Supporting Information for:

Mechanistic details for oxidative addition of $PhICl_2$ to gold(I) complexes

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Computational details

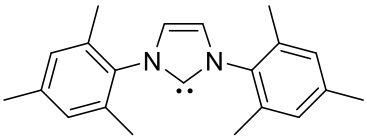
Gaussian 16[1] was used to fully optimize all the structures reported in this paper at the M06 hybrid functional of Truhlar and Zhao[2] level of theory. For all of the calculations, solvent effects were considered using the SMD solvation model of Truhlar and workers[3] with dichloromethane as the solvent. For geometry optimizations, the SDD basis set with effective core potential (ECP) was chosen to describe gold and iodine and the 6-31G(d) basis set was employed for all other atoms.[4-6] This basis set combination will be referred to as BS1. Frequency calculations were carried out at the same level of theory as those for 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.[7] To further refine the energies obtained from the SMD/M06/SDD,6-31G(d) calculations, we carried out single-point energy calculations using the M06 functional method for all of the structures with a larger basis set def2-TZVP (BS2). [8] Grimme empirical dispersion was added with the GD3 term on all the single-point energy calculations.[9] A tight convergence criterion and ultrafine integral grid were also employed to increase the accuracy of the calculations. The free energy for each species in the solution was calculated using the equation,

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

where $\Delta G^{1atm\rightarrow 1M}$ = 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.[10]

NBO 7.0 program[11] was used to analyse Natural Bond Orbital (NBO) and Natural Localized Molecular Orbitals (NLMO).

The free energy barriers for the formation of the cation **8** was estimated according to the protocol presented by Hall and Hartwig.[12] In this protocol, for example, the Gibbs free energy barrier for a dissociation reaction such as A-B → A + B is estimated as $\Delta G^{\ddagger} \approx \Delta H = H_A + H_B - H_{A-B}$.



1,3-dihydro-1,3-bis(2,4,6-trimethylphenyl)-2H-imidazol2-ylidene

Fig. S1 N-Heterocyclic carbene (NHC) used in this work and ref 7.

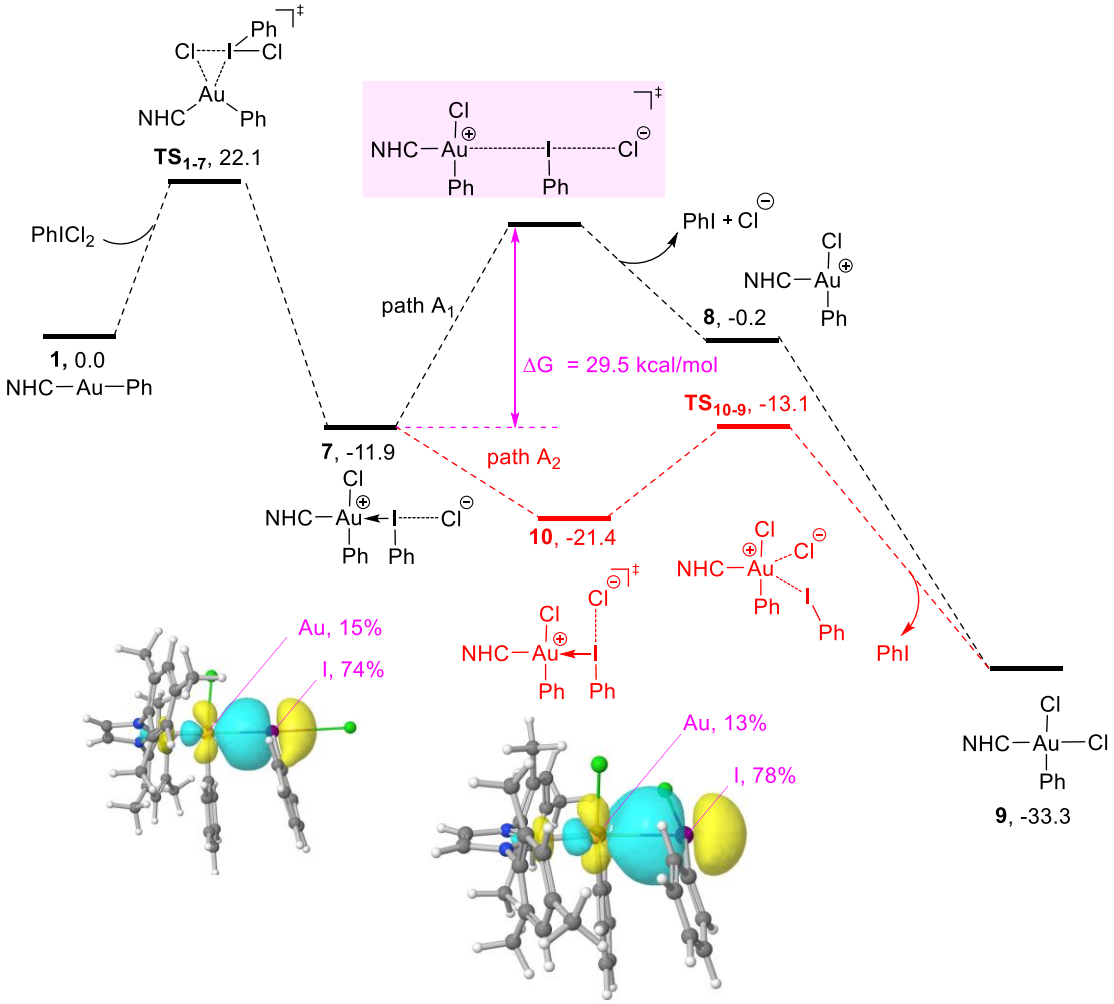


Fig. S2 Calculated free energy profile for oxidative addition of $PhICl_2$ to (NHC)AuPh (**1**) where NHC ligand is shown in Fig. S1 via pathway A. The relative free energy values are in kcal/mol. The figure includes the shape of the Au $d_{x^2-y^2}$ orbital determined by NLMO analysis for species **7** and **10**. Contribution of $d_{x^2-y^2}$ to the NLMO orbital in **7** and **10** are less than 50%, indicating that the $d_{x^2-y^2}$ orbital electrons are primarily localized on the iodine atom, and therefore the oxidation state of the Au atom in **7** and **10** are formally +3.

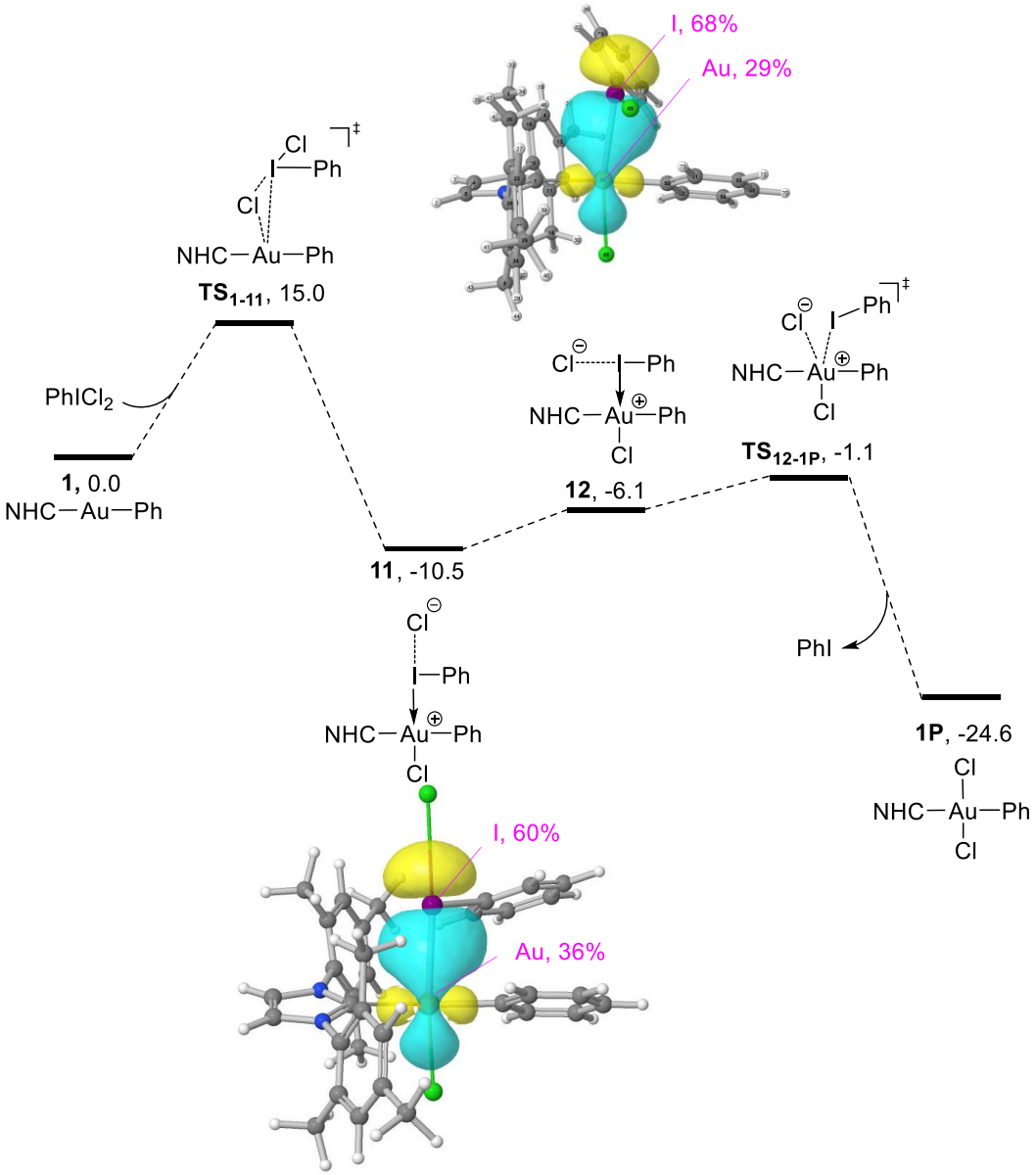


Fig. S3 Calculated free energy profile for oxidative addition of $PhICl_2$ to (NHC)AuPh (**1**) via pathway B leading to trans product **1P**. The relative free energy values are in kcal/mol. The figure includes the shape of the Au $d_{x^2-y^2}$ orbital determined by NLMO analysis for species **11** and **12**. Contribution of $d_{x^2-y^2}$ to the NLMO orbital in **11** and **12** are less than 50%, indicating that the $d_{x^2-y^2}$ orbital electrons are primarily localized on the iodine atom, and therefore the oxidation state of the Au atom in **11** and **12** are formally +3.

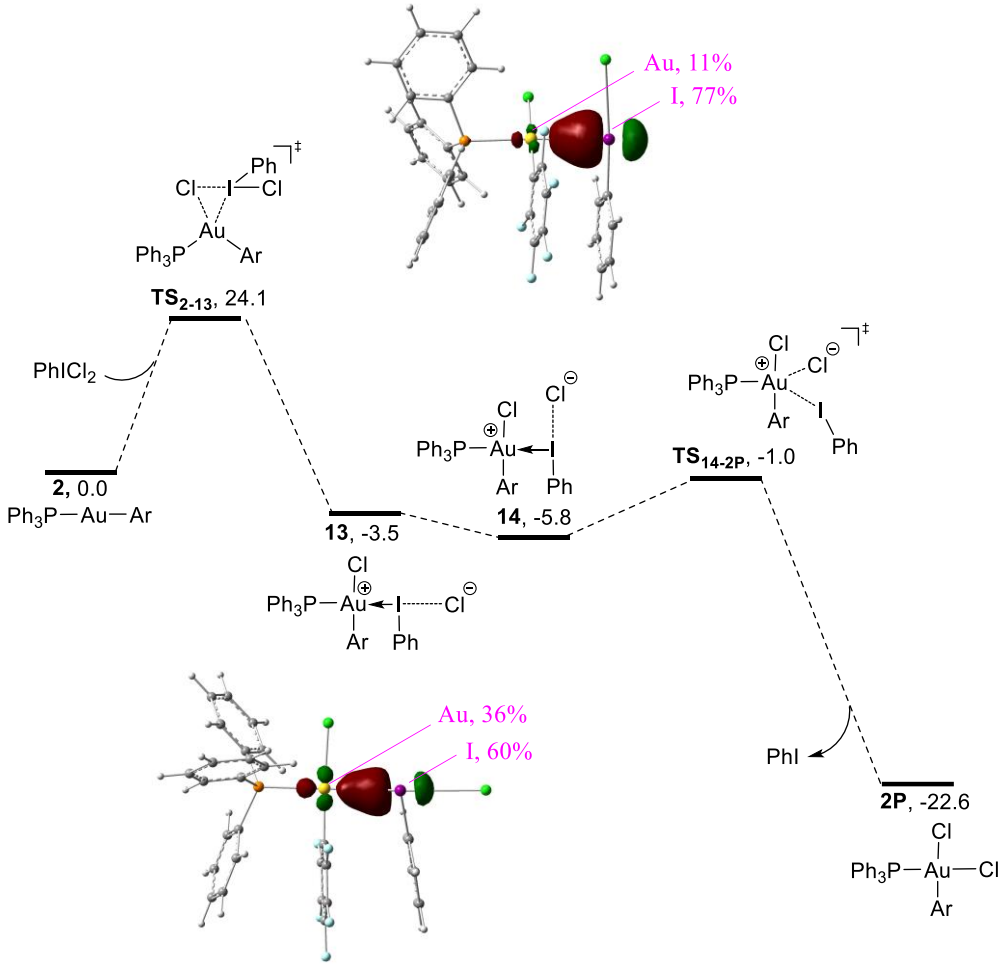


Fig. S4 Calculated free energy profile for oxidative addition of $PhICl_2$ to $(PPh_3)AuAr$ (**2**) where Ar = C_6F_5 via pathway A leading to cis product **2P**. The relative free energy values are in kcal/mol. The figure includes the shape of the Au $d_{x^2-y^2}$ orbital determined by NLMO analysis for species **13** and **14**. Contribution of $d_{x^2-y^2}$ to the NLMO orbital in **13** and **14** are less than 50%, indicating that the $d_{x^2-y^2}$ orbital electrons are primarily localised on the I atom, and therefore the oxidation state of the Au atom in **13** and **14** are formally +3.

