

“Supporting Information for”

Catalytic role of amines in activation of PhICl_2 : Fundamental mechanistic features revealed by a DFT-based investigation

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Computational details

Gaussian 16^{S1} was used to fully optimize all the structures reported in this paper at the M06-2X level of theory.^{S2} For all the calculations, solvent effects were considered using the SMD solvation model^{S3} in dichloromethane. The SDD basis set^{S4} with effective core potential (ECP) was chosen to describe iodine. The 6-31G(d) basis set^{S5} was used for other atoms. This basis set combination will be referred to as BS1. Frequency calculations were carried out at the same level of theory as those for the structural optimization. Transition structures were located using the Berny algorithm. Intrinsic reaction coordinate (IRC) calculations were used to confirm the connectivity between transition structures and minima.^{S6} To further refine the energies obtained from the SMD/M06-2X/SDD,6-31G(d) calculations, we carried out single-point energy calculations using the M06-2X functional method for all of the structures with a larger basis set (BS2). BS2 utilizes the def2-TZVP basis set^{S7} on all atoms. Tight convergence criterion and ultrafine integral grid were also employed to increase the accuracy of the calculations. In this work, the free energy for each species in solution was calculated using the following formula:

$$G = E(\text{BS2}) + G(\text{BS1}) - E(\text{BS1}) + \Delta G^{1\text{atm} \rightarrow 1\text{M}} \quad (1)$$

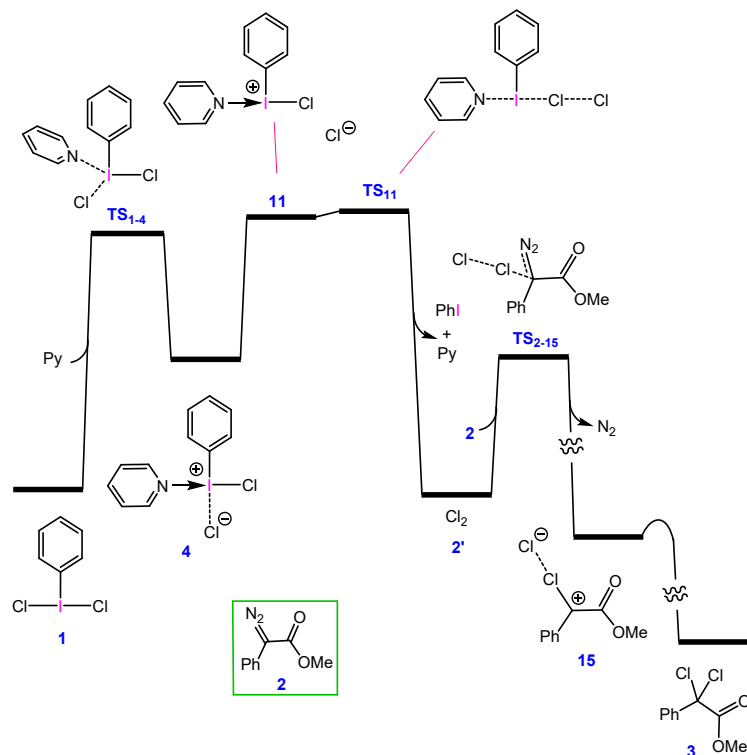
where $\Delta G^{1\text{atm} \rightarrow 1\text{M}} = 1.89$ kcal/mol is the free-energy change for compression of 1 mol of an ideal gas from 1 atm to the 1 M solution phase standard state.

The relative Gibbs energy of **TS**_{1'-4} (Fig. S1) is estimated on the basis of the methodology proposed by Hall and Hartwig. In this protocol, for example, the Gibbs free energy barrier for a dissociation reaction such as $A-B \rightarrow A + B$ is estimated as $\Delta G^\ddagger \approx \Delta H = H_A + H_B - H_{A-B}$.^{S8}

To validate the accuracy of the SMD/M06-2X/def2-TZVP//SMD/M06-2X/SDD,6-31G(d) calculations in determining the relative energies of species, we optimized all structures related to the most favourable pathway for the pyridine-catalysed dichlorination reaction using the triple-zeta def2-TZVP

Ahlrich's basis set and the corresponding ECP for the iodine atom. In addition, the single point calculations using the quadruple-*zeta* def2-QZVP Ahlrich's basis set and the corresponding ECP for the iodine atom were carried out to refine the energy values for the structures optimized by SMD/M06-2X/SDD,6-31G(d) and SMD/M06-2X/def2-TZVP; the Ahlrich basis sets have been benchmarked for non-covalent interactions (NCI) involving chlorine and reported suitable for mechanistic analysis of such systems;⁵⁹ the NCI analysis for some selected structures confirms the presence of van der Waals interactions in these systems (Figure S2). These additional results demonstrate that basis set dependence is insignificant (Table S1). For example, using SMD/M06-2X/def2-TZVP//SMD/M06-2X/SDD,6-31G(d), the relative free energies of **TS**₁₋₄, **4**, **11**, and **TS**₁₁ are 22.8, 11.1, 23.8, and 23.9 kcal/mol, respectively. Using SMD/M06-2X/def2-QZVP//SMD/M06-2X/def2-TZVP, the relative free energies are 24.5, 11.8, 22.3, and 23.2 kcal/mol, respectively. It follows from these results that the methodology used for studying the title reaction is adequately reliable.

Table S1. Basis set effect on the DFT-proposed mechanism for pyridine-catalysed dichlorination of diazo compound **2**.



method/basis set	TS ₁₋₄	4	11	TS ₁₁	2'	TS ₂₋₁₅	15	3
SMD/M06-2X/def2-TZVP//SMD/M06-2X/6-31G(d),SDD	22.8 (13.5)	11.1 (0.6)	23.8 (14.7)	23.9 (14.8)	-0.2 (8.6)	11.5 (12.0)	-27.9 (-16.6)	-57.0 (-48.9)
SMD/M06-2X/def2-QZVP//SMD/M06-2X/6-31G(d),SDD	22.9 (13.6)	10.8 (0.3)	21.1 (12.0)	21.7 (12.6)	0.4 (9.2)	12.6 (13.1)	-28.3 (-17.0)	-55.3 (-47.2)
SMD/M06-2X/def2-TZVP//SMD/M06-2X/def2-TZVP	24.5 (13.9)	12.1 (1.2)	24.9 (15.0)	25.5 (15.2)	2.8 (10.5)	15.3 (14.3)	-25.4 (-15.2)	-54.0 (-47.0)
SMD/M06-2X/def2-QZVP//SMD/M06-2X/def2-TZVP	24.5 (13.9)	11.8 (0.9)	22.3 (12.4)	23.2 (12.9)	3.5 (11.2)	16.5 (15.5)	-25.8 (-15.6)	-52.2 (-45.2)

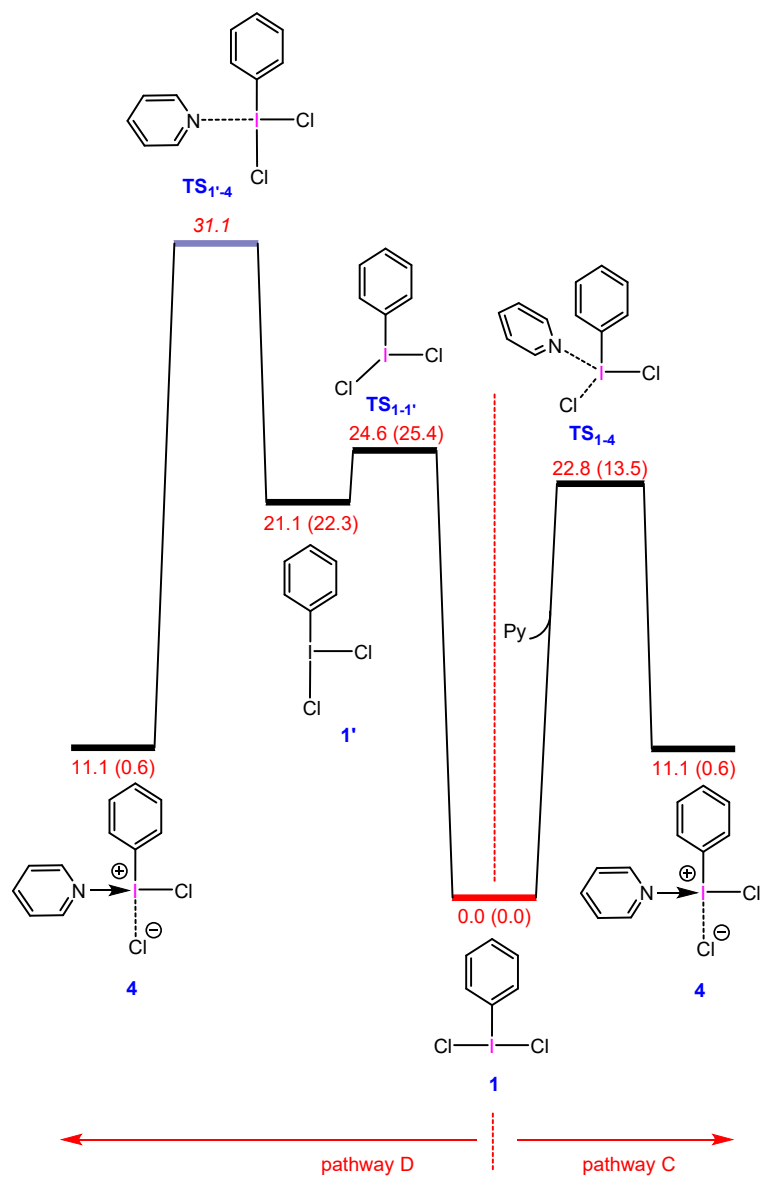


Fig. S1. Calculated mechanism for formation of activated complex **4**.

