100	-0.33751200
B	-2.20656700	-0.41635200	0.12190000
C	-3.59297300	-0.66368500	-0.64559500
H	-4.43345800	-0.17159400	-0.14428000
H	-3.57260700	-0.30515000	-1.68027400
H	-3.83033300	-1.73274900	-0.68118700
C	-2.21066200	-0.79138400	1.69010800
H	-1.24679000	-0.59940800	2.17755300
H	-2.96917600	-0.22527200	2.24165900
H	-2.43598200	-1.85330700	1.83706700
C	-0.59200300	1.34244000	-0.18906700
O	0.01000400	2.37555100	-0.26497700
O	-1.82896300	1.11917400	-0.00142000

Zero-point correction= 0.199793 (Hartree/Particle)
Thermal correction to Energy= 0.212311
Thermal correction to Enthalpy= 0.213255
Thermal correction to Gibbs Free Energy= 0.161192
Sum of electronic and zero-point Energies= -580.025968
Sum of electronic and thermal Energies= -580.013450
Sum of electronic and thermal Enthalpies= -580.012506
Sum of electronic and thermal Free Energies= -580.064568

Toluene

2

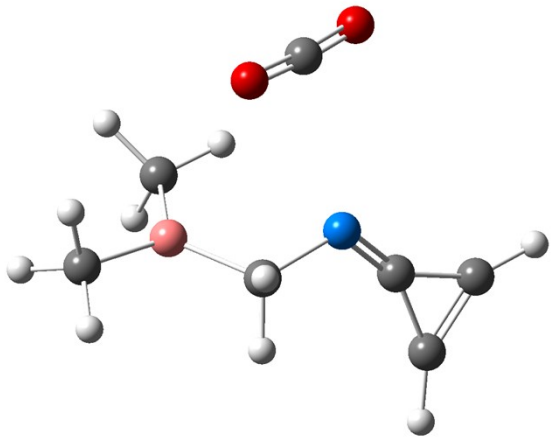
2



C	-0.54250600	-0.71314300	1.01930400
H	-0.05614400	-0.17529500	1.84144700
H	-0.98937700	-1.62954900	1.40919600
B	-1.51750500	0.16489200	0.13549600
N	0.41244800	-1.08204400	-0.04437300
C	1.47215800	-0.39989200	-0.11234700
C	2.71198600	-0.10578800	-0.73018100
C	2.37982200	0.60905400	0.33520000
H	3.44303200	-0.28479300	-1.50275300
H	2.66643400	1.40427000	1.00496700
C	-1.24783000	1.70328300	-0.02852500
H	-0.30059600	2.05221800	0.38715400
H	-1.32545800	2.03535600	-1.06733600
H	-2.04864600	2.22995600	0.50883000
C	-2.71029400	-0.53798900	-0.59991200
H	-3.16730100	0.04229900	-1.40321400
H	-2.41055200	-1.51434600	-0.99102300
H	-3.49101300	-0.74341700	0.14463300

Zero-point correction= 0.146096 (Hartree/Particle)
Thermal correction to Energy= 0.156263
Thermal correction to Enthalpy= 0.157207
Thermal correction to Gibbs Free Energy= 0.109577
Sum of electronic and zero-point Energies= -313.987032
Sum of electronic and thermal Energies= -313.976864
Sum of electronic and thermal Enthalpies= -313.975920
Sum of electronic and thermal Free Energies= -314.023550

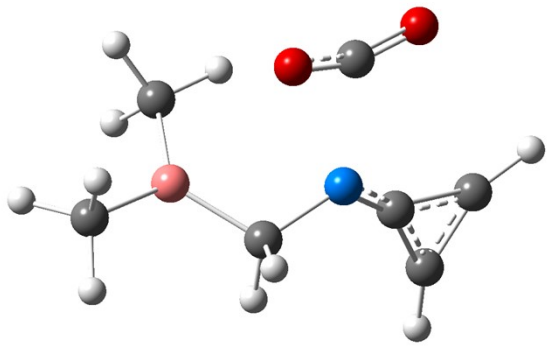
CM_2



C	0.15995700	-1.06755700	-0.76129900
H	0.52173400	-0.94200900	-1.78947100
H	-0.29289400	-2.07556300	-0.73730800
B	1.40928900	-1.12253000	0.20140300
N	-0.80881400	-0.01771800	-0.47322100
C	-1.98035900	-0.35699100	-0.16707000
C	-3.30491200	-0.02151100	0.21101800
C	-3.02062700	-1.30837600	0.08009300
H	-4.05625200	0.71480400	0.44871000
H	-3.39545800	-2.31771600	0.14247100
C	2.67346000	-1.92037600	-0.27662500
H	3.23210000	-2.38790100	0.53735200
H	2.47221900	-2.66524500	-1.04997700
H	3.35083000	-1.18063600	-0.72584900
C	1.39248400	-0.46393900	1.62318000
H	1.19441700	-1.27083300	2.34315500
H	2.36517900	-0.05249000	1.90594100
H	0.61768300	0.28967400	1.77362300
C	0.75212600	2.17340100	-0.21962400
O	1.59720300	1.60766400	-0.77248000
O	-0.02558700	2.81942200	0.33733600