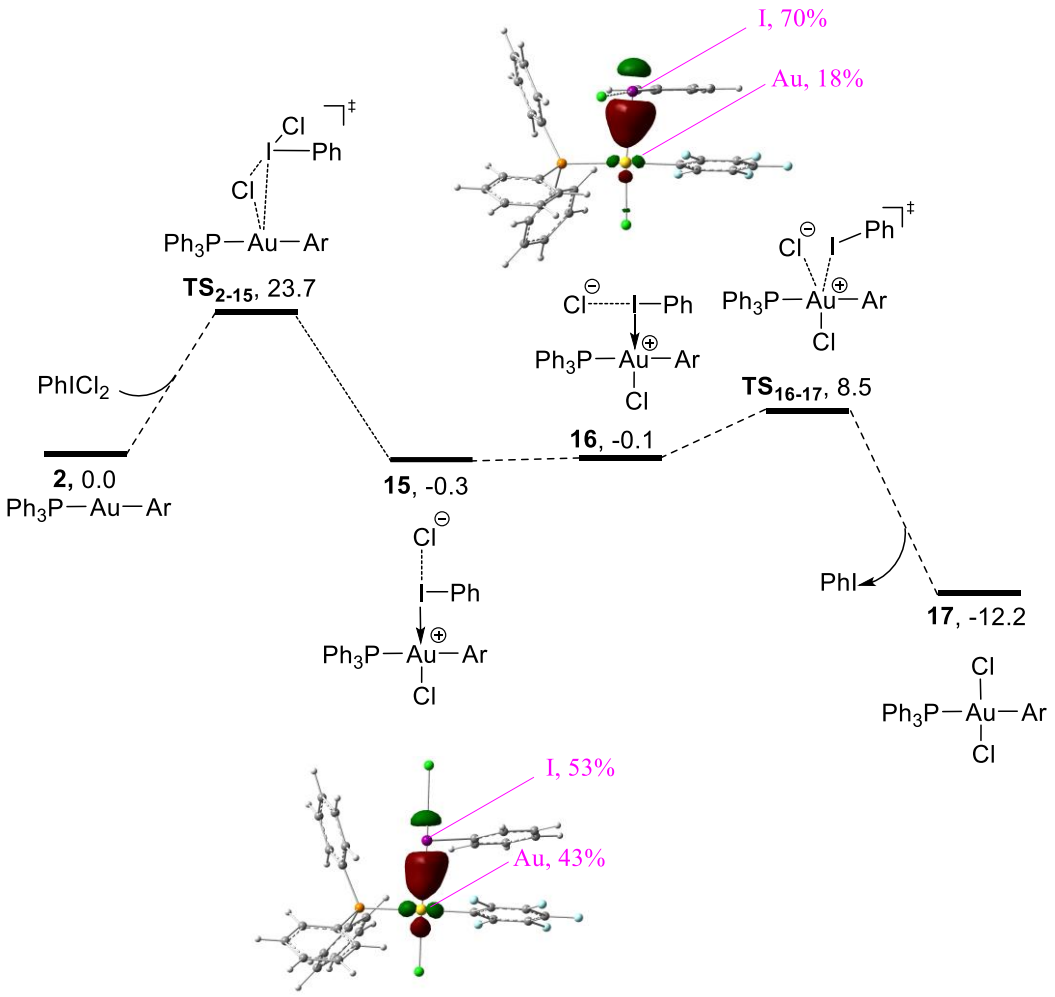


Fig. S5 Calculated free energy profile for oxidative addition of $PhICl_2$ to (PPh_3)AuAr (**2**) via pathway B leading to trans product **17**. The relative free energy values are in kcal/mol. The figure includes the shape of the Au $d_{x^2-y^2}$ orbital determined by NLMO analysis for species **15** and **16**. Contribution of $d_{x^2-y^2}$ to the NLMO orbital in **15** and **16** are less than 50%, indicating that the $d_{x^2-y^2}$ orbital electrons are primarily localised on the I atom, and therefore the oxidation state of the Au atom in **15** and **16** are formally +3.

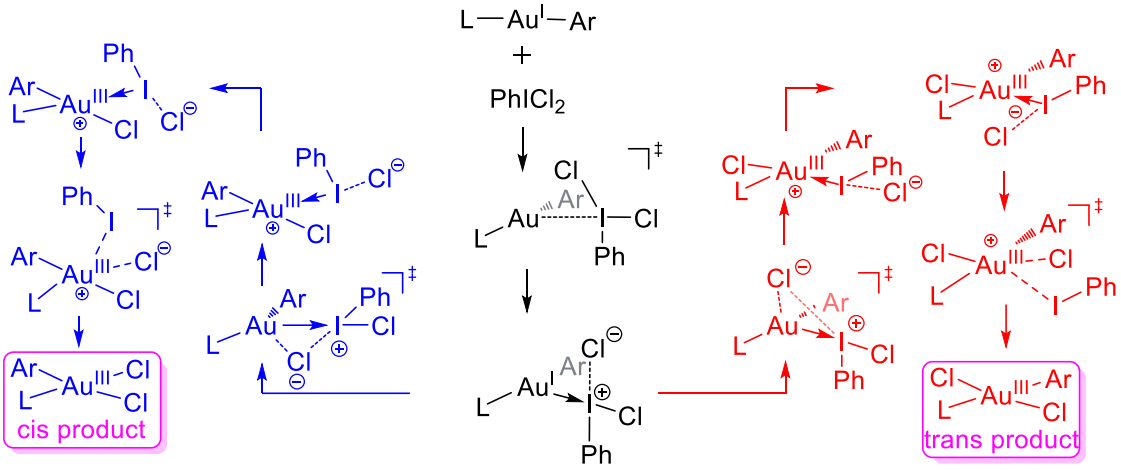


Fig. S6. Stepwise mechanism (pathway C) discovered in this work

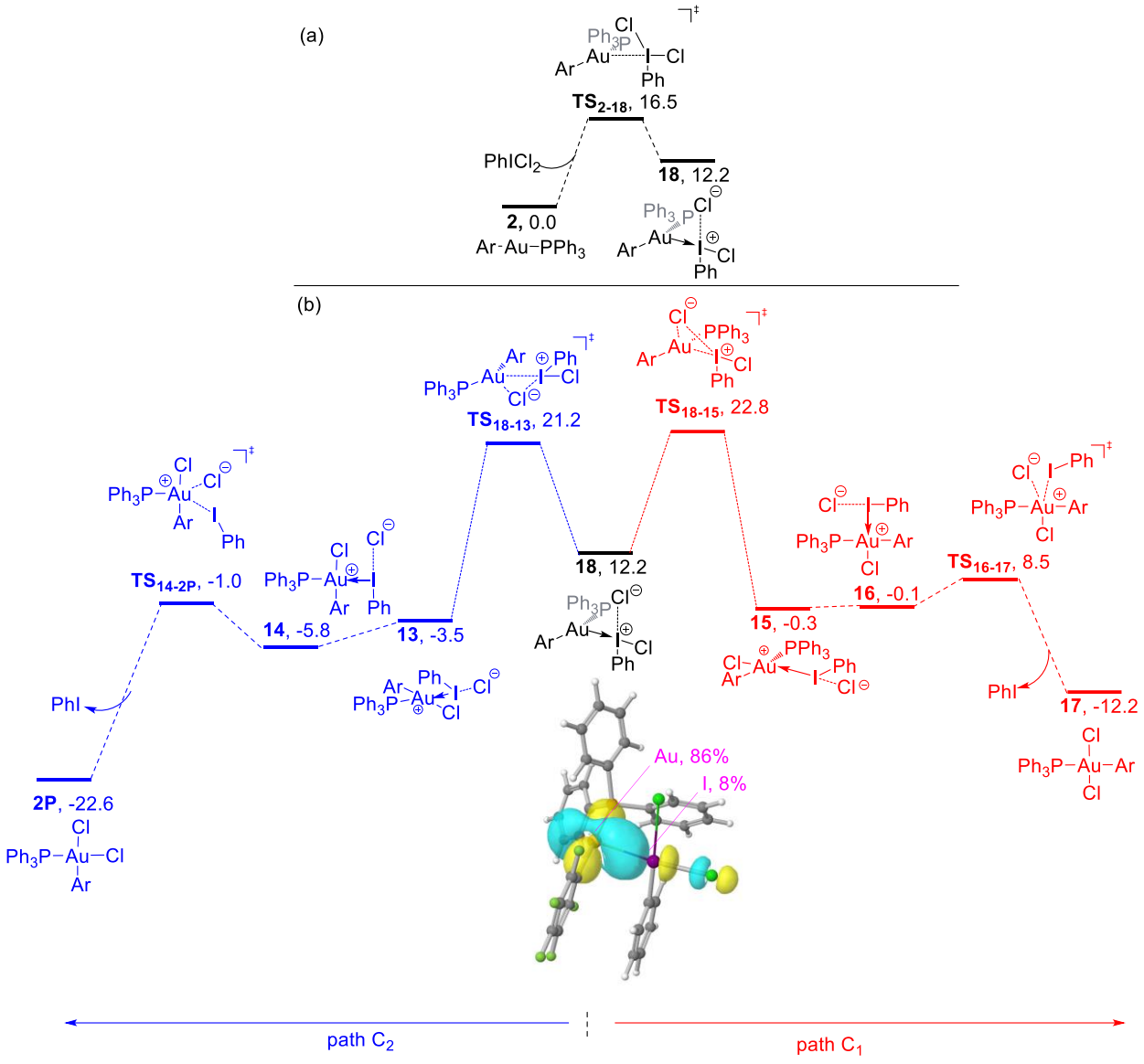


Fig. S7 Calculated free energy profile for oxidative addition of $PhICl_2$ to $(PPh_3)AuAr$ via stepwise pathway (path C). The relative free energies are in kcal/mol. The figure includes the shape of the Au $d_{x^2-y^2}$ orbital determined by NLMO analysis for structure **18**. Contribution of $d_{x^2-y^2}$ to the NLMO orbital in 18 is greater than 50%, indicating that the $d_{x^2-y^2}$ orbital electrons are still primarily localised on the Au atom, and therefore the oxidation state of the Au atom in **18** is formally +1.