NCI analysis. To evaluate whether a weak noncovalent interaction exists between two chlorine atoms in our systems, we performed NCI analysis for structures **15**, **TS₂₋₁₅**, and **TS₁₁** using the Multiwfn 3.7 package.^{S10} This method is used for distinguishing hydrogen bonds, van der Waals interactions and repulsive steric clashes^{S11} and has been reported as a powerful tool for assessing the characteristic of halogen bonds.^{S12} Plot of the reduced density gradient versus $\text{sign}(\lambda_2)\rho$ for these selected structures are shown in Figure S2. An attractive interaction is identified between two chlorine atoms in **15**, confirmed by one spike with a negative λ_2 . This result indicates the presence of a halogen bond between the two chlorine atoms in this molecule. For structure **TS₂₋₁₅**, no noncovalent interaction between two chlorines is detected by means of the NCI analysis. This is because, in this transition structure, a significant covalent bonding interaction still exists between the two chlorine atoms, a claim that finds support from Wiberg bond index (WBI) analysis showing a WBI value of 0.637 for this bond (Fig. S2a). In contrast, due to the early character of transition structure **TS₁₁**, there is a negligible covalent bonding between two chlorines in this structure, supported by a small WBI value of 0.02 (Fig. S2c). As a result, we identified an attractive noncovalent weak interaction midway between the two chlorine atoms in **TS₁₁** within the NCI framework.

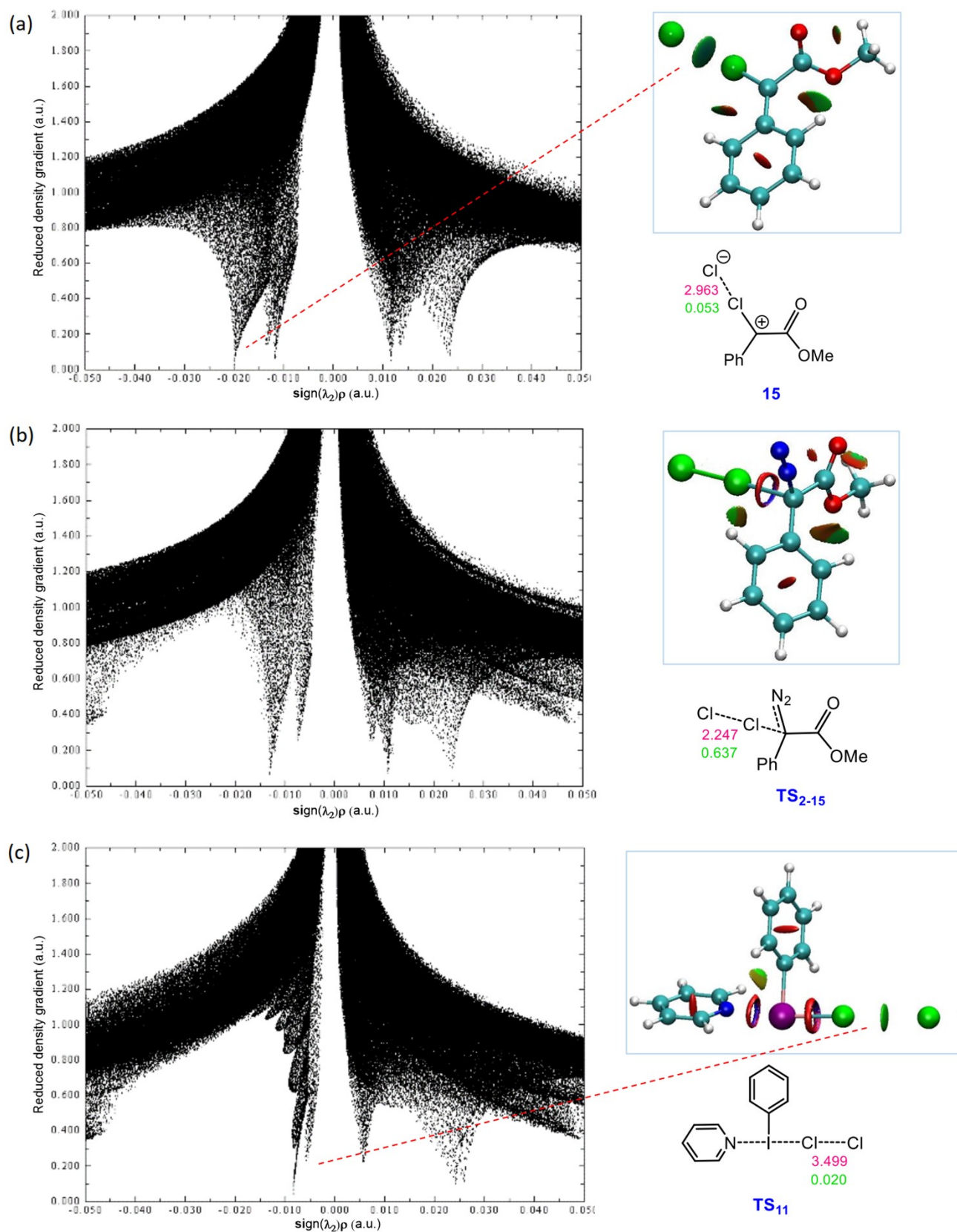


Fig. S2. NCI analysis for **TS₁₁**, **TS₂₋₁₅** and **15** calculated at the SMD/M06-2X/def2-TZVP//SMD/M06-2X/6-31G(d),SDD level of theory in dichloromethane. The Cl-Cl distances (Å) and the WBI values between two chlorine atoms are annotated in pink and green, respectively.

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Table S2. Total potential (E), enthalpy (H) and Gibbs free energies (G) of all structures optimized at the SMD/M06-2X/BS1 level of theory along with the total potential energies calculated by SMD/M06-2X/BS2//SMD/M06-2X/BS1, SMD/M06-2X/BS2//SMD/M06-2X/BS2, SMD/M06-2X/BS3//SMD/M06-2X/BS1 and SMD/M06-2X/BS3//SMD/M06-2X/BS2 and Cartesian coordinates for all of the calculated structures.

BS1 = 6-31G(d),SDD

BS2 = def2-TZVP

BS3 = def2-QZVP

4

E (SMD/M06-2X/BS1) = -1411.38013035 au

G (SMD/M06-2X/BS1) = -1411.241629 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1697.91806273 au

C	-3.60000100	2.32142500	-0.19192800
C	-3.34983400	1.65418500	1.00567100
C	-2.32964100	0.70695700	1.08033300
C	-1.58315500	0.45289800	-0.06433700
C	-1.81404100	1.10290300	-1.27017900
C	-2.83625800	2.04857100	-1.32545500
H	-4.39631300	3.05714300	-0.24305700
H	-3.94574000	1.86820600	1.88701200
H	-2.12689900	0.18065900	2.00781600
H	-1.21729900	0.87920900	-2.14867300
H	-3.03555400	2.56601700	-2.25835700
I	-0.00508100	-0.98535200	0.03062500
Cl	-1.82112400	-2.85812500	-0.07841000
C	3.02668100	2.99478000	0.06652600
C	2.03234400	2.87719700	1.03462100
C	1.19697600	1.77253500	1.00341000
C	2.29861300	0.91867400	-0.87398300
C	3.16113000	2.00388100	-0.90081300
H	3.69265600	3.85133000	0.06834400
H	1.89962400	3.62419000	1.80806900
H	0.39996400	1.62579800	1.72525200
H	2.36581800	0.10039800	-1.58147500
H	3.92310200	2.05785400	-1.66925300
N	1.34261400	0.83063300	0.06054300
Cl	2.76787400	-2.23161700	0.13571500

9

E (SMD/M06-2X/BS1) = -1310.26890063 au

G (SMD/M06-2X/BS1) = -1310.066569 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1596.91565895 au

C	-3.77179400	1.65706500	0.67685400
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C	-3.10302600	1.70535000	-0.54561400
C	-2.08309700	0.79883400	-0.82641700
C	-1.77125600	-0.13271800	0.15677700
C	-2.42222500	-0.22014300	1.38240500
C	-3.43726900	0.70117600	1.63437700
H	-4.56427400	2.36867000	0.88347400
H	-3.36988900	2.44811000	-1.28997900
H	-1.55260100	0.82392100	-1.77211900
H	-2.15438100	-0.97519600	2.11447000
H	-3.96540500	0.66216100	2.58109800
I	-0.18363100	-1.49816200	-0.22391200
Cl	-1.80693600	-3.17315900	-1.34959500
C	0.15091800	3.82106500	-0.15656300
C	0.45234100	2.68034400	0.58240200
C	1.03139100	1.57398600	-0.04687300
C	1.29810800	1.61400400	-1.42174600
C	0.99959200	2.76118600	-2.14728700
C	0.42238400	3.86543600	-1.52054000
H	-0.29808800	4.67337400	0.34248300
H	0.23192400	2.67264600	1.64594000
H	1.72725000	0.75366000	-1.92238100
H	1.21100200	2.78567600	-3.21131200
H	0.18459500	4.75477400	-2.09492800
C	1.30640500	0.30900300	0.70639200
N	0.85659400	0.36028500	2.02179600
N	0.44384900	0.35192200	3.04689100
C	2.67797400	-0.34831000	0.75926100
O	3.07200300	-0.92603700	1.74123000
O	3.30424100	-0.22978600	-0.39083900
C	4.60659300	-0.85039700	-0.45198800
H	5.26296100	-0.39903800	0.29315400
H	4.51293600	-1.92275500	-0.27371100
H	4.96902200	-0.65385800	-1.45831700

15

E (SMD/M06-2X/BS1) = -1418.27635651 au

G (SMD/M06-2X/BS1) = -1418.166438 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1418.55456444 au

C	3.43499200	-0.99913700	0.16807300
C	2.37514700	-0.12092300	0.19853700
C	1.04215100	-0.61303300	0.04038600
C	0.82206800	-2.01165500	-0.14797300
C	1.89500800	-2.87056900	-0.18446700
C	3.19527000	-2.36598300	-0.02573200