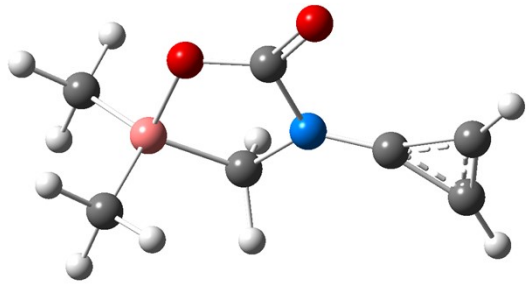
Zero-point correction= 0.158959 (Hartree/Particle)
Thermal correction to Energy= 0.172788
Thermal correction to Enthalpy= 0.173732
Thermal correction to Gibbs Free Energy= 0.116967
Sum of electronic and zero-point Energies= -502.584204
Sum of electronic and thermal Energies= -502.570374
Sum of electronic and thermal Enthalpies= -502.569430
Sum of electronic and thermal Free Energies= -502.626195

TS_2

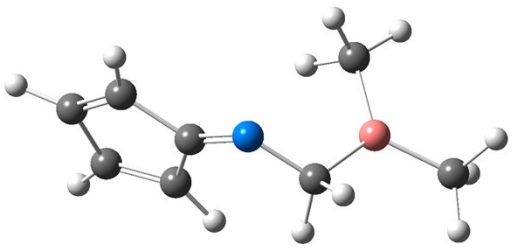


C	0.57203700	-0.95935200	-0.76087800
H	0.83324900	-0.75907300	-1.80600100
H	0.37168100	-2.04227000	-0.70402200
B	1.82808700	-0.68155600	0.16131300
N	-0.60145200	-0.17653900	-0.41549000
C	-1.70469200	-0.71542600	-0.13863900
C	-3.05658900	-0.59282700	0.25210900
C	-2.58749000	-1.81483900	0.04903100
H	-3.89737900	0.02429100	0.52482300
H	-2.79292900	-2.87318700	0.04534500
C	3.25127300	-0.96950200	-0.42975500
H	4.00207500	-1.22986100	0.31889200
H	3.26310900	-1.71469600	-1.22886200
H	3.58132800	-0.02560800	-0.88638900
C	1.67198200	-0.21457800	1.64811100
H	1.84758900	-1.09126000	2.28686300
H	2.44220000	0.50975800	1.92665700
H	0.69306000	0.19067500	1.90860200
C	-0.22130800	1.90662900	-0.19682300
O	0.90556000	1.92235500	-0.52077400
O	-1.25875300	2.30441300	0.16790200

Zero-point correction= 0.158929 (Hartree/Particle)
Thermal correction to Energy= 0.171811
Thermal correction to Enthalpy= 0.172755
Thermal correction to Gibbs Free Energy= 0.118609
Sum of electronic and zero-point Energies= -502.580594
Sum of electronic and thermal Energies= -502.567713
Sum of electronic and thermal Enthalpies= -502.566768

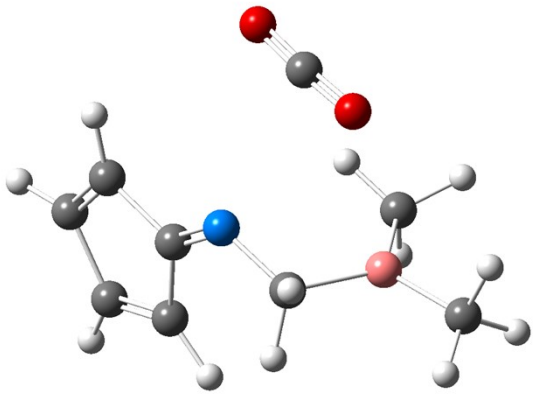
Sum of electronic and thermal Free Energies= -502.620914			
AD_2			
	C	-0.43278700	-1.18668200	-0.33431400
	H	-0.27185400	-2.02899500	0.33947600
	H	-0.39504800	-1.54193900	-1.36714600
	B	-1.76805800	-0.27251200	0.02326700
	N	0.64767200	-0.20583000	-0.14598700
	C	1.90716300	-0.43743700	-0.05049100
	C	3.20719100	0.01171300	0.12309300
	C	2.99880100	-1.29529400	-0.02454200
	H	3.88278500	0.83796400	0.26878100
	H	3.39086000	-2.29729100	-0.08337600
	C	-2.22494200	-0.45239900	1.55960300
	H	-1.39191000	-0.34971800	2.26675700
	H	-2.98147900	0.28350800	1.84969900
	H	-2.66309600	-1.44283500	1.72619800
	C	-2.95164800	-0.39198300	-1.05442700
	H	-3.77857900	0.29019500	-0.83300400
	H	-2.61814200	-0.17623400	-2.07544400
	H	-3.37212000	-1.40389500	-1.06197300
	C	0.15462700	1.17935800	-0.07724300
	O	-1.11659700	1.16643300	-0.10206700
	O	0.93593900	2.09218600	-0.01974100
Zero-point correction= 0.164286 (Hartree/Particle) Thermal correction to Energy= 0.175530 Thermal correction to Enthalpy= 0.176474 Thermal correction to Gibbs Free Energy= 0.127460 Sum of electronic and zero-point Energies= -502.612228 Sum of electronic and thermal Energies= -502.600985 Sum of electronic and thermal Enthalpies= -502.600040 Sum of electronic and thermal Free Energies= -502.649054				