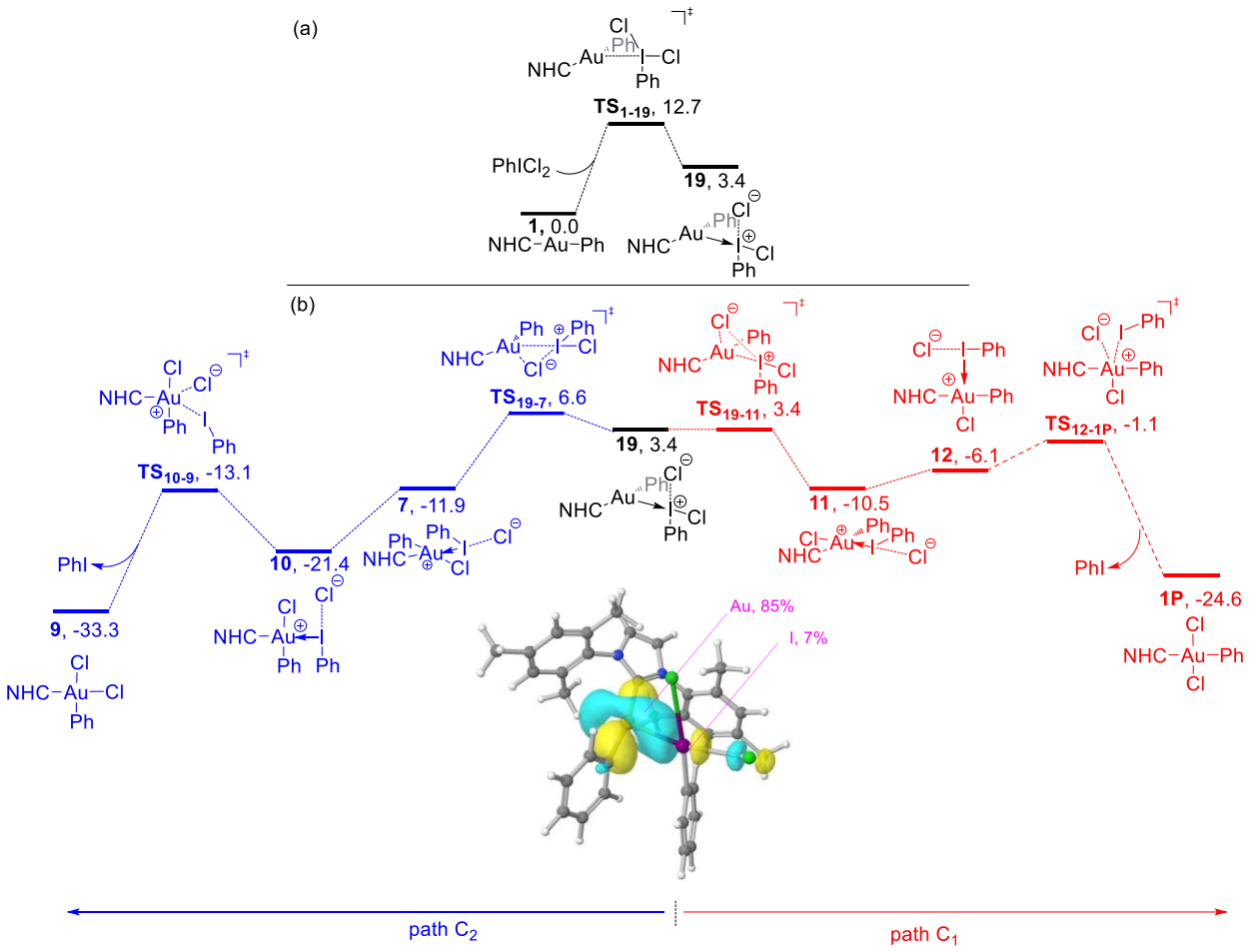


Fig. S8 Calculated free energy profile for oxidative addition of $PhICl_2$ to (NHC)AuPh via stepwise pathway (path C). The relative free energies are in kcal/mol. The figure includes the shape of the Au $d_{x^2-y^2}$ orbital determined by NLMO analysis for structure **19**. Contribution of $d_{x^2-y^2}$ to the NLMO orbital in **19** is greater than 50%, indicating that the $d_{x^2-y^2}$ orbital electrons are still primarily localized on the Au atom, and therefore the oxidation state of the Au atom in **19** is formally +1.

Further investigations for determining gold oxidation state. We conducted an NBO analysis to determine the occupancies of the gold $d_{x^2-y^2}$ orbital and the NPA charge on the gold center in various complexes formed during pathway C for both oxidative addition of $PhICl_2$ to complex **2** (Table S1) and to complex **1** (Table S2). The results of the analysis shed light on the electronic structure of the complexes and provide insight into the mechanism of oxidative addition. The conclusions drawn from the NLMO calculations are found to be in excellent agreement with those obtained from the two new analyses. For instance, the occupancy of the gold $d_{x^2-y^2}$ orbital decreases from 1.73 in **18** to 1.58 in **15** and further to 1.54 in **16**. The occupancy of the gold $d_{x^2-y^2}$ orbital in **17** with a value of 1.48 is very similar to those in **15** and **16**. The NPA charge on the gold center follows a similar trend, increasing from 0.57 in **18** to 0.77 in **15** and reaching 0.86 in **16**. Notably, the NPA charge on the gold centre in **17** with a value of 0.94 is almost close to those in **18** and **15**. These results indicate that the gold centre in **15** and **16** should have a formal oxidation state of +3, in agreement with the prediction from NLMO calculations.

Table S1 NBO analysis for the occupancies of the gold $d_{x^2-y^2}$ orbital (P_{dx2-y2}) and the NPA charge on the gold centre (NPA_{Au}) in various complexes formed during pathway C for oxidative addition of $PhICl_2$ to **2**.

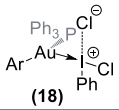
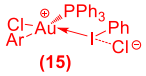
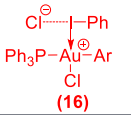
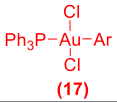
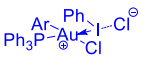
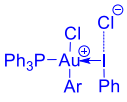
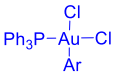
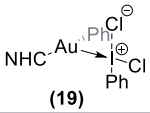
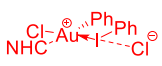
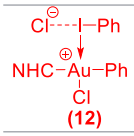
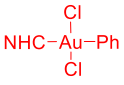
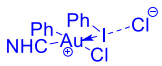
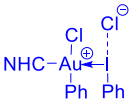
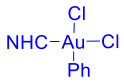
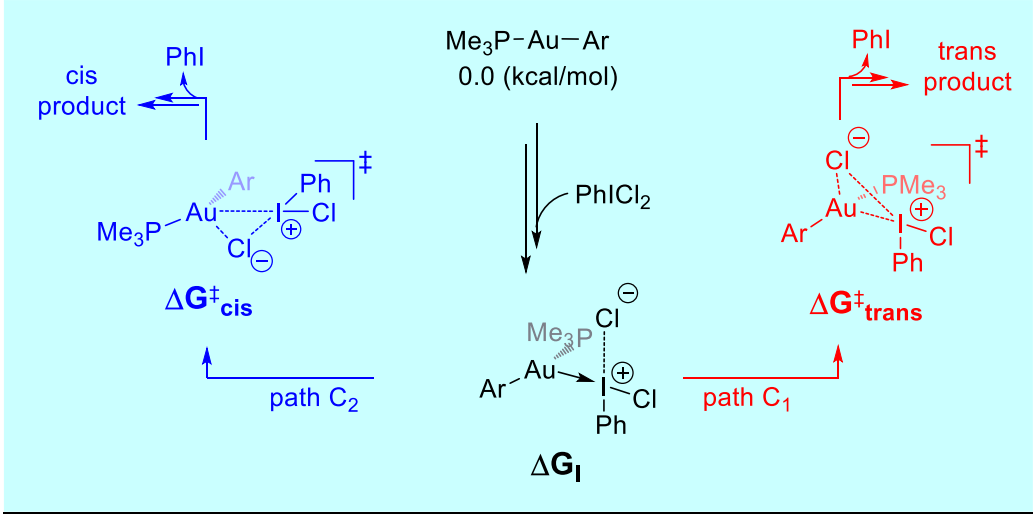
	Structure	P_{dx2-y2}	NPA_{Au}
	$Ar-Au-PPh_3$ **(2)**	1.86	0.32
	 **(18)**	1.73	0.57
path C_1	 **(15)**	1.58	0.77
path C_1	 **(16)**	1.54	0.86
path C_1	 **(17)**	1.48	0.94
path C_2	 **(13)**	1.57	0.78
path C_2	 **(14)**	1.56	0.83
path C_2	 **(2P)**	1.51	0.91

Table S2 NBO analysis for the occupancies of the gold $d_{x^2-y^2}$ orbital (P_{dx2-y2}) and the NPA charge on the gold centre (NPA_{Au}) in various complexes formed during pathway C for oxidative addition of $PhICl_2$ to **1**.

	Structure	P_{dx2-y2}	NPA_{Au}
	NHC–Au–Ph **(1)**	1.81	0.28
	 **(19)**	1.74	0.66
path C_1	 **(11)**	1.54	0.86
path C_1	 **(12)**	1.54	0.93
path C_1	 **(1P)**	1.46	1.01
path C_2	 **(7)**	1.53	0.87
path C_2	 **(10)**	1.51	0.91
path C_2	 **(9)**	1.47	0.97



Me$_3$P–Au–Ar	$d_{x^2-y^2}$	E($d_{x^2-y^2}$)	ΔG_I	$\Delta G^{\ddagger}_{cis}$	$\Delta G^{\ddagger}_{trans}$
(**i**) Me$_3$P–Au–OMe	HOMO-1	-6.4	7.4	13.1	9.7
(**ii**) Me$_3$P–Au–F	HOMO-1	-6.4	8.3	13.4	12.7
(**iii**) Me$_3$P–Au–Cl	HOMO-1	-6.5	8.8	13.5	12.6
(**iv**) Me$_3$P–Au–CN	HOMO-1	-6.6	10.9	15.5	13.3
(**v**) Me$_3$P–Au–C$_6$H$_2$(CN)$_3$	HOMO	-7.0	12.5	19.7	16.8
(**vi**) Me$_3$P–Au–C$_6$F$_5$	HOMO-1	-7.1	14.5	21.6	22.6

Fig. S9 Calculated relative free energy values for ΔG_I, $\Delta G^{\ddagger}_{cis}$, and $\Delta G^{\ddagger}_{trans}$ in oxidative addition of $PhICl_2$ to gold(I) complexes (**i**) – (**vi**). Shape and energy (in eV) of the Au $d_{x^2-y^2}$ orbital in gold(I) complexes (**i**) – (**vi**). The relative free energies are given in kcal/mol.

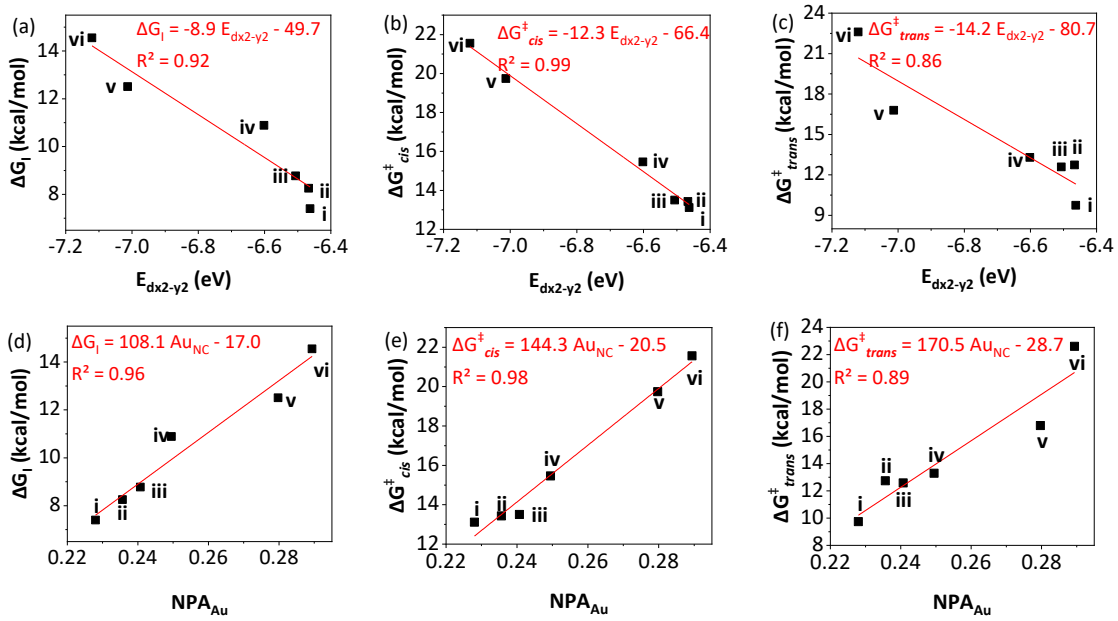


Fig. S10 (a) Plot of ΔG_I for the formation of the iodonium complex versus $E_{dx2\text{-}y2}$. (b) ΔG_{cis} for pathway C_2 versus $E_{dx2\text{-}y2}$. (c) $\Delta G^{\ddagger}_{trans}$ for pathway C_1 versus $E_{dx2\text{-}y2}$. (d) ΔG_I for the formation of the iodonium complex versus the NPA charge on the gold centre (NPA_{Au}). (e) ΔG_{cis} for pathway C_2 versus NPA_{Au}. (f) $\Delta G^{\ddagger}_{trans}$ for pathway C_1 versus NPA_{Au}. The observed correlations make it evident that a decrease in the positive charge of the gold centre leads to higher energy levels of the gold(I) $d_{x^2-y^2}$ orbital, which in turn results in stronger coordination with the iodonium and a lowered barrier to oxidative addition.