H	4.44843600	-0.63636700	0.29280300
H	2.55507500	0.93775100	0.35134800
H	-0.18735400	-2.39011000	-0.26757100
H	1.73885700	-3.93266600	-0.33292600
H	4.03607600	-3.05264800	-0.05232000
C	-0.02438700	0.28458300	0.09260000
C	0.17484600	1.77566500	0.30473000
O	-0.22024900	2.31760400	1.30116100
O	0.78261700	2.32517900	-0.72556600
C	0.96925700	3.75599000	-0.63975000
H	-0.00022500	4.24620300	-0.54028300
H	1.60254400	3.99285600	0.21665400
H	1.45371200	4.03707600	-1.57185500
Cl	-1.63437100	-0.17202900	0.01360600
Cl	-4.45105200	-1.08408800	-0.10413800

Cl⁻

E (SMD/M06-2X/BS1) = -460.313950773 au

G (SMD/M06-2X/BS1) = -460.328974 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -460.355413773 au

Cl	0.00000000	0.00000000	0.00000000
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Cl₂

E (SMD/M06-2X/BS1) = -920.277078700 au

G (SMD/M06-2X/BS1) = -920.297643 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -920.363316311 au

Cl	0.00000000	0.00000000	1.00755000
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Cl	0.00000000	0.00000000	-1.00755000
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2

E (SMD/M06-2X/BS1) = -607.433529208 au

G (SMD/M06-2X/BS1) = -607.311778 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -607.681406007 au

C	-3.17006600	0.49571200	0.43586900
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C	-1.86210600	0.96698000	0.40720600
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C	-0.81599500	0.14600400	-0.03947900
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C	-1.11275000	-1.15887300	-0.45762400
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C	-2.42264600	-1.62701900	-0.41188400
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C	-3.45758600	-0.80624200	0.03130400
---	-------------	-------------	------------

H	-3.96419900	1.14815900	0.78574200
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H	-1.65379000	1.97980400	0.74241500
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H	-0.32121600	-1.80345700	-0.81916300
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H	-2.63371800	-2.64145300	-0.73656700
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H	-4.47741000	-1.17653400	0.06005600
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C	0.56147000	0.67365300	-0.09028400
N	0.71303400	1.97918500	-0.17820500
N	0.84635300	3.09434300	-0.25295000
C	1.85576000	-0.00936000	0.00239100
O	2.92500600	0.56307200	-0.06918200
O	1.72406800	-1.32609700	0.18920600
C	2.95592600	-2.04807300	0.29724100
H	3.54661300	-1.93239300	-0.61386300
H	3.53149200	-1.69134600	1.15385600
H	2.67187600	-3.08995900	0.43697200

N₂

E (SMD/M06-2X/BS1) = -109.480264686 au

G (SMD/M06-2X/BS1) = -109.492893 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -109.530305870 au

N	0.00000000	0.00000000	0.54903100
N	0.00000000	0.00000000	-0.54903100

PhI

E (SMD/M06-2X/BS1) = -242.911245883 au

G (SMD/M06-2X/BS1) = -242.851785 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -529.265362662 au

C	-3.34874900	0.00000000	0.00012100
C	-2.65078100	-1.20554100	0.00000900
C	-1.25616200	-1.21410700	-0.00011500
C	-0.57676100	-0.00001700	-0.00018100
C	-1.25614400	1.21411600	-0.00013400
C	-2.65071500	1.20557100	0.00002600
H	-4.43416000	0.00002600	0.00031800
H	-3.18820000	-2.14887400	0.00008800
H	-0.71298800	-2.15289900	-0.00019000
H	-0.71291900	2.15287700	-0.00026800
H	-3.18814400	2.14889200	0.00017300
I	1.55985400	-0.00000300	0.00002900

1

E (SMD/M06-2X/BS1) = -1163.19091141 au

G (SMD/M06-2X/BS1) = -1163.134871 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1449.64242301 au

C	3.71221400	-0.08680500	-0.00032600
C	3.02572900	0.10330600	1.19747100
C	1.63230000	0.12539300	1.21446600
C	0.97672500	-0.04510400	0.00318800
C	1.62403500	-0.24080000	-1.20831700

C	3.01743800	-0.26081500	-1.19558000
H	4.79734000	-0.09789500	-0.00256900
H	3.56928600	0.23729300	2.12686400
H	1.08494100	0.27581500	2.13831000
H	1.07014200	-0.36960300	-2.13152400
H	3.55379200	-0.40803100	-2.12716300
I	-1.15397200	0.03262800	-0.00275200
Cl	-0.96458600	2.61863300	-0.08891700
Cl	-1.20280300	-2.55615600	0.09341800

10

E (SMD/M06-2X/BS1) = -951.036335640 au

G (SMD/M06-2X/BS1) = -950.895114 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1237.53577238 au

C	-1.57521000	3.54891900	-0.09700600
C	-1.61236300	2.85684300	1.11171400
C	-1.29524500	1.50018800	1.15527200
C	-0.95030100	0.88804400	-0.04095900
C	-0.90674800	1.53947900	-1.26550700
C	-1.22481300	2.89669800	-1.27781000
H	-1.82448200	4.60466900	-0.11974300
H	-1.88859400	3.36637200	2.02890800
H	-1.32447500	0.94739600	2.08793700
H	-0.64158000	1.01776500	-2.17843900
H	-1.20182200	3.43799600	-2.21771900
I	-0.45023900	-1.18633000	0.01439800
Cl	-2.95852600	-1.73313200	-0.01559600
C	4.30262200	0.42980500	0.06829700
C	3.55838300	0.40834800	1.24501100
C	2.24932600	-0.04319900	1.20038800
C	2.40541300	-0.44193200	-1.09888600
C	3.71898800	-0.00059800	-1.12015500
H	5.32931300	0.77978400	0.07782200
H	3.97750100	0.73508800	2.18912500
H	1.61675400	-0.08037100	2.08133100
H	1.89245400	-0.78952700	-1.98960100
H	4.26567400	0.00271500	-2.05551000
N	1.70522000	-0.45410000	0.04510800

3

E (SMD/M06-2X/BS1) = -1418.32847218 au

G (SMD/M06-2X/BS1) = -1418.213551 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1418.60603972 au

C	-3.24353000	0.97070800	0.34046100
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C	-1.85977300	1.15341300	0.30929900
C	-1.02496400	0.09091300	-0.02321700
C	-1.58471600	-1.15756900	-0.32589900
C	-2.96014800	-1.33480700	-0.29172200
C	-3.79662500	-0.26794000	0.04202400
H	-3.88295600	1.80829700	0.60002000
H	-1.45211700	2.12857800	0.54596600
H	-0.94224900	-1.99348100	-0.58651900
H	-3.38050200	-2.30780800	-0.52490200
H	-4.87285800	-0.40691400	0.06762100
C	0.48786000	0.21340200	-0.10161400
C	1.18746100	-0.78632500	0.86824500
O	0.52254400	-1.37998900	1.67543800
O	2.50344800	-0.95007700	0.86253300
C	3.47638300	-0.39825200	-0.03734600
H	3.54824500	-1.02430600	-0.92741300
H	3.25925400	0.63234000	-0.31211100
H	4.41387900	-0.43548900	0.51717800
Cl	1.06917700	1.84669700	0.37287600
Cl	0.99021600	-0.12092900	-1.80611100

Pyridine

E (SMD/M06-2X/BS1) = -248.179243021 au

G (SMD/M06-2X/BS1) = -248.116564 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -248.276593636 au

C	-0.00003400	-1.38136900	-0.00000100
C	1.19669500	-0.67106800	0.00000900
C	1.14146700	0.72049800	-0.00002000
C	-1.14142900	0.72055300	0.00002300
C	-1.19672600	-0.67101900	-0.00000900
H	-0.00005100	-2.46726400	0.00000000
H	2.15483900	-1.17941100	0.00003100
H	2.05908900	1.30472500	0.00000400
H	-2.05902800	1.30481800	-0.00000600
H	-2.15490000	-1.17930500	-0.00003200
N	0.00003100	1.41583800	-0.00000200

12

E (SMD/M06-2X/BS1) = -708.129304288 au

G (SMD/M06-2X/BS1) = -708.065589 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -708.263298038 au

Cl	0.00000000	2.18195700	0.00000000
C	0.00000000	-2.24167200	0.00000000
C	0.00000000	-1.54218100	-1.20465800
C	0.00000000	-0.16237600	-1.19068300
C	0.00000000	-0.16237600	1.19068300

C	0.00000000	-1.54218100	1.20465800
H	0.00000000	-3.32616600	0.00000000
H	0.00000000	-2.04975400	-2.16127800
H	0.00000000	0.45570100	-2.08015700
H	0.00000000	0.45570100	2.08015700
H	0.00000000	-2.04975400	2.16127800
N	0.00000000	0.47510500	0.00000000

TS₈

E (SMD/M06-2X/BS1) = -1770.59754446 au

G (SMD/M06-2X/BS1) = -1770.398880 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -2057.28050587 au

C	-3.56548700	2.78452300	0.92896800
C	-2.75438000	2.86667100	-0.20021300
C	-1.99860800	1.76514100	-0.60199700
C	-2.07322800	0.60507200	0.15872300
C	-2.88388300	0.49254200	1.28260400
C	-3.63651900	1.60092300	1.66394200
H	-4.15052900	3.64540600	1.23621300
H	-2.70895300	3.78432500	-0.77761500
H	-1.36951700	1.81706100	-1.48449900
H	-2.92171100	-0.42985500	1.85333700
H	-4.27448800	1.53740400	2.53943700
I	-0.83763100	-1.05340500	-0.38931300
Cl	-3.15510500	-2.21093400	-1.26988900
C	3.32870300	2.82917700	-0.61860400
C	2.66370700	1.89368700	0.15779500
C	1.69307200	1.05615100	-0.42242600
C	1.40932600	1.17047700	-1.79034900
C	2.10105900	2.09285600	-2.56758500
C	3.05257700	2.92500800	-1.98407800
H	4.06691000	3.47969500	-0.16203100
H	2.88284000	1.81808100	1.21856200
H	0.67674400	0.52210600	-2.25765900
H	1.88998000	2.16117900	-3.62919800
H	3.58176200	3.65185400	-2.59218300
C	1.00450600	0.06004500	0.41450500
N	0.25343900	1.06518000	1.67024200
N	-0.15555100	1.77040200	2.40537700
C	1.77145400	-0.82608300	1.41924800
O	1.18545200	-1.43190500	2.27993300
O	3.07153600	-0.75286200	1.24988400
C	3.83440100	-1.68855200	2.03110100
H	3.67408300	-1.50801200	3.09547700
H	3.53029500	-2.70369500	1.76738100
H	4.87317700	-1.51320900	1.75959200
Cl	1.75642900	-2.52839800	-0.96134200