3

3				
	C	-2.26024200	-1.01385600	0.21397200
	C	-3.14771800	-0.02622600	0.37312700
	C	-2.52425700	1.25277200	-0.04006000
	C	-1.26774200	1.03526300	-0.45116900
	H	-2.37589600	-2.06734900	0.41703000
	H	-4.15969800	-0.11561700	0.73999100
	H	-3.02838400	2.20839200	-0.00635900
	H	-0.56716400	1.77314900	-0.80879700
	C	-1.00564200	-0.42294700	-0.31288300
	N	0.03883900	-1.10592700	-0.54225000
	C	1.24467900	-0.46714900	-0.99888400
	H	1.79281300	-1.16880700	-1.63724200
	H	1.06148800	0.42418400	-1.61806500
	B	2.23494600	-0.00202800	0.14961800
	C	3.65053200	0.51802200	-0.27231400
	H	4.39617300	-0.19496900	0.10221100
	H	3.80671800	0.62966200	-1.34654900
	H	3.88577900	1.46593500	0.22113200
	C	1.78542300	-0.04706200	1.64469100
	H	1.41160900	-1.04222100	1.90724300
	H	2.55600900	0.24659000	2.35836700
	H	0.92376400	0.61978200	1.77982200
Zero-point correction= 0.182489 (Hartree/Particle)				

Thermal correction to Energy= 0.193668
Thermal correction to Enthalpy= 0.194612
Thermal correction to Gibbs Free Energy= 0.144541
Sum of electronic and zero-point Energies= -391.419844
Sum of electronic and thermal Energies= -391.408665
Sum of electronic and thermal Enthalpies= -391.407720
Sum of electronic and thermal Free Energies= -391.457792

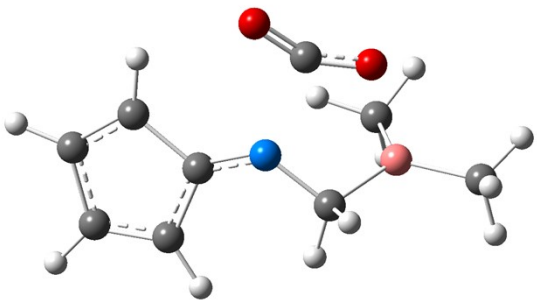
CM_3



C	2.34660600	0.98376400	-0.17681700
C	3.47421100	0.42074500	0.26939600
C	3.29667900	-1.05037200	0.30770300
C	2.06862100	-1.37241500	-0.11927900
H	2.12500200	2.02892000	-0.32692500
H	4.38147500	0.92888400	0.56148400
H	4.05966700	-1.74199900	0.63620500
H	1.65028700	-2.36281200	-0.20014400
C	1.37209500	-0.10085900	-0.45179100
N	0.19019200	0.11739600	-0.85892600
C	-0.74241300	-0.96110500	-1.05041500
H	-1.36720400	-0.72984900	-1.91826600
H	-0.26024100	-1.92812900	-1.26244300
B	-1.70040500	-1.22757400	0.18842500
C	-2.99479400	-2.07072400	-0.06756900
H	-3.27511300	-2.69806100	0.78154200
H	-3.81302600	-1.34841500	-0.19449800
H	-2.97071600	-2.67889400	-0.97402300
C	-1.32887900	-0.75206600	1.63098400
H	-0.66092600	0.10952300	1.68854600
H	-2.20481300	-0.57931100	2.26048100
H	-0.78545500	-1.58801800	2.09637600
C	-1.55702700	2.13483900	-0.01357800
O	-0.73608700	2.83655500	0.39125400
O	-2.42876900	1.47762300	-0.39747600