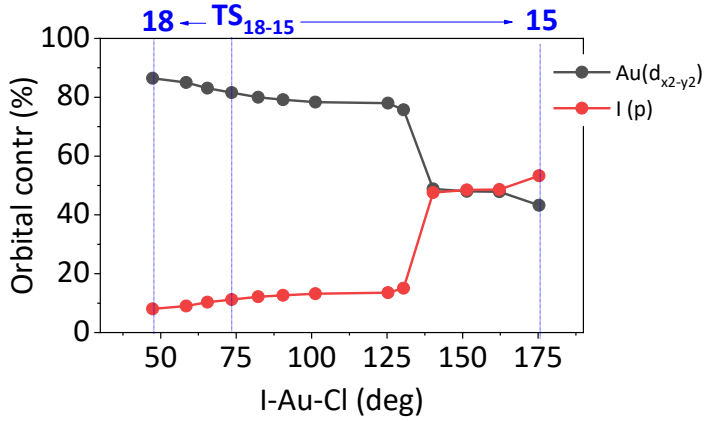


Fig. S11 Plot of the population changes of gold $d_{x^2-y^2}$ and iodine p orbitals against the I-Au-Cl angle along the IRC for transformation **18** ⟶ **15**. The analysis indicates that the oxidation state of gold remains +1 in the transition structure **TS18-15**, and that gold oxidation primarily occurs at the late stages of transformation **18** ⟶ **15**.

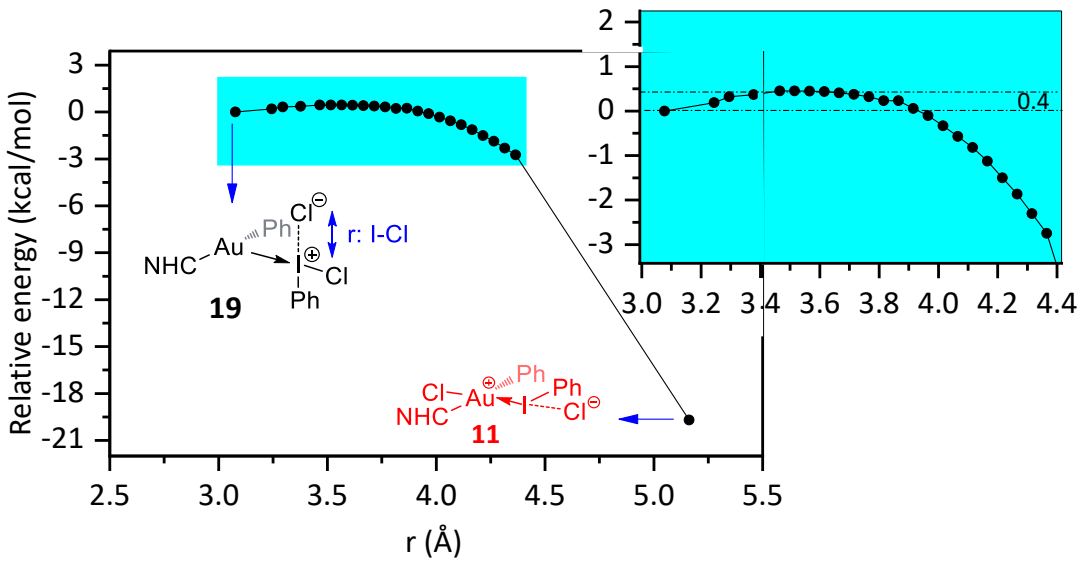


Fig. S12 Scan of the distance between iodine and chloride starting from structure **19.** It is obvious from this figure that the potential energy surface near intermediate **19** is considerably flat, which elucidates the difficulty in locating the transition structure $\mathbf{TS_{19\text{-}11}}$. Our scan calculations predict an activation energy barrier of approximately 0.4 kcal/mol for the conversion of intermediate **19** to **11**.

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Table S2. Total potential (E), enthalpy (H) and Gibbs free energies (G) of all structures optimized at the SMD/M06/BS1 level of theory along with the total potential energies calculated by SMD/M06/BS2//SMD/M06/BS1 in dichloromethane.
BS1 = 6-31G(d), SDD
BS2 = def2-TZVP

2
E (M06-SMD/SDD) = -1899.028326 au
H (M06-SMD/SDD) = -1898.676376 au
G (M06-SMD/SDD) = -1898.768065 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -1899.635025 au

Au -0.56832200 0.01207300 -0.02511300
P 1.79160800 0.00916700 0.00227800
C -2.64986700 0.00315600 -0.02441200
C -3.39374000 1.17103700 0.00223500
C -3.38300300 -1.17178100 -0.03718400
C -4.78208700 1.19259200 0.01528800
C -4.77105800 -1.20646600 -0.02507100
C -5.47422900 -0.01028700 0.00165500
H 5.16463500 3.38998900 -1.40429500
H 1.81911800 4.85003800 0.87223700
H 3.95630100 5.26969900 -0.32318200
C 2.52570700 -0.96970900 -1.34958500
C 3.67830900 -1.74023700 -1.17514300
C 1.91207500 -0.91328300 -2.60586700
C 4.21063900 -2.44667800 -2.25012000
H 4.16259100 -1.79031100 -0.19957200
C 2.45124800 -1.61516800 -3.67814800
H 1.00718100 -0.31789600 -2.74075200
C 3.59910600 -2.38418300 -3.49940100
H 5.10686300 -3.04855600 -2.10931100
H 1.96896800 -1.56892700 -4.65298800
H 4.01650400 -2.94057500 -4.33703700
F -2.75465100 -2.36170400 -0.06191500
F -5.43657600 -2.36096100 -0.03729600
F -6.80353900 -0.01670100 0.01418400
F -5.45828000 2.34063600 0.04101600
F -2.77568500 2.36656600 0.01675400
C 2.46850700 -0.69982400 1.53943000
C 3.61601800 -0.20068100 2.16077200
C 1.81043500 -1.80845800 2.08357500
C 4.09928000 -0.80879100 3.31645100
H 4.13453600 0.66329200 1.74444500
C 2.30103800 -2.41683000 3.23316800
H 0.90897600 -2.19345100 1.60278400
C 3.44442600 -1.91506800 3.85114100
H 4.99148300 -0.41484400 3.80025700
H 1.78489300 -3.27872600 3.65243700
H 3.82440900 -2.38611500 4.75619500
C 2.51018200 1.67727700 -0.14632400
C 3.71306400 1.91583800 -0.81682700
C 1.83015000 2.73957800 0.45945600
C 4.22947200 3.20689900 -0.87774800
H 4.24796900 1.09395500 -1.29352100
C 2.35320400 4.02671100 0.40115800
H 0.88517000 2.55443500 0.97412900
C 3.55151000 4.26038900 -0.26962700
C 3.27338500 -1.54582600 -1.48965900
C 4.68881300 -2.01417400 0.89103200
C 5.36317800 -1.67631800 -0.28164200
C 4.66246900 -1.44356900 -1.46257900
C 3.30140400 -2.11094300 0.89795100
I 0.50244400 -2.00585100 -0.28416600
H 5.19353100 -1.17550800 -2.37379900
H 6.44804300 -1.59012800 -0.27251900
H 2.76188200 -2.36115600 1.80852800
H 2.70035700 -1.33274400 -2.39214600
H 5.24070500 -2.19569900 1.81118500
Cl 0.48531300 -0.11370700 -3.09160300
C 1.79856300 1.50830900 0.11084700
C 2.45142300 2.35903700 -0.76850700
C 2.54043900 1.06850600 1.19530500
C 3.78020300 2.73006300 -0.60880300
C 3.87266900 1.40468200 1.39054300
C 4.49569900 2.24196200 0.47602300
Cl 0.61134200 -4.58946800 0.27321600
C -2.58589800 -0.87337100 1.46026500
C -3.13950700 -2.13474500 1.22700400
C -1.92501700 -0.61802300 2.67059700
C -3.03871300 -3.12896600 2.19859200
H -3.64581400 -2.34958200 0.28612300
C -1.83717500 -1.60994700 3.63857700
H -1.47270200 0.35924800 2.85114300
C -2.39076200 -2.86849200 3.40151500
H -3.47005700 -4.11056100 2.01039800
H -1.32952600 -1.40326200 4.57917100
H -2.31233200 -3.64783300 4.15752200
C -3.57711400 -0.18365800 -1.19813400
C -4.96758600 -0.17357800 -1.02940800
C -3.01656300 -0.66655700 -2.38298500
C -5.78912600 -0.65369200 -2.04111000
H -5.40640400 0.20567300 -0.10563600
C -3.84864700 -1.14525200 -3.39303800
H -1.93331700 -0.64691000 -2.52995900
C -5.22901800 -1.14107100 -3.22192900
H -6.86973900 -0.64665700 -1.90992000
H -3.41151100 -1.51612600 -4.31851700
H -5.87612800 -1.51460000 -4.01398200
C -3.23918000 1.91591000 0.78684800
C -4.08945100 1.94626000 1.89530500
C -2.94286400 3.10072800 0.10043500
C -4.64000200 3.15538100 2.30999200
H -4.32391900 1.02817000 2.43402400
C -3.49918200 4.30433500 0.51790100
H -2.27670300 3.07705500 -0.76477200
C -4.34586500 4.33128300 1.62380700
H -5.30413400 3.17765800 3.17227600
H -3.26717100 5.22270100 -0.01835300
H -4.77790300 5.27448300 1.95369400
F 1.98413200 0.26719600 2.12342700
F 1.80461900 2.88064200 -1.81941700
F 4.37630200 3.55054700 -1.47173800
F 5.76811700 2.58359200 0.64431700
F 4.55647000 0.94018800 2.43506100

$TS_{2\text{-}15}$
E (M06-SMD/SDD) = -3062.164853 au
H (M06-SMD/SDD) = -3061.708486 au
G (M06-SMD/SDD) = -3061.827678 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.321856 au

Au -0.17069800 0.87911600 -0.18300900
P -2.49599000 0.38394200 0.14551900
C 2.63649400 -1.87808500 -0.30157300

15
E (M06-SMD/SDD) = -3062.210578 au
H (M06-SMD/SDD) = -3061.752530 au
G (M06-SMD/SDD) = -3061.873009 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.360484 au

Au 0.12500900 -0.78267000 -0.13719200
P 2.48564700 -0.21180700 0.10782600
C -1.88595100 -1.29362200 -0.31967000
C -2.49065700 -1.40011500 -1.55726000
C -2.65584100 -1.56684600 0.79565800
C -3.82747700 -1.75048400 -1.69694800
C -3.99805200 -1.90743800 0.69619400
C -4.58239500 -2.00356000 -0.56000700
F -2.12640000 -1.47961200 2.02365600
F -4.72967500 -2.13295900 1.78289400
F -5.86407000 -2.32945800 -0.67267700
F -4.39100500 -1.83965700 -2.89787100
F -1.79757800 -1.13835000 -2.67676800
C -2.54123300 1.70426700 0.48408100
C -2.61241200 1.67938800 1.87002900
C -3.87144600 1.57016300 2.45720100
C -5.01172700 1.49608400 1.66167500
C -4.90755000 1.53684500 0.27258400
C -3.65966800 1.64464000 -0.33659600
H -1.71200400 1.72958000 2.48058500
H -3.95458200 1.54227200 3.54198500
H -5.99121900 1.40659700 2.12745400
H -5.80093400 1.48359600 -0.34730100
H -3.56531900 1.67641900 -1.42065600
I -0.60966100 1.85134800 -0.42039400
Cl 0.66638900 -3.13304700 0.27988700
Cl -1.24909500 4.74357700 -0.71885200
C 2.94693500 -0.67133800 1.80127700
C 2.09480300 -0.26168300 2.83650100
C 4.06983500 -1.44847400 2.09063300
C 2.38407000 -0.60326900 4.15134900
H 1.20030900 0.32469100 2.61184700
C 4.34846000 -1.79447400 3.41018500
H 4.72495000 -1.79249800 1.29154600
C 3.51183600 -1.37059400 4.43773600
H 1.72265400 -0.27927200 4.95260200
H 5.22348500 -2.40223300 3.63288900
H 3.73324500 -1.64558400 5.46743600
C 3.58123800 -1.02511200 -1.08780800
C 4.93549300 -0.66501900 -1.12178400
C 3.08090500 -1.94823000 -2.00921400
C 5.78296200 -1.24875700 -2.05457400
H 5.32474700 0.07403900 -0.42014500
C 3.93449700 -2.52114200 -2.94774900
H 2.02645900 -2.22147600 -1.99111100
C 5.28211700 -2.17647400 -2.96673400
H 6.83563000 -0.97311900 -2.07526300
H 3.54157800 -3.23833100 -3.66588700
H 5.94751100 -2.62737400 -3.70099100
C 2.82634400 1.56581100 -0.10464100
C 3.14551100 2.40511500 0.96430600
C 2.66476200 2.10500200 -1.38973800
C 3.29850200 3.77279100 0.74861300
H 3.27880700 1.99812000 1.96588300
C 2.82199400 3.47011300 -1.59750300
H 2.41395800 1.45440100 -2.23059100
C 3.13336700 4.30569100 -0.52604900
H 3.54964300 4.42323100 1.58441300
H 2.69424300 3.88330600 -2.59627400
H 3.24767700 5.37587500 -0.68790600