TS₁₋₄

E (SMD/M06-2X/BS1) = -1411.35808386 au

G (SMD/M06-2X/BS1) = -1411.221549 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1697.89756019 au

C	1.08770600	3.82177200	0.36706900
C	0.69782500	3.24148300	-0.84178800
C	0.62566500	1.85737100	-0.96518200
C	0.97153700	1.09152300	0.14223600
C	1.36559800	1.63467900	1.35690500
C	1.41882100	3.02611600	1.46001700
H	1.13117700	4.90253000	0.45524100
H	0.44191000	3.86628600	-1.69129900
H	0.30397100	1.39172400	-1.89083600
H	1.62220000	1.00167300	2.19962100
H	1.71972500	3.47901400	2.39903200
I	0.88896900	-1.03579300	-0.00438300
Cl	3.23622700	-0.94764900	-1.08834900
Cl	-0.95745000	-2.65595600	1.36789500
C	-2.22450200	1.01146700	0.46909600
C	-3.55461600	1.39633300	0.32762900
C	-4.36783200	0.66947700	-0.53660900
C	-3.82581600	-0.41590800	-1.21935000
C	-2.48961700	-0.73560500	-1.00258500
N	-1.70872200	-0.03277300	-0.18067100
H	-5.40890700	0.94383600	-0.67539200
H	-1.54832100	1.55883000	1.12328900
H	-3.93532700	2.24663200	0.88244900
H	-4.42203500	-1.00921800	-1.90359900
H	-2.02650700	-1.58583700	-1.49840100

TS₁₋₁₂

E (SMD/M06-2X/BS1) = -1411.35469813 au

G (SMD/M06-2X/BS1) = -1411.220007 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1697.88769919 au

C	-2.27141200	3.61087700	-0.05927700
C	-1.56163000	3.05076200	-1.11883400
C	-1.26980100	1.68700400	-1.12798000
C	-1.70025000	0.91900000	-0.05355700
C	-2.41205300	1.44783200	1.01475500
C	-2.69636600	2.81243400	1.00090300
H	-2.49786500	4.67228800	-0.06128000
H	-1.23578800	3.66917500	-1.94912800
H	-0.72471000	1.24232200	-1.95386800
H	-2.74909900	0.81649400	1.82891900
H	-3.25361700	3.24643100	1.82490200
I	-1.24552000	-1.16428800	-0.03892500

Cl	1.37425400	-0.65989900	0.01442000
Cl	-4.38360000	-1.47591100	0.02228000
C	6.07124800	0.37412600	0.12253300
C	5.31717400	0.41034400	1.29267400
C	3.96480100	0.10181800	1.22480300
C	4.10178100	-0.26599100	-1.07698400
C	5.45824600	0.03165600	-1.08012500
H	7.12968300	0.61127200	0.14769400
H	5.76044600	0.67190700	2.24647400
H	3.31447400	0.10959000	2.09381700
H	3.55759800	-0.54065400	-1.97509400
H	6.01368100	-0.00666900	-2.00994000
N	3.40660500	-0.22218200	0.05902200

TS₄

E (SMD/M06-2X/BS1) = -1411.30401568 au

G (SMD/M06-2X/BS1) = -1411.172353 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1697.82957875 au

C	0.88954300	3.89050300	-0.17163100
C	0.90810800	3.07987100	-1.30735100
C	0.42188300	1.77739700	-1.24752200
C	-0.07128600	1.30896400	-0.02986500
C	-0.10544600	2.10381200	1.11554100
C	0.38205500	3.40625000	1.03306000
H	1.26987900	4.90546300	-0.22737300
H	1.30020800	3.46104000	-2.24462700
H	0.43410300	1.13799400	-2.12366800
H	-0.49728800	1.71534000	2.04945200
H	0.36504300	4.03933400	1.91429000
I	-0.78781900	-0.65751900	0.08660300
Cl	-3.89661900	-1.95755300	0.02199500
Cl	-3.42423000	0.61967400	-0.17549700
C	2.65816200	-2.19050800	-0.27354700
C	4.02615300	-2.43987500	-0.33704600
C	4.90345600	-1.41579300	0.00809700
C	4.38237800	-0.18661400	0.40173000
C	2.99885100	-0.03178800	0.43241000
N	2.15659700	-1.01207600	0.10170000
H	5.97688300	-1.57345500	-0.02919400
H	1.93676400	-2.96154700	-0.53483000
H	4.38781100	-3.41298600	-0.65071700
H	5.02815700	0.63900100	0.67994600
H	2.54799300	0.91349400	0.73115100

11

E (SMD/M06-2X/BS1) = -1411.35374169 au

G (SMD/M06-2X/BS1) = -1411.217499 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1697.89566043 au

C	-0.91364900	3.96440200	0.23944100
C	-0.85485300	3.18622400	1.39388300
C	-0.55774400	1.82647400	1.31308300
C	-0.33286600	1.30002600	0.04924000
C	-0.37932600	2.04072200	-1.12270700
C	-0.67722000	3.39776900	-1.01163600
H	-1.14050800	5.02272800	0.31492500
H	-1.03327700	3.63321600	2.36620600
H	-0.50109500	1.21008600	2.20349700
H	-0.18105300	1.58762700	-2.08831700
H	-0.71746900	4.00700000	-1.90848100
I	0.12271600	-0.77406600	-0.10774600
Cl	7.21389400	-0.78932200	0.12360800
Cl	2.60666100	-0.18233600	-0.16188400
C	-2.70600800	-1.56812200	1.06913400
C	-4.07575000	-1.76591600	1.14721300
C	-4.86607100	-1.42596300	0.05289700
C	-4.26765700	-0.89867600	-1.08837700
C	-2.89255500	-0.72587000	-1.10342100
N	-2.14880900	-1.05770700	-0.03811200
H	-5.94056700	-1.57116200	0.08877700
H	-2.03433900	-1.81026400	1.88631300
H	-4.5052800	-2.17776200	2.05263300
H	-4.84944200	-0.62412600	-1.96014400
H	-2.36628000	-0.31615100	-1.95986800

TS₁₁

E (SMD/M06-2X/BS1) = -1411.35221931 au

G (SMD/M06-2X/BS1) = -1411.215977 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1697.89545304 au

C	-0.14420300	3.90811900	0.25891400
C	-0.46933600	3.13066100	1.36893800
C	-0.39826600	1.74050400	1.29951900
C	-0.00208800	1.18120600	0.09288500
C	0.32961600	1.92034400	-1.03396200
C	0.25349900	3.30897900	-0.93449100
H	-0.19724300	4.98976000	0.32630600
H	-0.77185100	3.60039000	2.29903400
H	-0.63976700	1.12350900	2.15824600
H	0.64486900	1.44071200	-1.95437400
H	0.50915200	3.91665600	-1.79613500
I	0.11298700	-0.94572900	-0.03582200
Cl	6.12562200	-0.61788100	-0.04460800
Cl	2.63230400	-0.80459500	0.04011800
C	-2.93995300	-1.42912500	0.85912600
C	-4.32736500	-1.41018500	0.85030600

C	-4.98098700	-0.72085800	-0.16695800
C	-4.23135700	-0.07193100	-1.14498500
C	-2.84783500	-0.13282200	-1.07457700
N	-2.23471100	-0.79776900	-0.08706300
H	-6.06507600	-0.68906900	-0.19776400
H	-2.37288600	-1.94705200	1.62646500
H	-4.87521900	-1.92586800	1.63013700
H	-4.70371400	0.47416900	-1.95295300
H	-2.20871100	0.35751900	-1.80291400

TS'₁

E (SMD/M06-2X/BS1) = -1163.13091651 au

G (SMD/M06-2X/BS1) = -1163.077818 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1449.58326090 au

C	4.23869600	0.90879000	0.00451700
C	3.57322900	0.74430000	-1.21043700
C	2.27877800	0.23516300	-1.23659500
C	1.69716900	-0.09496400	-0.01484700
C	2.33013000	0.05701000	1.21646800
C	3.62436800	0.56765900	1.20968700
H	5.24741100	1.30865000	0.01211700
H	4.05787800	1.01337000	-2.14283600
H	1.74407600	0.10440300	-2.17057100
H	1.83418600	-0.20993000	2.14297400
H	4.14897500	0.69993600	2.14981100
I	-0.25226000	-0.89442800	-0.03136700
Cl	-4.97993500	0.59460900	-0.02554400
Cl	-1.49753300	1.16894900	0.13484900

TS₉

E (SMD/M06-2X/BS1) = -1770.58948271 au

G (SMD/M06-2X/BS1) = -1770.391076 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -2057.26612764 au

C	3.31263600	2.63780100	-0.46997600
C	3.05172800	2.08774500	0.78473700
C	2.33831400	0.89665600	0.89788900
C	1.89909100	0.28194700	-0.26937000
C	2.15344000	0.80484600	-1.53595800
C	2.86790900	1.99794400	-1.62556500
H	3.86908900	3.56648900	-0.54702300
H	3.40131300	2.58557500	1.68378500
H	2.13187300	0.46122000	1.86951100
H	1.80764600	0.29499900	-2.42968700
H	3.07766100	2.42167200	-2.60248900
I	0.74771500	-1.48606400	-0.12136900
Cl	3.38481200	-2.95411800	0.53395200
C	-0.10350400	3.49065100	0.24734700