Zero-point correction= 0.195699 (Hartree/Particle)
Thermal correction to Energy= 0.210719
Thermal correction to Enthalpy= 0.211663
Thermal correction to Gibbs Free Energy= 0.151327
Sum of electronic and zero-point Energies= -580.012533
Sum of electronic and thermal Energies= -579.997513
Sum of electronic and thermal Enthalpies= -579.996569
Sum of electronic and thermal Free Energies= -580.056904

TS_3

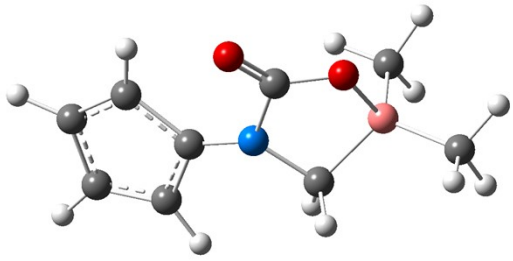


C	2.32687100	0.81351900	0.24021400
C	3.48083000	0.15879700	0.38945700
C	3.29787700	-1.26289400	0.00037300
C	2.03368000	-1.46888900	-0.38009700
H	2.11280200	1.85099100	0.43005500
H	4.41519300	0.57491900	0.73613300
H	4.08478100	-2.00292100	0.02684800
H	1.59437400	-2.39093700	-0.72241000
C	1.32439800	-0.16768300	-0.25514300
N	0.10951600	0.10277500	-0.50101600
C	-0.88714300	-0.85708500	-0.90359500
H	-1.23985700	-0.56273600	-1.89617900
H	-0.48521900	-1.87242800	-0.96902200
B	-2.10832500	-0.81990600	0.14014400
C	-3.55660300	-1.08122500	-0.40693500
H	-4.34114300	-0.81210300	0.30263100
H	-3.75622900	-0.58041100	-1.35636600

	H	-3.65819400	-2.15836200	-0.59440100
	C	-1.79364300	-0.95178600	1.67451900
	H	-0.80861600	-0.58765100	1.97544900
	H	-2.54731200	-0.46082700	2.29375800
	H	-1.83288100	-2.01843700	1.93198400
	C	-0.84569600	1.80483100	-0.10671700
	O	-0.04963900	2.66481100	-0.10393500
	O	-1.95612600	1.39462600	-0.00413400

Zero-point correction= 0.196623 (Hartree/Particle)
Thermal correction to Energy= 0.210273
Thermal correction to Enthalpy= 0.211217
Thermal correction to Gibbs Free Energy= 0.155450
Sum of electronic and zero-point Energies= -579.999886
Sum of electronic and thermal Energies= -579.986237
Sum of electronic and thermal Enthalpies= -579.985292
Sum of electronic and thermal Free Energies= -580.041059

AD_3



C	2.32656600	0.85919500	0.33588500
C	3.50026800	0.23122500	0.41759000
C	3.35364800	-1.17899200	-0.04943100
C	2.08577600	-1.40542500	-0.39671500
H	2.08483900	1.87425900	0.59160800
H	4.42832400	0.65828000	0.76721700
H	4.16565200	-1.88968000	-0.09490000
H	1.65054200	-2.30893200	-0.78825800
C	1.35628800	-0.13697900	-0.18312600
N	0.10473000	0.03212300	-0.40153900
C	-0.88935000	-0.98531700	-0.71803800
H	-1.08275400	-0.92798100	-1.79367500
H	-0.52093600	-1.97151900	-0.45170400
B	-2.19636200	-0.42069500	0.13294100
C	-3.60177000	-0.67514300	-0.58778100
H	-4.42588900	-0.20211900	-0.04496100
H	-3.62941200	-0.29671600	-1.61476100
H	-3.82957000	-1.74559900	-0.63218800
C	-2.12797200	-0.82593000	1.68924800
H	-1.15020500	-0.63784600	2.15032900
H	-2.86722600	-0.27454800	2.27838500
H	-2.34418900	-1.89066400	1.82589200
C	-0.60656100	1.36133100	-0.18976000
O	0.00593700	2.38474300	-0.25828100
O	-1.83241600	1.11874200	0.01401100

Zero-point correction= 0.200350 (Hartree/Particle)
Thermal correction to Energy= 0.212844
Thermal correction to Enthalpy= 0.213788
Thermal correction to Gibbs Free Energy= 0.161810
Sum of electronic and zero-point Energies= -580.018983
Sum of electronic and thermal Energies= -580.006488
Sum of electronic and thermal Enthalpies= -580.005544
Sum of electronic and thermal Free Energies= -580.057522