16
E (M06-SMD/SDD) = -3062.210741 au
H (M06-SMD/SDD) = -3061.752589 au
G (M06-SMD/SDD) = -3061.871844 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.361477 au

Au -0.09342100 -0.62246700 0.26894800
P 2.27879400 0.01578000 0.38787900
C -2.13346200 -1.04239600 0.39025200
C -2.75020100 -2.01150600 -0.37721700
C -2.91234500 -0.30907600 1.26602600
C -4.11834000 -2.24032600 -0.29549500
C -4.28265500 -0.50847900 1.36658500
C -4.88450100 -1.48106700 0.57980900
F -2.36354800 0.64572400 2.02904400
F -5.02143700 0.23310400 2.18523100
F -6.19293400 -1.68351900 0.66053300
F -4.70167000 -3.16879800 -1.04514000
F -2.04214100 -2.74741800 -1.23929700
C -1.93110500 2.20249100 -0.93311900
C -1.34197100 3.27064900 -0.26349600
C -2.15570600 4.13319900 0.46764600
C -3.53170900 3.92108200 0.51984300
C -4.10564200 2.85423500 -0.16689200
C -3.30450100 1.98385200 -0.90377500
H -0.26398200 3.42752700 -0.30651300
H -1.70979800 4.97250800 0.99862700
H -4.16155500 4.59434100 1.09833300
H -5.18150200 2.69065700 -0.12700100
H -3.74493600 1.13875200 -1.43280800
I -0.68620000 0.79990700 -1.98324300
Cl 0.20807000 -2.00519000 2.18115700
Cl 0.93177000 -1.37604000 -3.48835100
C 2.52388000 0.53489700 2.11140500
C 1.57427400 1.39293300 2.68252700
C 3.59166200 0.06964000 2.88015000
C 1.70889400 1.79884200 4.00384800
H 0.71945800 1.73757700 2.09532400
C 3.71700600 0.47515000 4.20638600
H 4.32256500 -0.61571500 2.45322800
C 2.78118200 1.33854300 4.76648000
H 0.96916500 2.46556100 4.44292500
H 4.54953600 0.10797700 4.80370000
H 2.88115900 1.64924800 5.80495200
C 3.41370300 -1.34095500 0.00042800
C 4.78323200 -1.07797900 -0.13698000
C 2.93094300 -2.64107300 -0.16936200
C 5.66006000 -2.11646700 -0.42433600
H 5.16265700 -0.06217100 -0.02164000
C 3.81461400 -3.67436900 -0.46357300
H 1.86362500 -2.84611100 -0.08633900
C 5.17560500 -3.41306100 -0.58726700
H 6.72389500 -1.91164600 -0.52865600
H 3.43424600 -4.68421200 -0.60376100
H 5.86435300 -4.22330000 -0.82023200
C 2.76612500 1.41529800 -0.66583900
C 2.89202600 2.71169800 -0.15680700
C 2.94473400 1.18146500 -2.03546400
C 3.19090700 3.76668600 -1.01470700
H 2.76941200 2.90312600 0.90848600
C 3.24819800 2.24033400 -2.88301300
H 2.81052700 0.17932200 -2.44885900
C 3.36727400 3.53290200 -2.37584600
H 3.29484400 4.77316500 -0.61323800
H 3.38609900 2.05250400 -3.94654900
H 3.60236500 4.36023000 -3.04336400

17
E (M06-SMD/SDD) = -2819.373607 au
H (M06-SMD/SDD) = -2819.014610 au
G (M06-SMD/SDD) = -2819.111875 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2820.047654 au

Au 0.51311500 -0.04871400 0.06083800
P -1.93265300 0.01903500 -0.02238300
C 2.59315400 -0.05805400 0.06906100
C 3.30656500 1.11170600 0.24147000
C 3.29699400 -1.23217500 -0.11206500
C 4.69525600 1.12448700 0.23677100
C 4.68552800 -1.25413300 -0.12355700
C 5.38342100 -0.06708100 0.05254600
F 2.65107000 -2.39294400 -0.28406700
F 5.35081600 -2.39098500 -0.30001100

F 6.71045900 -0.07136500 0.04478700
F 5.37018200 2.25684800 0.40494000
F 2.66968700 2.27616200 0.41992600
Cl 0.59561200 0.43103600 -2.25266800
Cl 0.57648000 -0.48262300 2.37137100
C -2.78160100 -0.03271300 1.58341800
C -3.43167200 1.08209500 2.11742900
C -2.76348000 -1.23842000 2.29685200
C -4.06235800 0.98857000 3.35521100
H -3.45990600 2.02218000 1.56868700
C -3.39760200 -1.32484100 3.52879500
H -2.25543800 -2.11131600 1.88501600
C -4.04567300 -0.21061300 4.05977000
H -4.57303400 1.85816600 3.76486600
H -3.38351200 -2.26410400 4.07843800
H -4.54055700 -0.28019900 5.02694900
C -2.61433900 -1.37328300 -0.96491700
C -4.00189900 -1.56801800 -1.00527700
C -1.76578400 -2.27195200 -1.61605300
C -4.52910300 -2.64115400 -1.71236700
H -4.66859300 -0.88101900 -0.48282900
C -2.30063000 -3.34992300 -2.31558900
H -0.68510900 -2.13346400 -1.57356400
C -3.67885300 -3.53103000 -2.36710400
H -5.60697300 -2.78800300 -1.74676100
H -1.63557900 -4.04973200 -2.81789900
H -4.09552700 -4.37440600 -2.91503200
C -2.37470300 1.58347300 -0.82774700
C -3.22566300 1.64269100 -1.93253200
C -1.78186800 2.75466900 -0.33687900
C -3.49731600 2.87108200 -2.52926000
H -3.67275900 0.73500400 -2.33545900
C -2.06414900 3.97731400 -0.93244500
H -1.09637800 2.70848400 0.51244600
C -2.92218600 4.03504000 -2.02956700
H -4.15978200 2.91445100 -3.39182600
H -1.60516500 4.88531600 -0.54605000
H -3.13573900 4.99261200 -2.50133600

$TS_{2\text{-}13}$
E (M06-SMD/SDD) = -3062.159339 au
H (M06-SMD/SDD) = -3061.703159 au
G (M06-SMD/SDD) = -3061.824960 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.318450 au

Au -0.08754800 0.22906700 -0.50812000
P -2.49640000 0.21880700 -0.05343500
C 1.47039100 1.60182800 -0.21660600
C 2.33038800 2.00149400 -1.22592300
C 1.65654100 2.21008100 1.01435600
C 3.33606700 2.94047800 -1.03738900
C 2.64880700 3.15223800 1.25235500
C 3.49430700 3.51859600 0.21446800
F 0.86586700 1.89156600 2.05836300
F 2.80269400 3.70746400 2.45350100
F 4.44982600 4.41951400 0.41842800
F 4.14615900 3.29610100 -2.03287900
F 2.22101400 1.47421100 -2.45928000
C 2.00758400 -2.14889800 1.08290600
C 1.40220600 -3.34619000 1.44913900
C 1.14583200 -3.55347200 2.80179800
C 1.49662000 -2.58459500 3.73985400
C 2.10540400 -1.39564000 3.34097300
C 2.36990900 -1.16332400 1.99537500
H 1.13398000 -4.09334000 0.70521500
H 0.67257600 -4.48064400 3.11946800
H 1.29420000 -2.75804900 4.79527900
H 2.37878000 -0.64208800 4.07682700
H 2.84932500 -0.24237500 1.66727400
I 2.42360100 -1.82393000 -0.97325000
Cl -0.41031600 -2.25405800 -1.77465500
Cl 4.98440200 -2.42750900 -0.59236800
C -3.47513900 -0.68073700 -1.29399900
C -4.18760300 -1.84262800 -0.99013800
C -3.41019400 -0.23662200 -2.62185500
C -4.84257100 -2.54214500 -2.00106200
H -4.23243300 -2.20790000 0.03545400
C -4.07288300 -0.93207400 -3.62438700
H -2.83343400 0.65698600 -2.86948100
C -4.78895000 -2.08791400 -3.31472500
H -5.39641000 -3.44731700 -1.75731100
H -4.02219800 -0.57821200 -4.65269500
H -5.30006100 -2.63824600 -4.10298600
C -2.87048900 -0.54218700 1.56090200
C -4.11625500 -0.36691000 2.17520000
C -1.89580400 -1.32574300 2.18543700
C -4.38325100 -0.97641300 3.39533100
H -4.88093200 0.24527300 1.69521900
C -2.16865400 -1.93645200 3.40669900
H -0.91732000 -1.45339100 1.71386500
C -3.41001000 -1.76221100 4.01046100
H -5.35368400 -0.83752400 3.86886200
H -1.40544200 -2.54657100 3.88801900
H -3.62092000 -2.23761800 4.96707700
C -3.21687400 1.89368900 0.04637200
C -4.47386700 2.21386200 -0.47433700
C -2.47206700 2.87684200 0.70852300
C -4.97527100 3.50561500 -0.33786400
H -5.06471200 1.45509500 -0.98721000
C -2.98131800 4.16247900 0.85070400
H -1.49172400 2.63004200 1.12046500
C -4.23137400 4.47905100 0.32286700
H -5.95353300 3.74996700 -0.74874800
H -2.39702900 4.92155600 1.36809400
H -4.62595200 5.48855200 0.42617300

13
E (M06-SMD/SDD) = -3062.221553 au
H (M06-SMD/SDD) = -3061.762861 au
G (M06-SMD/SDD) = -3061.880704 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.368861 au

Au -0.19690900 -0.90813800 -0.04631800
P -2.42060300 0.03580300 0.10619300
C 0.61290700 0.95736800 -0.26125300
C 0.90660000 1.45804900 -1.51661000
C 0.89604000 1.75040000 0.83685200
C 1.48584500 2.70857400 -1.68746000
C 1.48412000 3.00066200 0.70081800
C 1.78044000 3.47779500 -0.56958200
F 0.60920800 1.32368500 2.07267400
F 1.77229100 3.73766000 1.76673200
F 2.34856400 4.66696100 -0.71422700
F 1.76487500 3.17093400 -2.90070700
F 0.63366400 0.73788900 -2.61232800
C 3.45645500 -0.37046700 0.51281700
C 3.50162100 -0.23740100 1.89465200
C 4.18834400 0.85211900 2.42781200
C 4.81169200 1.76966300 1.58603300
C 4.76085100 1.60334800 0.20374700
C 4.07918200 0.52200300 -0.35040300
H 3.00633000 -0.95748400 2.54371100
H 4.23300900 0.97870600 3.50800200
H 5.34322600 2.61957600 2.01000300
H 5.25262800 2.31806700 -0.45426800
H 4.03284000 0.38327400 -1.42930500
I 2.35731500 -2.00624600 -0.31430600
Cl -1.04893800 -3.15772800 0.13961400
Cl 5.19960400 -3.34055700 -0.64156100
C -2.42316300 1.82103300 0.41570800
C -2.60229200 2.33817400 1.70175800
C -2.15394000 2.68585300 -0.65470300
C -2.51540600 3.71080500 1.91336800
H -2.81823900 1.67742200 2.53995500

C -2.07443300 4.05467400 -0.43530600
H -2.00959300 2.29108900 -1.66137000
C -2.25057000 4.56764400 0.84935800
H -2.66072600 4.10987800 2.91531000
H -1.87026000 4.72304800 -1.26992700
H -2.18289700 5.64061500 1.01951600
C -3.28460600 -0.80265400 1.45573500
C -4.55074000 -1.36149500 1.26721600
C -2.64109200 -0.91813100 2.69475900
C -5.17944900 -2.00962000 2.32635100
H -5.04629100 -1.29933200 0.29963300
C -3.27911900 -1.56041700 3.74725000
H -1.63660600 -0.51410300 2.83165700
C -4.54871500 -2.10560400 3.56264800
H -6.16587000 -2.44527600 2.17964700
H -2.77901000 -1.64726900 4.70976800
H -5.04369300 -2.61685100 4.38627900
C -3.28619500 -0.22681600 -1.46131800
C -4.50488200 0.43112800 -1.68197800
C -2.75713600 -1.06820700 -2.44472000
C -5.19139900 0.22935900 -2.87254300
H -4.91572100 1.09842200 -0.92385500
C -3.44877800 -1.25813900 -3.63689000
H -1.80719500 -1.57916700 -2.28556800
C -4.66362000 -0.61404000 -3.84861000
H -6.13947400 0.73651200 -3.04055400
H -3.03307900 -1.91165800 -4.40118200
H -5.20233300 -0.76583500 -4.78221000

14
E (M06-SMD/SDD) = -3062.226401 au
H (M06-SMD/SDD) = -3061.767736au
G (M06-SMD/SDD) = -3061.884648au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.373486 au