C	-0.63784600	2.39610000	-0.41639100
C	-1.11712800	1.29877800	0.31759200
C	-1.03863200	1.30200500	1.71920600
C	-0.51247800	2.41095000	2.36849600
C	-0.04620600	3.50532000	1.64068300
H	0.26275500	4.33515200	-0.32665700
H	-0.69831200	2.41340500	-1.50082100
H	-1.38208100	0.45117300	2.29262900
H	-0.45985900	2.41350500	3.45212600
H	0.36702700	4.36541300	2.15769100
C	-1.69588600	0.15377000	-0.38490600
N	-1.41960500	0.05512900	-1.75975500
N	-1.24427700	0.01031100	-2.84888000
C	-2.39791800	-1.11641000	0.06547200
O	-2.57751100	-2.03142100	-0.69633400
O	-2.74985500	-1.04353300	1.32594100
C	-3.45327300	-2.19894300	1.83106200
H	-4.37099900	-2.34511200	1.25964300
H	-2.81334500	-3.07983100	1.75771100
H	-3.67464000	-1.96536400	2.86985000
Cl	-3.83201200	1.02998000	-0.96348500

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E (SMD/M06-2X/BS1) = -1770.61749782 au

G (SMD/M06-2X/BS1) = -1770.418175 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -2057.30067252 au

C	-3.47028500	2.15427600	0.69446900
C	-2.59774600	1.94507300	1.76102800
C	-1.27497400	1.57633600	1.52223800
C	-0.86254800	1.42526500	0.20291900
C	-1.70953500	1.64723400	-0.87881600
C	-3.02848000	2.01202500	-0.62063600
H	-4.50042400	2.43575800	0.88876100
H	-2.94240000	2.06845400	2.78267500
H	-0.58712100	1.41048900	2.34427500
H	-1.35427300	1.53238300	-1.89743700
H	-3.70827200	2.18260700	-1.44932600
I	1.13356300	0.80077800	-0.19378400
Cl	1.86538300	3.33847600	-0.32479700
C	-2.58453100	-1.44851500	-2.51920900
C	-1.31206400	-1.47494100	-1.96335900
C	-1.15209700	-1.55516200	-0.57317300
C	-2.27858400	-1.59386200	0.25443300
C	-3.54963700	-1.55085700	-0.31353300
C	-3.70883900	-1.48030600	-1.69476400
H	-2.69529800	-1.39150200	-3.59709300
H	-0.44348600	-1.42029300	-2.61604900

H	-2.17472400	-1.64728900	1.33044900
H	-4.41898900	-1.57467600	0.33573000
H	-4.70313300	-1.44884000	-2.12847100
C	0.23405100	-1.53366600	-0.00719100
N	1.11464500	-2.27314200	-0.80489900
N	1.88057600	-2.77750200	-1.41901800
C	0.55926200	-1.92553400	1.42551400
O	1.40889700	-2.73048400	1.70713000
O	-0.16682300	-1.22191100	2.27485400
C	0.10070600	-1.46592600	3.67064100
H	-0.06105700	-2.51990800	3.90095000
H	1.12877600	-1.18209000	3.90134300
H	-0.60562600	-0.83903500	4.21102100
Cl	3.77555000	-0.60096200	-0.83920900

TS₁₀

E (SMD/M06-2X/BS1) = -1558.45500031 au

G (SMD/M06-2X/BS1) = -1558.174387 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1845.19134875 au

C	4.96129000	-2.91124000	-0.79654000
C	4.20617900	-2.08224500	0.02326900
C	4.24031300	-0.69358300	-0.16108100
C	5.03579600	-0.14379800	-1.17209000
C	5.77779000	-0.98476600	-1.99679500
C	5.74545700	-2.36473000	-1.81238700
H	4.93098100	-3.98541200	-0.64592400
H	3.58549500	-2.51484100	0.80417000
H	5.07796900	0.92922500	-1.31423900
H	6.39092800	-0.55343600	-2.78144600
H	6.33012900	-3.01368200	-2.45647100
C	3.44802400	0.17492400	0.74505500
N	3.58230900	-0.12612300	2.07072400
N	3.61589100	-0.40698300	3.14531600
C	3.18339000	1.64364100	0.60520500
O	3.03242500	2.37181100	1.55683300
O	3.06394500	1.98655600	-0.66638300
C	-2.39087600	3.71101000	-0.47310100
C	-1.93762900	2.93814700	-1.54104200
C	-1.62361700	1.59284300	-1.35237200
C	-1.77335500	1.06269900	-0.07618100
C	-2.22175700	1.80712500	1.00864100
C	-2.53241400	3.14901300	0.79470700
H	-2.63552000	4.75660900	-0.62982900
H	-1.82913400	3.37584200	-2.52812200
H	-1.27471000	0.98095200	-2.17704700
H	-2.33161500	1.35929800	1.99011400
H	-2.88559600	3.75183600	1.62504300

I	-1.33916600	-0.98904200	0.22307900
Cl	1.23057700	-0.45042500	0.55281300
C	2.68273800	3.35460100	-0.89726700
H	3.41235700	4.02979400	-0.44740600
H	2.66641500	3.46985400	-1.97911800
H	1.69216800	3.53688800	-0.47510700
C	-4.74630600	-2.16459300	0.16255200
C	-6.11745000	-2.36918800	0.04794200
C	-6.91003000	-1.31480600	-0.39667400
C	-6.30308800	-0.10201800	-0.70870300
C	-4.92332900	0.00881400	-0.56214200
N	-4.16107400	-1.00126900	-0.13484100
H	-7.98379600	-1.43684600	-0.49876100
H	-4.08947300	-2.96094200	0.50644600
H	-6.54709500	-3.33174400	0.30236300
H	-6.88103400	0.74594200	-1.05914600
H	-4.41007500	0.93969700	-0.79450400

6

E (SMD/M06-2X/BS1) = -1349.17707306 au

G (SMD/M06-2X/BS1) = -1348.895903 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1635.93596499 au

O	0.00388600	0.47773800	0.28558900
Br	-0.00983500	-1.26833600	-0.37130000
O	2.10277400	1.65691600	-1.05786100
H	1.22346800	1.31387200	-0.78668400
H	2.61735700	1.45075100	-0.25689000
O	2.38925000	0.50213600	1.53716800
H	2.77763500	-0.34803700	1.28226100
H	1.46310900	0.46885700	1.17805600
O	-2.35814400	0.54115400	1.57467300
H	-1.44063200	0.49823400	1.19315900
H	-2.77425900	-0.28745600	1.29325500
O	-2.09835300	1.64044900	-1.07046900
H	-1.22096700	1.29897000	-0.79140900
H	-2.61681400	1.44945100	-0.26907500

Phi

E (SMD/M06-2X/BS1) = -242.905483781 au

G (SMD/M06-2X/BS1) = -242.845994 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -529.259553873 au

I	-1.55945200	-0.00001400	0.00004200
C	0.57646800	0.00029100	-0.00029800
C	1.25541600	1.21429100	-0.00029700
C	1.25572700	-1.21433100	-0.00012100

C	2.65035800	1.20554900	0.00016400
H	0.71281500	2.15304500	-0.00025700
C	2.65003000	-1.20578100	0.00001800
H	0.71326400	-2.15286000	-0.00026000
C	3.34799400	0.00008300	0.00021800
H	3.18806900	2.14841800	0.00007300
H	3.18767500	-2.14864200	-0.00002900
H	4.43316800	0.00017300	0.00014100

Et₃N

E (SMD/M06-2X/BS1) = -292.260941254 au

G (SMD/M06-2X/BS1) = -292.085705 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -292.376625288 au

N	0.51463800	0.10153600	0.00000000
C	-0.64302700	0.99836000	0.00000000
H	-0.55799400	1.65326500	0.87280400
H	-0.55799400	1.65326500	-0.87280400
C	0.59782000	-0.74027300	1.19287900
H	-0.21076000	-1.49449700	1.21917800
H	1.53638600	-1.30266400	1.11727100
C	0.59782000	-0.74027300	-1.19287900
H	1.53638600	-1.30266400	-1.11727100
H	-0.21076000	-1.49449700	-1.21917800
C	0.59782000	0.04653800	-2.49697300
H	0.86251600	-0.61424700	-3.32788300
H	-0.38202200	0.47981200	-2.71977900
H	1.33214100	0.85788900	-2.45549800
C	-2.01950000	0.32852400	0.00000000
H	-2.16537000	-0.29879700	0.88597200
H	-2.80478200	1.09124000	0.00000000
H	-2.16537000	-0.29879700	-0.88597200
C	0.59782000	0.04653800	2.49697300
H	-0.38202200	0.47981200	2.71977900
H	0.86251600	-0.61424700	3.32788300
H	1.33214100	0.85788900	2.45549800

TS₁₋₂₀

E (SMD/M06-2X/BS1) = -1455.45265847 au

G (SMD/M06-2X/BS1) = -1455.203631 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1742.01226787 au

C	-2.56392200	3.51228500	0.42233300
C	-1.97834300	3.07587400	-0.76427500
C	-1.68337400	1.72576800	-0.94790900
C	-1.98606300	0.85271200	0.08730000
C	-2.56762200	1.25173300	1.28219200
C	-2.85866200	2.60605600	1.43906800

H	-2.79322400	4.56465700	0.55514400
H	-1.75270000	3.78104800	-1.55754100
H	-1.23088600	1.37353000	-1.86861600
H	-2.79294500	0.53697500	2.06586400
H	-3.31485900	2.94695600	2.36273100
I	-1.51553900	-1.21017500	-0.17336200
Cl	0.98636800	-0.61669800	0.01913200
Cl	-4.25137200	-1.62187600	-0.34441700
N	3.46687300	0.12566000	0.22262500
C	4.14103600	-0.28064100	-1.00844300
H	4.01816400	-1.36243600	-1.11318700
H	3.60088700	0.16847700	-1.84679000
C	3.95931200	-0.52511400	1.43568100
H	4.94639300	-0.11814400	1.72038500
H	3.26605200	-0.25091600	2.23945500
C	3.38284900	1.57103100	0.42884700
H	2.71477300	1.72526400	1.28439500
H	4.36747700	1.97814400	0.72157500
C	2.85102900	2.34438500	-0.76914400
H	2.66254800	3.38084800	-0.47393700
H	3.56288700	2.36185200	-1.59990200
H	1.91048300	1.91248100	-1.12484600
C	5.62419300	0.08620000	-1.08651900
H	6.19725800	-0.38579300	-0.28134100
H	6.04198000	-0.25352900	-2.03939200
H	5.77384900	1.16917900	-1.02099600
C	4.04407900	-2.04142900	1.33956000
H	4.84806200	-2.37004100	0.67410700
H	4.24739200	-2.45514700	2.33170100
H	3.09983600	-2.46115800	0.97870900

TS₁₋₁₈

E (SMD/M06-2X/BS1) = -1455.44144917 au

G (SMD/M06-2X/BS1) = -1455.185738 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1741.99755299 au

C	-2.84566400	3.03387200	0.07477300
C	-2.68231700	2.24999100	1.21670700
C	-1.99316600	1.04127700	1.14756200
C	-1.49524800	0.65032800	-0.09034900
C	-1.66654600	1.39200400	-1.25141500
C	-2.34437600	2.60700500	-1.15273900
H	-3.37601700	3.97821900	0.14189200
H	-3.08601200	2.57670400	2.16941100
H	-1.86325200	0.42517100	2.03078500
H	-1.28080300	1.04302100	-2.20365800
H	-2.48487200	3.21014500	-2.04371100
I	-0.41632000	-1.17885300	-0.25540600

Cl	-2.47547700	-2.41240100	0.73131000
Cl	1.46987400	-1.14287200	-2.47978000
N	1.69874600	0.59603900	0.59943200
C	1.40411400	2.00539700	0.29442000
H	0.37637000	2.19770100	0.61863900
H	2.04488900	2.65536000	0.91245700
C	1.49581700	0.36423600	2.03896000
H	0.42098600	0.47791600	2.22923700
H	1.99401500	1.16152100	2.61356000
C	3.02229700	0.17282900	0.11808100
H	3.03013400	0.29291900	-0.96472800
H	3.11478500	-0.90119100	0.30137900
C	1.56797100	2.36820000	-1.17402600
H	1.09396200	1.62441000	-1.82088700
H	1.10534200	3.34231800	-1.35940500
H	2.62171400	2.43865600	-1.46076500
C	4.19928200	0.92215100	0.74570000
H	4.21099400	0.83373600	1.83700900
H	5.13509700	0.50237900	0.36437700
H	4.18372500	1.98621900	0.48927700
C	1.96787300	-0.98999000	2.55135600
H	1.56440600	-1.81701100	1.96034000
H	3.05825200	-1.07163600	2.55231900
H	1.62501700	-1.11379700	3.58278000

TS_{19-cl2}

E (SMD/M06-2X/BS1) = -1455.44742513 au

G (SMD/M06-2X/BS1) = -1455.194308 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1742.00242088 au

C	0.39552000	4.08022600	-0.28739300
C	0.49267100	3.46971900	0.96207800
C	0.45547300	2.08088800	1.07161200
C	0.31786700	1.34128700	-0.09762500
C	0.23488600	1.91901200	-1.35848300
C	0.27078000	3.31056700	-1.44192300
H	0.42414600	5.16243000	-0.36189100
H	0.59949100	4.07043700	1.85934900
H	0.53172500	1.59629100	2.03897900
H	0.14847400	1.30937700	-2.25174100
H	0.20630500	3.78663600	-2.41479000
I	0.22230600	-0.77469700	0.04005100
Cl	5.53247900	-1.19088900	0.09057500
Cl	2.79134100	-0.96558200	0.06592900
N	-2.36356400	-0.42437000	-0.00729100
C	-2.83253700	-1.75127800	0.43988300
H	-2.39571200	-2.49537800	-0.23374400
H	-2.39985100	-1.93369500	1.42788000

C	-2.78480500	-0.07957200	-1.38279000
H	-3.85675700	0.16769700	-1.37313900
H	-2.25336700	0.84204500	-1.64513500
C	-2.76481700	0.67640900	0.89235800
H	-2.27102900	1.58024900	0.51959300
H	-3.84700500	0.84493100	0.78677000
C	-2.42220600	0.45929000	2.35789800
H	-2.60153300	1.39110100	2.90189600
H	-3.04260000	-0.31682600	2.81504900
H	-1.37116500	0.18588800	2.49559900
C	-4.34791500	-1.91318300	0.49085600
H	-4.80474200	-1.76775200	-0.49293900
H	-4.58811400	-2.92628400	0.82612800
H	-4.80661500	-1.21001000	1.19273900
C	-2.52089200	-1.15220300	-2.42826200
H	-3.14814700	-2.03566900	-2.27999100
H	-2.75691700	-0.74147500	-3.41404000
H	-1.47294400	-1.46744000	-2.43806700

22

E (SMD/M06-2X/BS1) = -568.107488926 au

G (SMD/M06-2X/BS1) = -568.008786 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -568.338885070 au

C	-2.79345400	0.30105300	-0.13377600
C	-1.50429500	0.84917500	-0.35084700
N	-0.63560300	-0.09480300	0.04342000
H	-1.20068600	1.78648800	-0.78320200
N	-1.17609800	-1.18186100	0.49827800
O	-2.50355300	-0.97250700	0.39392300
C	0.79912100	-0.01294800	0.01074100
C	1.40725600	1.20741300	0.28282200
C	1.52634800	-1.15939100	-0.29210200
C	2.79654900	1.27595400	0.24639500
H	0.81032400	2.07760700	0.53498800
C	2.91447200	-1.07268900	-0.31654000
H	1.01277100	-2.08856700	-0.51249600
C	3.54826600	0.14028500	-0.05054000
H	3.28967600	2.21843000	0.45926600
H	3.49936600	-1.95507800	-0.55341100
H	4.63143400	0.20089900	-0.07552300
O	-3.93726700	0.66297600	-0.29872700

TS₂₂₋₂₃

E (SMD/M06-2X/BS1) = -1488.38724556 au

G (SMD/M06-2X/BS1) = -1488.292307 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1488.69475670 au

C	1.42569600	2.05779800	0.46267400
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C	0.59461000	0.94146500	0.86664000
N	-0.47115700	0.99423500	-0.02676800
H	0.39845800	0.67091800	1.89501600
N	-0.30325800	1.81178700	-0.98766700
O	0.83714100	2.46427100	-0.77184800
C	-1.66586200	0.20024000	0.02791200
C	-2.79909100	0.64960800	-0.64721100
C	-1.64705500	-0.98179300	0.76191000
C	-3.94657500	-0.13081000	-0.59164900
H	-2.78417200	1.58926800	-1.18769700
C	-2.80999900	-1.74372000	0.80823100
H	-0.75038600	-1.31396300	1.27331900
C	-3.95354100	-1.32334000	0.13252100
H	-4.84066400	0.20120100	-1.10798800
H	-2.81473600	-2.67056600	1.37104400
H	-4.85603600	-1.92421400	0.17314800
O	2.41251300	2.58380100	0.87365600
Cl	1.83192000	-0.73031200	0.14383400
Cl	3.10232100	-2.48122200	-0.55891800

19

E (SMD/M06-2X/BS1) = -1455.45055493 au

G (SMD/M06-2X/BS1) = -1455.197859 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1742.00777213 au

C	-0.88607900	3.92503100	0.00000000
C	-0.73651700	3.25146300	-1.21083200
C	-0.43111400	1.89172000	-1.22606800
C	-0.27838300	1.25492900	0.00006400
C	-0.43177900	1.89163500	1.22616000
C	-0.73718500	3.25137400	1.21086300
H	-1.12822500	4.98269900	-0.00003000
H	-0.86302700	3.77704000	-2.15138700
H	-0.32200600	1.35400300	-2.16206400
H	-0.32318000	1.35384600	2.16217000
H	-0.86421800	3.77687400	2.15139200
I	0.16964900	-0.82449800	0.00015500
Cl	-7.05782400	-1.05368900	-0.00021100
Cl	-2.37998200	-1.30227100	0.00013900
N	2.44945900	-0.29203300	-0.00008100
C	3.09324300	-1.64134200	-0.00005200
H	2.72405000	-2.17314400	0.88047400
H	2.72390100	-2.17325300	-0.88045000
C	2.79349600	0.51763600	1.20968700
H	3.83769800	0.82898200	1.09537900

H	2.18344300	1.42391000	1.15652200
C	2.79338300	0.51744800	-1.21000200
H	2.18375600	1.42399500	-1.15662000
H	3.83776400	0.82829100	-1.09604600
C	2.60036700	-0.18713600	-2.54045300
H	2.77230100	0.54491900	-3.33415900
H	3.31367400	-1.00311200	-2.68228100
H	1.58756300	-0.58100300	-2.66482700
C	4.61373900	-1.60070900	-0.00021400
H	5.01010400	-1.10454400	0.88972100
H	4.97894500	-2.63125300	-0.00006900
H	5.00993000	-1.10485600	-0.89039600
C	2.60119000	-0.18708800	2.54016200
H	3.31503200	-1.00262300	2.68183200
H	2.77276500	0.54504000	3.33387700
H	1.58865000	-0.58161700	2.66466500

24

E (SMD/M06-2X/BS1) = -1027.66044199 au

G (SMD/M06-2X/BS1) = -1027.573284 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1027.92885155 au