Au -0.05283700 -0.85214800 -0.07730600
P -2.13448400 0.26110600 0.30957400
C 0.80018000 0.93820300 -0.58763500
C 1.00628500 1.29284200 -1.90925100
C 1.25161200 1.80332200 0.39450400
C 1.66686400 2.46439900 -2.25462600
C 1.91537000 2.98188600 0.08068200
C 2.12834500 3.30775300 -1.25160900
F 1.04983200 1.53219900 1.68806000
F 2.36107600 3.78338200 1.04089300
F 2.76599900 4.42560100 -1.56804300
F 1.85958700 2.78704800 -3.52747900
F 0.54971300 0.51601800 -2.89425000
C 3.24132900 -0.98158500 1.15650700
C 2.96285600 -1.45628700 2.43491700
C 3.41821600 -0.73225300 3.53544000
C 4.13289200 0.44921800 3.34992500
C 4.40367800 0.91073800 2.06401500
C 3.96174100 0.19144600 0.95470900
H 2.39280100 -2.37527500 2.57289300
H 3.20998100 -1.09479200 4.54092000
H 4.48111200 1.01339100 4.21336000
H 4.95876000 1.83654600 1.91813000
H 4.16166000 0.55163300 -0.05505700
I 2.46156100 -2.03370600 -0.55403700
Cl -0.97966500 -2.94022600 0.67880300
Cl 1.18735800 -3.35096600 -3.05512900
C -2.72991300 -0.27673100 1.92629400
C -4.01910700 -0.79365200 2.07461600
C -1.86807100 -0.19312400 3.02800500
C -4.45238400 -1.19966500 3.33317000
H -4.68331800 -0.88609500 1.21679500
C -2.31264300 -0.59783100 4.27905700
H -0.84851100 0.17701500 2.90725100
C -3.60447700 -1.09945100 4.43149600
H -5.45675000 -1.60157200 3.45054000
H -1.64484900 -0.53224700 5.13564200
H -3.94734000 -1.42309800 5.41253700
C -2.00577100 2.06427600 0.29041200
C -1.85168700 2.70246800 -0.94890700
C -2.00291900 2.81304800 1.47063700
C -1.69375300 4.07986400 -1.00029400
H -1.85150400 2.12120000 -1.87238700
C -1.84340600 4.19411500 1.40873800
H -2.12961900 2.32759500 2.43684000
C -1.68490600 4.82541000 0.17893200
H -1.57446800 4.57367300 -1.96285500
H -1.84610200 4.77666400 2.32774200
H -1.55550300 5.90529700 0.13588200
C -3.28147600 -0.19221900 -1.01059200
C -4.48938600 0.51703900 -1.09436400
C -2.98822100 -1.19597000 -1.93882500
C -5.40232500 0.20304400 -2.09209500
H -4.71571100 1.31136500 -0.38283500
C -3.90625300 -1.49360000 -2.94100000
H -2.04772500 -1.74527400 -1.88883900
C -5.10970700 -0.79955100 -3.01501500
H -6.34153200 0.74913400 -2.15357500
H -3.67321100 -2.27038900 -3.66605900
H -5.82393700 -1.03612400 -3.80155200

2P
E (M06-SMD/SDD) = -2819.391952 au
H (M06-SMD/SDD) = -2819.031629 au
G (M06-SMD/SDD) = -2819.129698 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2820.064800 au

Au -0.20722800 -1.47309800 0.06676900
P -1.18984100 0.68324100 -0.05492300
C 1.65768300 -0.64269000 0.05816800
C 2.39444800 -0.55846700 -1.10926000
C 2.23463400 -0.18809400 1.22965000
C 3.67904200 -0.03109500 -1.11987300
C 3.51406900 0.35084000 1.24922200
C 4.23870600 0.42253800 0.06712200
F 1.55850100 -0.24320300 2.38208800
F 4.04954500 0.79198800 2.38101500
F 5.46326700 0.93080900 0.07047700
F 4.37212800 0.04934900 -2.24967400
F 1.87275900 -0.96287700 -2.27221000
Cl -2.40919600 -2.46183400 0.04782000
Cl 0.86565800 -3.62547100 0.21119200
C -0.01871300 2.03208700 0.25560100
C 0.85948600 2.40460300 -0.77128100
C 0.06336900 2.65260000 1.50481400
C 1.80723600 3.39361900 -0.54555700
H 0.80253000 1.92117000 -1.74759700
C 1.01896800 3.64060100 1.72356800
H -0.61707600 2.37461700 2.30807500
C 1.88978000 4.00947900 0.70302100
H 2.48629000 3.68202700 -1.34587400
H 1.07771900 4.12487000 2.69626700
H 2.63639700 4.78188300 0.87827500
C -2.49523500 0.76185000 1.19438500
C -3.77014400 1.23589700 0.87933500
C -2.20689300 0.31749000 2.49101900
C -4.74692600 1.28583500 1.86949600
H -4.00914000 1.55725600 -0.13314900
C -3.18704100 0.37564700 3.47266900
H -1.22019600 -0.08286200 2.72902300
C -4.45640600 0.86044500 3.16174700
H -5.74137700 1.65349000 1.62415500
H -2.96279100 0.03044500 4.47995800
H -5.22564300 0.89703500 3.93106500
C -1.85237600 0.95440400 -1.71627100
C -2.31298000 2.23522200 -2.05448000
C -1.88693000 -0.07434500 -2.66179400
C -2.82525700 2.47001600 -3.32397300
H -2.27054400 3.04782800 -1.32858900

C -2.39297600 0.17354400 -3.93384700
H -1.52002200 -1.06901700 -2.40926300
C -2.86516200 1.44020200 -4.26215900
H -3.18820800 3.46260700 -3.58320700
H -2.41537100 -0.62882600 -4.66850100
H -3.26191400 1.62984100 -5.25792100

TS_{2-18}
E (M06-SMD/SDD) = -3062.170510 au
H (M06-SMD/SDD) = -3061.714174 au
G (M06-SMD/SDD) = -3061.833396 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.333321 au

Au -0.02217400 -0.77865000 -0.43777900
P 2.30696400 -0.43670800 -0.00846900
C -2.02035900 -1.38467200 -0.55580100
C -2.87112300 -1.18528700 -1.63170400
C -2.59315200 -1.98000200 0.55860400
C -4.21739500 -1.53127200 -1.60834400
C -3.93139600 -2.33799000 0.63239800
C -4.75050300 -2.10745900 -0.46456900
F -1.85317000 -2.21835700 1.65811500
F -4.44183000 -2.88573100 1.73448500
F -6.03479800 -2.44292800 -0.42155000
F -5.00200900 -1.31701500 -2.66273300
F -2.42137900 -0.62871500 -2.76569000
C -1.48845900 1.54378600 1.45582300
C -0.45070000 1.63182600 2.37737900
C -0.68047600 1.15556300 3.66489000
C -1.92326300 0.62110200 4.00044200
C -2.95061000 0.56201900 3.05849300
C -2.73797000 1.01585900 1.76093200
H 0.51314900 2.05702100 2.10081200
H 0.11687400 1.21002500 4.40458800
H -2.09552100 0.24814700 5.00818500
H -3.91925000 0.14357900 3.32721300
H -3.52198800 0.95161500 1.00669500
I -1.12425600 2.25304300 -0.53304200
Cl 0.41743500 1.47067500 -2.88087700
Cl -2.42886800 4.44332100 0.07426400
C 2.78272600 1.17411800 0.70821300
C 2.64605900 2.32970000 -0.07172600
C 3.18461800 1.28540800 2.04310600
C 2.91337100 3.57798400 0.48001200
H 2.31663000 2.24983800 -1.11020800
C 3.44379200 2.53924200 2.59163100
H 3.29226300 0.39544300 2.66278800
C 3.30828500 3.68479600 1.81295800
H 2.81000900 4.47147300 -0.13378400
H 3.75538300 2.61759400 3.63189800
H 3.51131000 4.66388600 2.24374000
C 3.36489600 -0.71434700 -1.46254500
C 4.56854200 -0.03584900 -1.66747200
C 2.95171000 -1.69008000 -2.37579800
C 5.35108700 -0.33415500 -2.77962200
H 4.89673700 0.72663200 -0.96084100
C 3.73978400 -1.98934000 -3.48066900
H 2.00307500 -2.20898000 -2.22245800
C 4.93856400 -1.30904500 -3.68382600
H 6.28671600 0.19909200 -2.93938300
H 3.41213400 -2.74694300 -4.19031400
H 5.55186900 -1.53703100 -4.55406100
C 2.85500500 -1.66952100 1.22155600
C 4.19592200 -2.05618400 1.31388200
C 1.92105600 -2.18923400 2.12330600
C 4.59410900 -2.95542900 2.29678700
H 4.93138300 -1.65221600 0.61731600
C 2.32423100 -3.08612500 3.10848400
H 0.87308100 -1.89138100 2.04772000
C 3.65952900 -3.46989700 3.19360200
H 5.63833300 -3.25601400 2.36327200
H 1.59182300 -3.48990000 3.80538100
H 3.97463400 -4.17550700 3.96054000

18
E (M06-SMD/SDD) = -3062.177531 au
H (M06-SMD/SDD) = -3061.720667 au
G (M06-SMD/SDD) = -3061.840026 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.340455 au

Au 0.03979300 -0.87722800 -0.38332900
P 2.35360200 -0.51584100 0.14238000
C -1.97208200 -1.33043400 -0.64405600
C -2.64682100 -1.20173400 -1.84817800
C -2.72299100 -1.73982800 0.44761000
C -4.00123000 -1.47942200 -1.97844100
C -4.07757900 -2.02367100 0.36302500
C -4.71846100 -1.88954200 -0.86212100
F -2.15209000 -1.85454000 1.65706800
F -4.77078100 -2.39893200 1.43417400
F -6.01299600 -2.15608600 -0.96600200
F -4.62099900 -1.35297100 -3.14747900
F -2.00041400 -0.78606200 -2.94420400
C -1.92744300 1.55153600 1.42994400
C -1.19917000 1.56890500 2.61671600
C -1.86296200 1.28155900 3.80632800
C -3.22385400 0.98152100 3.79048100
C -3.93596700 0.97285100 2.59162000
C -3.28844500 1.26299500 1.39439100
H -0.13278000 1.80069700 2.61236400
H -1.31420700 1.29170300 4.74616400
H -3.73621100 0.75174800 4.72290300
H -4.99863600 0.73622700 2.58687000
H -3.82882100 1.24737900 0.44772900
I -0.88605000 1.86894300 -0.40839900
Cl 0.66645600 2.23020700 -2.95714500
Cl -1.37494200 4.42129800 -0.26600300
C 2.83218400 -1.82602400 1.31169600
C 1.85771500 -2.32020400 2.18796400
C 4.13907800 -2.31675600 1.37648400
C 2.19141500 -3.29351000 3.12393100
H 0.83553600 -1.93489400 2.13824400
C 4.46578100 -3.29407600 2.31073100
H 4.90241600 -1.93979300 0.69568300
C 3.49469100 -3.78127400 3.18271300
H 1.43150100 -3.67523800 3.80332700
H 5.48380200 -3.67657900 2.35756500
H 3.75490900 -4.54774300 3.91065200
C 3.44278200 -0.63347600 -1.30190300
C 4.71478300 -0.05249600 -1.32004900
C 2.98307800 -1.34468400 -2.41450300
C 5.52141900 -0.19287700 -2.44400900
H 5.07185200 0.51429300 -0.45979900
C 3.79496000 -1.48356700 -3.53489800
H 1.98013800 -1.77826800 -2.40433900
C 5.06236500 -0.90724100 -3.54849100
H 6.50998000 0.26245900 -2.45985200
H 3.43193200 -2.03115500 -4.40260400
H 5.69448600 -1.00803900 -4.42909700
C 2.71087500 1.06660200 0.96706300
C 2.95441500 1.13384800 2.34190100
C 2.62963500 2.24474500 0.21348400
C 3.11217800 2.37321700 2.95821200
H 3.02470300 0.22231600 2.93548400
C 2.78885100 3.47743100 0.83621100
H 2.41898400 2.20376500 -0.85886900
C 3.02590800 3.54326800 2.20851100
H 3.30601100 2.42134700 4.02840000
H 2.72027700 4.38970400 0.24528500
H 3.14618800 4.51050300 2.69361800

TS_{18-15}

E (M06-SMD/SDD) = -3062.170322 au
H (M06-SMD/SDD) = -3061.712962 au
G (M06-SMD/SDD) = -3061.829641 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.326841 au

Au 0.02249700 -0.89279800 -0.18900000
P 2.31947500 -0.27784700 0.33244600
C -1.99570400 -1.42803300 -0.13674100
C -2.75766900 -1.82493200 -1.22692200
C -2.67606700 -1.28851300 1.06627600
C -4.11778900 -2.09461500 -1.13156200
C -4.03287400 -1.54030300 1.20212800
C -4.75850800 -1.94583000 0.09024000
F -2.03321500 -0.87223000 2.16838700
F -4.64783800 -1.37722400 2.37049800
F -6.05679800 -2.19280800 0.19603500
F -4.81476000 -2.48214600 -2.19557000
F -2.20749400 -1.95545400 -2.43578200
C -1.84111500 2.09016300 0.54670700
C -1.09724600 2.58505800 1.61249400
C -1.76909600 2.86872800 2.79890600
C -3.14175700 2.65311200 2.89639400
C -3.86176700 2.15801300 1.81033500
C -3.21236600 1.86841200 0.61409300
H -0.02189900 2.74154300 1.53026400
H -1.21001500 3.25472700 3.64923100
H -3.65715500 2.87202800 3.82951300
H -4.93396300 1.98896900 1.89226100
H -3.75833600 1.46762700 -0.23938100
I -0.82811600 1.56132700 -1.25236200
Cl 1.04249300 -0.79102900 -3.01900000
Cl -1.49030500 3.95784000 -2.30665600
C 2.32064000 0.47257200 1.99276700
C 1.38501500 -0.01262300 2.91580800
C 3.18984800 1.50091600 2.36686000
C 1.31469300 0.52774900 4.19403200
H 0.70896900 -0.82112800 2.62750300
C 3.10728300 2.04820000 3.64488500
H 3.92881500 1.88123800 1.66263300
C 2.17045000 1.56679700 4.55531600
H 0.58376500 0.14525200 4.90429400
H 3.78168600 2.85397400 3.92923700
H 2.10880100 2.00001900 5.55219100
C 3.33388300 0.79324800 -0.72504200
C 4.48598000 0.31189400 -1.35012900
C 2.93132800 2.11767200 -0.93738800
C 5.22308200 1.14648400 -2.18517100
H 4.80809000 -0.71704400 -1.19486900
C 3.67237200 2.94669400 -1.76999700
H 2.03832100 2.50770700 -0.44767700
C 4.81682600 2.45972700 -2.39870300
H 6.11858600 0.76431300 -2.67187300
H 3.35311400 3.97501000 -1.93058200
H 5.39317200 3.10818700 -3.05633000
C 3.17789300 -1.87476000 0.48335700
C 4.01011800 -2.16406200 1.56921900
C 2.97970300 -2.82993800 -0.52404100
C 4.63949000 -3.40227300 1.64547300
H 4.16961900 -1.42382100 2.35312800
C 3.61717400 -4.06327000 -0.44089000
H 2.34143800 -2.59137900 -1.37863700
C 4.44170100 -4.35082000 0.64417400
H 5.28870000 -3.62643000 2.49007800
H 3.46549000 -4.80268800 -1.22517700
H 4.93414000 -5.31952900 0.71051400

TS_{18-13}
E (M06-SMD/SDD) = -3062.168249 au
H (M06-SMD/SDD) = -3061.711718 au
G (M06-SMD/SDD) = -3061.831945 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.324949 au

Au -0.41222700 0.02285100 -0.36210600
P -2.75612100 0.23856600 0.15913600
C 1.45005400 1.00447700 -0.49324900
C 2.03671100 1.26895600 -1.72392700
C 1.95426500 1.67606300 0.61325400
C 3.07670100 2.17734500 -1.86223200
C 3.00188400 2.57675700 0.51361700
C 3.56312600 2.82621200 -0.73423600
F 1.44856300 1.44592100 1.82943200
F 3.47562800 3.20188600 1.58460200
F 4.56493800 3.68345900 -0.84608400
F 3.62051100 2.42215700 -3.04823700
F 1.62103900 0.63119400 -2.82178800
C 3.64411800 -0.92111000 0.72571300
C 3.66915900 -0.72773600 2.10328500
C 4.77528700 -0.08957200 2.65603900
C 5.82463300 0.32692000 1.83876200
C 5.78630300 0.10210700 0.46440900
C 4.68478500 -0.52673400 -0.10953800
H 2.83916200 -1.05163600 2.72860600
H 4.81525700 0.08193700 3.72997500
H 6.68414000 0.82864600 2.27926000
H 6.61257600 0.42157700 -0.16796600
H 4.63714600 -0.70075400 -1.18361500
I 1.91887500 -1.81785100 -0.15909700
Cl -0.74761100 -2.69393800 -1.50350200
Cl 3.08142600 -4.19417500 0.01101700
C -3.88404900 -0.18315600 -1.20410700
C -5.08759300 -0.85920300 -0.99122900
C -3.52972400 0.22181200 -2.49533300
C -5.93272200 -1.12178400 -2.06602100
H -5.36843600 -1.17922200 0.01237800
C -4.38031700 -0.03651400 -3.56331100
H -2.57993100 0.73393500 -2.66279400
C -5.58126800 -0.71010400 -3.34842900
H -6.86899800 -1.65150600 -1.89872100
H -4.10037500 0.27786100 -4.56718600
H -6.24318300 -0.92071500 -4.18682500
C -3.23862300 -0.80141500 1.57644100
C -4.03907200 -0.31594600 2.61387400
C -2.79214100 -2.12886900 1.60058700
C -4.39012000 -1.15455600 3.66862400
H -4.39137800 0.71537600 2.60211400
C -3.15289200 -2.96149000 2.65402000
H -2.16860900 -2.50766600 0.78571100
C -3.94840200 -2.47435500 3.68934800
H -5.01250500 -0.77292700 4.47632400
H -2.80684300 -3.99359600 2.66812100
H -4.22356600 -3.12653800 4.51666500
C -3.17438400 1.94839300 0.63340800
C -4.42265300 2.50705100 0.34558300
C -2.22610900 2.69582200 1.34020600
C -4.71657600 3.80252700 0.76142500
H -5.16884900 1.93096400 -0.20197500
C -2.52754000 3.98654500 1.76099900
H -1.24877100 2.26186500 1.56124400
C -3.77150400 4.54110000 1.46843400
H -5.68868500 4.23538300 0.53158300
H -1.78600100 4.56352000 2.31091500
H -4.00380600 5.55495100 1.79011500

$PhICl_2$
E (M06-SMD/SDD) = -1163.143055 au
H (M06-SMD/SDD) = -1163.041354 au
G (M06-SMD/SDD) = -1163.088741 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -1449.705015 au

C 0.98167800 -0.04103400 0.00179400
C 1.63710800 0.20282500 1.20037800
C 3.02031700 -0.32799600 -1.18072800

C 3.71302000 -0.08329500 0.00188800
C 3.02832900 0.17948500 1.18530200
C 1.62884300 -0.30800900 -1.19620500
I -1.15014300 0.03013100 -0.00154500
H 3.57457300 0.36886700 2.10723200
H 4.80131900 -0.09645100 0.00112100
H 1.07430500 -0.49500300 -2.11312500
H 1.08822000 0.40976600 2.11643400
H 3.56077200 -0.53198300 -2.10296200
Cl -1.20517300 -2.58250100 0.12466800
Cl -0.98290800 2.64226500 -0.12475100

PhI

E (M06-SMD/SDD) = -242.847963 au
H (M06-SMD/SDD) = -242.751345 au
G (M06-SMD/SDD) = -242.789978 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -529.316991 au

C -0.58091500 0.00000900 -0.00012100
C -1.25872700 -1.21416100 -0.00011600
C -2.65213200 -1.20507400 0.00003000
C -3.34883500 -0.00000600 0.00015300
C -2.65213400 1.20506900 0.00002300
C -1.25873300 1.21417500 -0.00011400
H -0.71312700 -2.15569000 -0.00043100
H -3.19214600 -2.15067100 -0.00003300
H -4.43746200 -0.00002700 0.00030300
H -3.19216800 2.15065100 -0.00001800
H -0.71314700 2.15571100 -0.00042800
I 1.56145100 -0.00000100 0.00002800

1

E (M06-SMD/SDD) = -1290.766533 au
H (M06-SMD/SDD) = -1290.247072 au
G (M06-SMD/SDD) = -1290.346037 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -1291.209771 au

C 0.06328000 -1.26837500 -0.00646500
H -1.23947200 -4.27986300 -0.00437600
N 1.16057300 -2.06352000 -0.00677700
C 0.80895000 -3.40652100 -0.00597600
C -0.54374900 -3.45025300 -0.00610000
N -0.98060000 -2.13295200 -0.00683600
H 1.55709400 -4.18925300 -0.00429400
C 2.48995500 -1.67066200 -2.51352600
C -2.21410100 -1.62247700 2.53218900
C 2.51094100 -1.57876800 0.00901300
C 3.11620800 -1.31731000 1.24289700
C 4.43222000 -0.85662700 1.23234000
C 5.12984200 -0.65268200 0.04073100
C 4.48718900 -0.93001300 -1.16694800
C 3.17281600 -1.39333700 -1.20927700
C 2.37352200 -1.50553500 2.53029200
H 4.92664500 -0.65194300 2.18391300
C 6.53396500 -0.12865800 0.05776500
H 5.02444400 -0.78187700 -2.10556300
C -2.35819100 -1.73204600 0.01241100
C -3.03359100 -1.58756900 -1.20563500
C -4.36769100 -1.18989600 -1.16125900
C -5.02125100 -0.94155100 0.04862100
C -4.30917800 -1.09701900 1.23723500
C -2.97049800 -1.49223900 1.24565700
C -2.33900100 -1.83146300 -2.51028400
H -4.91394500 -1.06877000 -2.09882900
C -6.46461900 -0.53774200 0.05926800
H -4.80729200 -0.90526400 2.18938200
H 1.61324400 -0.72179000 2.66699100
H 3.05742000 -1.45506400 3.38548500
H 1.84755400 -2.46947100 2.56960300
H 3.18587600 -1.54742300 -3.35126100
H 1.64592400 -0.98406600 -2.67584200
H 2.08349600 -2.69068200 -2.55780600
H 6.54423700 0.97087700 0.05908600
H 7.09744100 -0.45600800 -0.82494500
H 7.07581100 -0.45648000 0.95393300
H -6.66538400 0.25010500 -0.67865000
H -6.77358800 -0.16912300 1.04484900
H -7.11537100 -1.38634700 -0.19620300
H -1.52516800 -0.77601000 2.67253000
H -1.60678800 -2.53741900 2.56709500
H -2.89946700 -1.63479100 3.38769400
H -3.03932100 -1.73589900 -3.34797000
H -1.88985700 -2.83333600 -2.55676500
H -1.52458000 -1.10943700 -2.67023200
Au -0.02660900 0.81797700 -0.01821000
H 1.99309100 3.24342800 -0.04197100
C -0.14281900 2.88283100 -0.03368400
C -1.38338200 3.55080400 -0.03539100
C 1.00199600 3.70355800 -0.04296000
C -1.47913600 4.94205600 -0.04634900
C 0.91867100 5.09574600 -0.05398900
C -0.32529300 5.72228300 -0.05572600
H -0.39500000 6.80991000 -0.06434400
H 1.83019500 5.69484700 -0.06115300
H -2.45978600 5.41973900 -0.04747300
H -2.30748300 2.96734400 -0.02812000

$TS_{1\text{-}11}$

E (M06-SMD/SDD) = -2453.913980 au
H (M06-SMD/SDD) = -2453.291862 au
G (M06-SMD/SDD) = -2453.417229 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.909737 au

C 1.83233400 1.38195700 -0.08428000
H 4.56721200 2.83934200 -1.14660100
N 1.45408900 2.67933400 -0.17686300
C 2.49826000 3.47479800 -0.62501100
C 3.55517700 2.64961900 -0.81237100
N 3.12599500 1.37230500 -0.47914200
H 2.38291900 4.54218100 -0.76370800
C -0.38349600 3.17345600 -2.32830500
C 4.18444900 0.40141500 2.00982800
C 0.13745600 3.14339000 0.15032100
C -0.20328300 3.32106000 1.49491900
C -1.50637400 3.73288000 1.78341200
C -2.44366700 3.96815400 0.77871300
C -2.05653900 3.78648900 -0.55177900
C -0.77086000 3.37098900 -0.89352900
C 0.77677300 3.06168000 2.59829700
H -1.79119500 3.87993100 2.82688300
C -3.84314800 4.39092000 1.10383000
H -2.78150400 3.96449600 -1.34807300
C 3.95747500 0.20218000 -0.50166100
C 4.21537500 -0.41565300 -1.73223300
C 5.03020600 -1.54490800 -1.72718600
C 5.57734000 -2.05411700 -0.54676100
C 5.29539200 -1.40547900 0.65444700
C 4.48533900 -0.26958800 0.70397600
C 3.62103500 0.10477000 -3.00450700
H 5.24165500 -2.04563400 -2.67402900
C 6.46046100 -3.26437000 -0.58559500
H 5.71966200 -1.78951200 1.58388000
H 0.87250600 1.98213300 2.79842700
H 0.45002400 3.54171900 3.52827100
H 1.78244200 3.43129100 2.35534700
H -1.27449800 3.15487800 -2.96810700
H 0.16656100 2.23431700 -2.48539300
H 0.26625800 3.98434700 -2.68799500
H -4.55987800 3.60055300 0.83663500
H -4.13279600 5.28623800 0.53733900
H -3.96312800 4.60860400 2.17194900