C	2.59779500	-0.37759800	-0.07770900
C	1.38331900	0.35054800	0.04805000
N	0.38723000	-0.53221900	-0.13463700
N	0.79286700	-1.74173100	-0.37825600
O	2.14246000	-1.67016700	-0.34339600
C	-1.03261200	-0.29659200	-0.08545900
C	-1.80268800	-1.11635700	0.73108300
C	-1.57478600	0.72076000	-0.86263700
C	-3.17670700	-0.89986400	0.76848000
H	-1.33134800	-1.89343500	1.32304300
C	-2.94997900	0.92356800	-0.80778100
H	-0.94202100	1.32270900	-1.50649200
C	-3.74666300	0.11760800	0.00492900
H	-3.79915600	-1.52487300	1.39971400
H	-3.39783400	1.70859800	-1.40744300
H	-4.81847900	0.28323300	0.04168200
O	3.77155200	-0.10338300	0.00285200
Cl	1.20764600	1.98102200	0.47943300

23

E (SMD/M06-2X/BS1) = -1488.39229955 au

G (SMD/M06-2X/BS1) = -1488.296797 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1488.69715763 au

C	-1.64738200	-2.10049900	0.26161700
C	-0.83886100	-0.92108300	0.73188100
N	0.41543300	-1.17668600	0.01514800
H	-0.66972200	-0.94722900	1.81101500
N	0.38425200	-2.19332600	-0.71907100
O	-0.79924000	-2.79221800	-0.64192800
C	1.57140000	-0.33622200	0.05359900
C	2.47133700	-0.38636100	-1.01244400
C	1.73860100	0.50795700	1.15030900
C	3.58713300	0.43503700	-0.95931700
H	2.28834200	-1.03129500	-1.86457700
C	2.86294000	1.32434100	1.17583100
H	1.02778700	0.53205000	1.97010500
C	3.78217200	1.28809400	0.12888500
H	4.29649800	0.42194600	-1.77933100
H	3.01429300	1.99222200	2.01612500
H	4.65185700	1.93624900	0.15404000
O	-2.74223700	-2.46911200	0.48937300
Cl	-1.57547200	0.63714800	0.23595300
Cl	-2.72094400	3.12221700	-0.55016700

TS₁

E (SMD/M06-2X/BS1) = -1770.60295032 au

G (SMD/M06-2X/BS1) = -1770.406411 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -2057.28217426 au

C	4.38023000	-2.34440900	-1.33279400
C	3.52818400	-1.81849500	-0.36987300
C	3.45577600	-0.43254700	-0.18708200
C	4.24108100	0.42283100	-0.96577200
C	5.08226400	-0.11425700	-1.93601000
C	5.15438100	-1.49281300	-2.12085100
H	4.43262700	-3.41893200	-1.47336100
H	2.91547800	-2.48180600	0.23486300
H	4.19923700	1.49608000	-0.82001900
H	5.68709900	0.55057600	-2.54384200
H	5.81365000	-1.90504800	-2.87801800
C	2.55931400	0.11329600	0.87364300
N	2.87695300	-0.38013000	2.13515600
N	3.05521200	-0.83036500	3.13082700
C	2.21329400	1.57729600	1.03321000
O	2.14537000	2.11381200	2.11086400
O	1.93453000	2.11594600	-0.13725500
C	-2.81471900	3.35308900	-0.87097800
C	-1.80719400	2.65903100	-1.53788600

C	-1.58384000	1.30863800	-1.26816000
C	-2.39242300	0.68581900	-0.32477400
C	-3.40812100	1.34999000	0.35005700
C	-3.61181500	2.69994900	0.06703900
H	-2.98349400	4.40319800	-1.08740800
H	-1.19246400	3.16108400	-2.27862200
H	-0.80117400	0.76407900	-1.78595600
H	-4.03633700	0.82718300	1.06200700
H	-4.40116400	3.23665800	0.58364300
I	-2.04823200	-1.37279700	0.11858500
Cl	0.57906800	-0.67264700	0.63393500
Cl	-5.18443200	-1.64408400	-0.37476800
C	1.48794100	3.48489500	-0.08949000
H	2.24941800	4.10758900	0.38318500
H	1.34265200	3.77598800	-1.12752200
H	0.55150500	3.54758100	0.46777000

TS₂₋₁₅

E (SMD/M06-2X/BS1) = -1527.71292772 au

G (SMD/M06-2X/BS1) = -1527.595330 au

E (SMD/M06-2X/BS2//SMD/M06-2X/BS1) = -1528.03940042 au

C	3.47753500	0.06039400	-0.97448200
C	2.28677400	0.63266200	-0.53480100
C	1.36444500	-0.14638200	0.16978500
C	1.65127900	-1.48858900	0.44550600
C	2.84967700	-2.04648400	0.01653300
C	3.76318900	-1.27479200	-0.70042500
H	4.18709700	0.66798600	-1.52695100
H	2.07867900	1.67548900	-0.74236600
H	0.93524700	-2.09786100	0.99131900
H	3.06410900	-3.08768600	0.23449300
H	4.69468400	-1.71365400	-1.04349200
C	0.08279800	0.43396700	0.66697200
N	-0.12262800	0.21994100	2.00603500
N	-0.34616500	-0.02046800	3.06609200
C	-0.48750400	1.77380300	0.31054900
O	-1.11963400	2.44576000	1.09057500
O	-0.26672100	2.06098600	-0.96178000
C	-0.86307200	3.28605800	-1.42245100
H	-1.94800100	3.23216800	-1.31661400
H	-0.47377000	4.13064600	-0.85122000
H	-0.58206000	3.36701500	-2.47050500
Cl	-1.60216900	-0.85079200	-0.10830000
Cl	-3.24102600	-2.14969100	-0.93129100

1

E (SMD/M06-2X/BS2) = -1449.64631097 au

G (SMD/M06-2X/ BS2) = -1449.592349 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -1449.69984567 au

C	3.68459600	-0.00027400	0.00001100
C	2.99565000	0.20680100	1.18826800
C	1.60709800	0.20787600	1.20087800
C	0.95080700	-0.00015100	-0.00000400
C	1.60708600	-0.20825700	-1.20086700
C	2.99564200	-0.20730100	-1.18824300
H	4.76704100	-0.00030400	0.00000700
H	3.53511700	0.36677700	2.11267300
H	1.05761700	0.36775300	2.11872200
H	1.05760600	-0.36805600	-2.11872600
H	3.53510200	-0.36731000	-2.11264700
I	-1.13892100	0.00009800	-0.00000300
Cl	-1.07710600	2.49087400	-0.10699300
Cl	-1.07789000	-2.49065000	0.10698700

2

E (SMD/M06-2X/BS2) = -607.682066754 au

G (SMD/M06-2X/ BS2) = -607.561413 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -607.730494352 au

C	-3.16366800	0.48900300	0.43354100
C	-1.86019400	0.95908800	0.40342100
C	-0.81622400	0.14096800	-0.03995100
C	-1.11297900	-1.16044700	-0.45363100
C	-2.41865500	-1.62707700	-0.40865400
C	-3.45047100	-0.80906000	0.03218800
H	-3.95597800	1.13990800	0.78123700
H	-1.65499800	1.96962700	0.73696700
H	-0.32586600	-1.80514400	-0.81506200
H	-2.62915100	-2.63907800	-0.73141300
H	-4.46741500	-1.17843500	0.06136600
C	0.55789100	0.66842400	-0.08905800
N	0.70107400	1.97446200	-0.17531000
N	0.82655400	3.07744900	-0.24834800
C	1.85228800	-0.00258900	-0.00070900
O	2.91359900	0.57637300	-0.07654800
O	1.73690500	-1.31573400	0.18937400
C	2.96980700	-2.03534900	0.29794800
H	3.55541400	-1.92322500	-0.61325700
H	3.54426800	-1.67523800	1.15010200

H 2.68953700 -3.07468100 0.44249500

3

E (SMD/M06-2X/BS2) = -1418.60647408 au

G (SMD/M06-2X/ BS2) = -1418.492457 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -1418.67734136 au

C	3.23573700	0.95825800	-0.33205300
C	1.85656000	1.14527000	-0.29442700
C	1.02261600	0.08887700	0.03630300
C	1.57668500	-1.15949400	0.32688200
C	2.94614200	-1.34188600	0.28557100
C	3.78310600	-0.27950500	-0.04408000
H	3.87579700	1.79212900	-0.58993000
H	1.45301000	2.12001500	-0.52561100
H	0.93341000	-1.99259900	0.58307700
H	3.36291500	-2.31542400	0.50931100
H	4.85570500	-0.42243200	-0.07525200
C	-0.48868100	0.21517900	0.11110200
C	-1.18207400	-0.74461000	-0.89831300
O	-0.52051700	-1.26661900	-1.74903100
O	-2.48593500	-0.95504500	-0.86997600
C	-3.46664500	-0.42271200	0.03304700
H	-3.53779300	-1.06213400	0.90960100
H	-3.25355200	0.60085000	0.32297500
H	-4.39945700	-0.45448000	-0.52411600
Cl	-1.06183300	1.85074000	-0.32271800
Cl	-0.99340700	-0.15949700	1.79317800

4

E (SMD/M06-2X/BS2) = -1697.92111179 au

G (SMD/M06-2X/ BS2) = -1697.784613 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -1697.99653471 au

C	3.64994800	2.22400900	0.19049000
C	3.39355800	1.54637600	-0.99498800
C	2.35250100	0.62953900	-1.06336700
C	1.59011400	0.41039800	0.07365800
C	1.83084400	1.07167300	1.26766000
C	2.87257100	1.98897500	1.31762400
H	4.46265800	2.93760100	0.23704600
H	4.00162600	1.73042400	-1.87127200
H	2.14546800	0.09502000	-1.98183100
H	1.22400500	0.87651800	2.14260800
H	3.07771500	2.51420500	2.24153500
I	0.00399900	-0.96913200	-0.01815200

Cl	1.65321400	-2.81597500	0.04276700
C	-3.00253300	3.02189400	-0.10079000
C	-2.02108600	2.88036900	-1.07175900
C	-1.18769700	1.78125300	-1.01776100
C	-2.26082100	0.98266400	0.88488400
C	-3.12409400	2.06146900	0.89163700
H	-3.66920300	3.87429700	-0.11975400
H	-1.89850800	3.60472300	-1.86428300
H	-0.40183900	1.61516500	-1.74420400
H	-2.31815000	0.18864100	1.61690700
H	-3.87743700	2.13530600	1.66294300
N	-1.31796800	0.86771200	-0.05256600
Cl	-2.72923200	-2.23541400	-0.11649500

11

E (SMD/M06-2X/BS2) = -1697.89919422 au

G (SMD/M06-2X/ BS2) = -1697.764337 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -1697.97822375 au

C	-0.81261700	3.94557800	0.31657100
C	-0.82636400	3.12812700	1.43974500
C	-0.54951700	1.77295600	1.32120000
C	-0.26974600	1.28105700	0.05737000
C	-0.24699000	2.06766800	-1.08210800
C	-0.52307800	3.42092900	-0.93659000
H	-1.02517400	5.00182200	0.41964100
H	-1.04584000	3.54188800	2.41524100
H	-0.54972000	1.12514500	2.18765700
H	-0.01141500	1.64732100	-2.05049800
H	-0.50885000	4.06230200	-1.80802000
I	0.13619600	-0.75873000	-0.13986000
Cl	7.05630200	-0.77823800	0.16440500
Cl	2.51750500	-0.31604600	-0.20674300
C	-2.67498600	-1.70611800	0.95968200
C	-4.03723900	-1.92312700	1.04092000
C	-4.85738100	-1.39089300	0.05724300
C	-4.29465300	-0.65955300	-0.97944600
C	-2.92548500	-0.48294700	-1.00035800
N	-2.15002300	-0.99865500	-0.04347700
H	-5.92764200	-1.54619100	0.09653700
H	-1.98135600	-2.09449700	1.69525000
H	-4.43859100	-2.49840400	1.86302700
H	-4.90057100	-0.23158100	-1.76534600
H	-2.42544300	0.07625400	-1.78215200

15

E (SMD/M06-2X/BS2) = -1418.55579946 au

G (SMD/M06-2X/ BS2) = -1418.446952 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -1418.63005553 au

C	3.63770800	-0.32062900	-0.13255100
C	2.43843400	0.33461100	-0.01191300
C	1.22858300	-0.41270500	0.03930900
C	1.27044600	-1.83201500	-0.03693600
C	2.47802600	-2.46789200	-0.15261600
C	3.65580100	-1.71466100	-0.19953500
H	4.56244200	0.23735400	-0.17412200
H	2.41356800	1.41506000	0.04256300
H	0.35129400	-2.40116600	-0.00075200
H	2.52340900	-3.54644500	-0.20762000
H	4.60578900	-2.22680700	-0.29124700
C	0.01910600	0.26725400	0.14729500
C	-0.03427300	1.77134200	0.32398800
O	0.35101100	2.28036000	1.33703200
O	-0.56749800	2.35547900	-0.71702800
C	-0.73247600	3.78760200	-0.62517800
H	-1.38411500	4.02332400	0.21378300
H	0.23890500	4.26095900	-0.49686400
H	-1.18713800	4.08398700	-1.56422300
Cl	-1.47151400	-0.46822400	0.15491400
Cl	-4.06733200	-1.85003600	-0.07213400

Cl₂

E (SMD/M06-2X/BS2) = -920.363579598 au

G (SMD/M06-2X/ BS2) = -920.384046 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -920.394920557 au

Cl	0.00000000	0.00000000	0.99428900
Cl	0.00000000	0.00000000	-0.99428900

N₂

E (SMD/M06-2X/BS2) = -109.530764525 au

G (SMD/M06-2X/ BS2) = -109.543410 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -109.537982915 au

N	0.00000000	0.00000000	0.54279400
N	0.00000000	0.00000000	-0.54279400

PhI

E (SMD/M06-2X/BS2) = -529.265994817 au

G (SMD/M06-2X/ BS2) = -529.206910 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -529.287101467 au

C	3.32061300	0.00000000	0.00003900
C	2.62467300	1.20155700	0.00001400
C	1.23501700	1.20941500	-0.00001600
C	0.55454300	0.00000000	-0.00001800
C	1.23501700	-1.20941500	-0.00002100
C	2.62467400	-1.20155700	0.00001400
H	4.40305800	0.00000000	0.00007100
H	3.16099500	2.14212700	0.00001700
H	0.69243700	2.14500800	-0.00003100
H	0.69243800	-2.14500800	-0.00003500
H	3.16099500	-2.14212700	0.00001700
I	-1.54107800	0.00000000	-0.00000200

Pyridine

E (SMD/M06-2X/BS2) = -248.276758749 au

G (SMD/M06-2X/ BS2) = -248.214603 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -248.298189374 au

C	0.00000100	1.37572600	0.00000000
C	1.19257000	0.66832400	-0.00000700
C	1.13976500	-0.71844100	0.00001200
C	-1.13976500	-0.71843800	-0.00001300
C	-1.19256700	0.66832900	0.00000700
H	0.00000400	2.45864400	0.00000000
H	2.14813600	1.17538400	-0.00002100
H	2.05500900	-1.30064400	-0.00001100
H	-2.05501200	-1.30063800	0.00001300
H	-2.14813400	1.17538700	0.00002200
N	-0.00000300	-1.40873400	0.00000100

TS₁₋₄

E (SMD/M06-2X/BS2) = -1697.90095193 au

G (SMD/M06-2X/ BS2) = -1697.764854 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -1697.97580467 au

C	1.07987900	3.80890500	0.30387200
C	0.71137100	3.21667200	-0.90113100
C	0.64256900	1.83653500	-1.00834200
C	0.96356500	1.07950900	0.10802900
C	1.33542100	1.63955400	1.31712400
C	1.38919900	3.02732300	1.40697900
H	1.12432700	4.88775500	0.37973000
H	0.47177100	3.83062800	-1.75968300
H	0.34127000	1.36234300	-1.93327500
H	1.57603400	1.01729900	2.16898900
H	1.67386500	3.48940100	2.34328700

I	0.90973700	-1.01371100	-0.02124400
Cl	3.18886200	-0.93811500	-0.91434500
Cl	-0.92249700	-2.72769500	1.19064300
C	-2.20805900	1.04634500	0.47471300
C	-3.54078000	1.42042100	0.38302700
C	-4.38585800	0.66629600	-0.41632600
C	-3.87095200	-0.43411800	-1.08617300
C	-2.53037000	-0.74318400	-0.91934300
N	-1.71758300	-0.01459600	-0.15884200
H	-5.43101600	0.93108900	-0.51533200
H	-1.51046200	1.61842200	1.07816100
H	-3.89855000	2.28407100	0.92679700
H	-4.49326300	-1.04948500	-1.72144400
H	-2.09105900	-1.60941500	-1.40101700

TS₁₁

E (SMD/M06-2X/BS2) = -1697.8988853 au

G (SMD/M06-2X/ BS2) = -1697.763282 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -1697.97750711 au

C	-0.12794100	3.89903100	0.25659200
C	-0.60559400	3.12145500	1.30397800
C	-0.54460600	1.73608500	1.23146400
C	-0.00591100	1.17539900	0.08629600
C	0.47780000	1.91982800	-0.97529400
C	0.41333400	3.30350200	-0.87542800
H	-0.17377200	4.97812800	0.32549500
H	-1.01920500	3.58858600	2.18810400
H	-0.90435400	1.12025500	2.04492500
H	0.90058100	1.44319600	-1.84974600
H	0.78763300	3.91170500	-1.68835100
I	0.09389800	-0.91131600	-0.04876300
Cl	6.27497700	-0.64944900	0.01302300
Cl	2.49949900	-0.83968200	0.02293100
C	-2.91363100	-1.42274500	0.85604700
C	-4.29585600	-1.43418800	0.85358400
C	-4.96573000	-0.76109500	-0.15698400
C	-4.23703100	-0.09840700	-1.13488100
C	-2.85779700	-0.12915500	-1.07033400
N	-2.22683700	-0.77826400	-0.08908400
H	-6.04766400	-0.75286400	-0.18335200
H	-2.33401500	-1.92880100	1.61848600
H	-4.82773800	-1.96089300	1.63310600
H	-4.72336500	0.43482400	-1.93929400
H	-2.23513100	0.37041000	-1.80279100

TS₂₋₁₅

E (SMD/M06-2X/BS2) = -1528.03953733 au

G (SMD/M06-2X/ BS2) = -1527.922503 au

E (SMD/M06-2X/BS3//SMD/M06-2X/BS2) = -1528.11848006 au

C	3.53141500	-0.01846800	-0.76476900
C	2.34321200	0.56184500	-0.34574800
C	1.31946700	-0.24365200	0.14683300
C	1.49649400	-1.62250200	0.23851200
C	2.69163000	-2.19274500	-0.16987300
C	3.70735600	-1.39286700	-0.67825000
H	4.32267600	0.60862900	-1.15454700
H	2.21840800	1.63476700	-0.40401000
H	0.70004600	-2.24820300	0.62229600
H	2.82507400	-3.26427200	-0.09863200
H	4.63656900	-1.84125200	-1.00581100
C	0.03363300	0.36414600	0.61719300
N	-0.12013400	0.22636900	1.99785700
N	-0.29390200	0.05299800	3.06305900
C	-0.39517400	1.76317500	0.25727600
O	-0.90398600	2.51278700	1.04700700
O	-0.19683300	1.99250400	-1.02112600
C	-0.66251300	3.26469000	-1.50684100
H	-1.73708300	3.34523100	-1.35304900
H	-0.14720200	4.07090900	-0.98805000
H	-0.42428000	3.27398200	-2.56540900
Cl	-1.61624500	-0.74833700	-0.05042600
Cl	-3.38860900	-1.98574700	-0.85853000