H 6.71700500 -3.61008700 0.42296400
H 7.39971400 -3.05373900 -1.11646000
H 5.97553300 -4.09447200 -1.11661400
H 3.16104800 0.17139900 2.34735800
H 4.25992000 1.49578300 1.94016200
H 4.87398400 0.05987300 2.79065700
H 3.93667600 -0.50750800 -3.85708900
H 3.91895800 1.14284100 -3.20714900
H 2.52128600 0.08168500 -2.96431800
C -0.36606600 -1.61405500 1.79163600
C -0.14394800 -2.98818700 1.61772400
C -1.26728400 -1.21709700 2.79294400
Au 0.67938100 -0.18770700 0.71746100
Cl -4.46613400 1.17352700 -1.07088300
C -2.98777800 -1.84013100 -0.99441300
C -3.19885100 -2.36431700 -2.26397000
C -4.08969400 -3.67474400 0.05030300
C -4.32032600 -4.22506000 -1.20693500
C -3.88172900 -3.57205100 -2.35827100
C -3.41832700 -2.46039300 0.17069200
I -2.02494300 0.05480600 -0.81423700
H -4.06521300 -4.00592600 -3.33933300
H -4.84549300 -5.17448600 -1.29324800
H -3.22947500 -2.01857700 1.14817700
H -2.83646800 -1.85234400 -3.15225600
H -4.42611900 -4.18760800 0.94973800
Cl 0.17929900 -1.49645800 -2.29736400
C -0.77826300 -3.92890600 2.43024800
C -1.90073700 -2.15347800 3.61054200
C -1.65848600 -3.51428100 3.42765000
H -1.48907400 -0.15493800 2.93560500
H -2.58957600 -1.81988500 4.38695200
H -2.15860600 -4.24932000 4.05750700
H -0.58725800 -4.99141600 2.27835000
H 0.53413700 -3.33534400 0.83547700

11
E (M06-SMD/SDD) = -2453.965089 au
H (M06-SMD/SDD) = -2453.340923 au
G (M06-SMD/SDD) = -2453.463825 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.954894 au

C 1.31600100 -1.56339700 -0.10300000
H 3.65581400 -3.66193200 0.80733900
N 0.68885400 -2.75603400 -0.21761900
C 1.54115300 -3.79547900 0.12819400
C 2.72195600 -3.23067200 0.47091400
N 2.56486600 -1.86052300 0.32216200
H 1.21801700 -4.82788300 0.09636300
C -1.17711100 -3.46415800 1.84828300
C 4.71034600 -1.67718900 -1.56881400
C -0.69040100 -2.92205700 -0.58119800
C -1.07206500 -2.74814600 -1.91538500
C -2.43086800 -2.86867400 -2.21815900
C -3.38151100 -3.15202500 -1.23867400
C -2.95138000 -3.33774500 0.07790900
C -1.60810500 -3.23841100 0.43114100
C -0.07828400 -2.43996000 -2.99365000
H -2.75112900 -2.73520100 -3.25308600
C -4.83927100 -3.23959300 -1.57362100
H -3.68547900 -3.55590800 0.85615300
C 3.59151800 -0.88439700 0.56012500
C 3.50882700 -0.06334700 1.68780500
C 4.49213900 0.91741600 1.84767400
C 5.52870000 1.07637200 0.93236800
C 5.58609300 0.21439600 -0.16696000
C 4.63057200 -0.77422900 -0.37644000
C 2.42567800 -0.19297700 2.71710900
H 4.44537400 1.56712200 2.72384600
C 6.57495100 2.13326600 1.11598100
H 6.39652500 0.32497300 -0.89014200
H 0.18002900 -1.37028800 -3.01684400
H -0.48565200 -2.70044100 -3.97770800
H 0.86387800 -2.98834800 -2.85628200
H -2.02454000 -3.34428800 2.53350500
H -0.38811900 -2.76660600 2.16193800
H -0.77932200 -4.47977100 1.98883600
H -5.43279100 -2.58039400 -0.92458200
H -5.22364000 -4.25834900 -1.42425000
H -5.03284200 -2.95761400 -2.61571400
H 6.61584000 2.80523600 0.24784400
H 7.57474400 1.68927500 1.22027700
H 6.38220800 2.74319200 2.00660300
H 3.73445100 -1.78349100 -2.06226100
H 5.05091000 -2.68617600 -1.29494800
H 5.41856700 -1.27952100 -2.30503200
H 2.82780700 -0.00375600 3.72029100
H 1.96131100 -1.18740000 2.72289800
H 1.62807300 0.54887600 2.55427200
Au 0.57746900 0.41326100 -0.52550000
H -1.34101700 1.79448200 -2.55136700
C -0.08787500 2.33988300 -0.87505900
C 0.39168600 3.37727600 -0.07777900
C -0.96913100 2.60450900 -1.92037200
C -0.02151500 4.68796200 -0.32669900
C -1.38048800 3.91554300 -2.16256700
C -0.90906500 4.95649600 -1.36540200
C -2.88279900 1.18323800 0.46254900
C -3.51038400 0.44221000 -0.52888600
C -4.56722300 1.03365900 -1.21836000
C -4.97343200 2.32753200 -0.90305300
C -4.32964700 3.04121400 0.10494500
C -3.26713000 2.47200700 0.80389400
H -3.18605200 -0.57075900 -0.76623600
H -5.07217400 0.47231300 -2.00321400
H -5.80014900 2.78321800 -1.44481300
H -4.64877200 4.05210600 0.35225000
H -2.75424200 3.02339600 1.58983400
I -1.24909300 0.29237000 1.51114000
Cl 2.08878900 0.71661000 -2.40351200
Cl -3.32559100 -0.09582800 3.78832600
H -1.23316300 5.97882000 -1.55499900
H -2.07330400 4.12005300 -2.97858800
H 0.35231700 5.49819600 0.29877700
H 1.08631300 3.17313800 0.74063700

12
E (M06-SMD/SDD) = -2453.961547 au
H (M06-SMD/SDD) = -2453.338357 au
G (M06-SMD/SDD) = -2453.456693 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.951550 au

C -0.75688800 -1.64804700 0.05568100
H -2.58156300 -4.26133000 -0.69052500
N 0.15735500 -2.64812400 0.05430800
C -0.43728900 -3.86575700 -0.24474300
C -1.75167000 -3.61523400 -0.43458100
N -1.92964800 -2.25310200 -0.24367600
H 0.14023600 -4.78016300 -0.29112900
C 1.90370900 -2.54704300 -2.19962800
C -3.82279000 -2.50016800 1.90435700
C 1.56624500 -2.51663700 0.30441400
C 2.03280600 -2.51092500 1.62587900
C 3.41126300 -2.42923000 1.82110400
C 4.30806500 -2.38985000 0.75195700
C 3.80030600 -2.42902500 -0.54594800
C 2.42985400 -2.49234600 -0.79735800
C 1.10784700 -2.61812600 2.79906000
H 3.79655600 -2.42667300 2.84287800
C 5.78378800 -2.32893200 1.00654700
H 4.48951600 -2.41168100 -1.39168100
C -3.20880000 -1.61422400 -0.38886800
C -3.51406600 -0.98024400 -1.59649000
C -4.77277800 -0.38679700 -1.71180100

C -5.70403000 -0.42795600 -0.67718100
C -5.36643600 -1.10056200 0.50025600
C -4.12902100 -1.71703900 0.66441300
C -2.55135900 -0.91258100 -2.74133700
H -5.02282800 0.12920700 -2.64086500
C -7.05519900 0.20126900 -0.83465900
H -6.09250500 -1.15357400 1.31378100
H 0.68602800 -1.64163400 3.07664100
H 1.64198700 -3.00683300 3.67419900
H 0.25519500 -3.28081200 2.59572900
H 2.71413900 -2.41114400 -2.92514500
H 1.14796500 -1.76795100 -2.38324700
H 1.42179800 -3.51116100 -2.41654200
H 5.28033100 -0.06016500 -3.48075700
H 6.35626800 -2.31155900 0.07134400
H 6.12056100 -3.19622600 1.59141200
H -7.03099500 1.03071500 -1.55204000
H -7.43324500 0.58502900 0.12133900
H -7.79118400 -0.52806600 -1.20354500
H -2.79193300 -2.34594100 2.24782400
H -3.95509000 -3.57907500 1.73349600
H -4.49736900 -2.21279100 2.71965400
H -1.76911200 -1.68140800 -2.68861500
H -2.07151300 0.07901200 -2.76594500
H -3.08239500 -1.03298600 -3.69438100
Au -0.36664200 0.39170300 0.70023500
H 1.70179100 1.37181600 2.69187100
C 0.11207400 2.24601900 1.50728500
C -0.60502900 3.38788800 1.17679500
C 1.16035400 2.28143300 2.42137000
C -0.25288200 4.59875600 1.77781700
C 1.50995400 3.50105500 3.00491300
C 0.80171100 4.65641200 2.68547600
C 2.73352500 0.96027500 -1.49817300
C 3.38006300 0.48327800 -2.63357100
C 4.76237600 0.30626300 -2.59563100
C 5.47370400 0.59266800 -1.43365400
C 4.80791900 1.06741500 -0.30601400
C 3.42938800 1.26751300 -0.33496000
H 2.82045700 0.25687400 -3.54061700
H 6.05307800 -1.43480400 1.58585200
H 6.55290200 0.45009900 -1.40723700
H 5.36343000 1.30200400 0.60089300
H 2.91352800 1.67523400 0.53423100
I 0.63376400 1.41857700 -1.66253600
Cl -1.43048800 0.00775400 2.80291400
Cl -2.23201300 2.65259600 -2.05173500
H 1.07173200 5.60513600 3.14704000
H 2.33207500 3.53864800 3.71889700
H -0.80751300 5.50136200 1.52321100
H -1.40875600 3.34721100 0.43701700

1P
E (M06-SMD/SDD) = -2211.130332 au
H (M06-SMD/SDD) = -2210.605475 au
G (M06-SMD/SDD) = -2210.708207 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2211.642282 au

C 0.00245400 -1.39464600 0.00110700
H -1.39080200 -4.35474700 0.06680900
N 1.07553800 -2.21477600 -0.04634200
C 0.68115300 -3.54562000 -0.02824600
C -0.67019700 -3.54749400 0.03258400
N -1.06832700 -2.21777000 0.04936300
H 1.40405400 -4.35085600 -0.06164700
C 2.19063400 -1.45981700 -2.58962800
C -2.18664600 -1.46101400 2.59108100
C 2.44261300 -1.77573400 -0.09286300
C 3.18372700 -1.77655500 1.09440000
C 4.50170600 -1.32724800 1.03172500
C 5.07726700 -0.90036700 -0.16627300
C 4.31076800 -0.94965000 -1.33135900
C 2.98656700 -1.38864700 -1.32257300
C 2.59496200 -2.26361300 2.38248600
H 5.09679900 -1.31300000 1.94665800
C 6.48648300 -0.39158700 -0.19719500
H 4.75757000 -0.64677000 -2.28014200
C -2.43657100 -1.78231800 0.09509400
C -3.17719100 -1.78557600 -1.09354900
C -4.49465400 -1.33743700 -1.03261300
C -5.07205800 -0.90958200 0.16524200
C -4.30682600 -0.95588100 1.33016600
C -2.98140000 -1.39415500 1.32305700
C -2.58563800 -2.27302100 -2.38023100
H -5.08929200 -1.32391000 -1.94804600
C -6.48477000 -0.41004400 0.18873600
H -4.75395100 -0.65078700 2.27798500
H 1.58701100 -1.85935300 2.54781600
H 3.22170300 -1.96764700 3.23178400
H 2.51368000 -3.36042200 2.39719900
H 2.84223500 -1.33663000 -3.46245600
H 1.42204400 -0.67378100 -2.63468400
H 1.66678200 -2.42133900 -2.68865800
H 6.51979600 0.68732100 0.01219100
H 6.94934800 -0.54480600 -1.18006900
H 7.11000700 -0.88531700 0.55879800
H -6.55244000 0.60126300 -0.23693900
H -6.87987900 -0.36389700 1.21078400
H -7.14747200 -1.05104700 -0.40745700
H -1.42254300 -0.67066900 2.63719500
H -1.65759500 -2.41959600 2.69072000
H -2.84001600 -1.34150800 3.46310400
H -3.21396800 -1.98292300 -3.23037200
H -2.49808400 -3.36937600 -2.39183900
H -1.57993600 -1.86350600 -2.54658800
Au -0.00097500 0.76785700 0.00028700
H 2.08929100 2.97598000 -0.51402900
C -0.00546600 2.83049200 -0.00025200
C -1.18271700 3.51142600 0.29055200
C 1.16824700 3.51738300 -0.29136400
C -1.18088900 4.90717700 0.29078700
C 1.15904200 4.91311800 -0.29245100
C -0.01274200 5.60678300 -0.00104400
Cl -0.78089600 0.90216300 -2.23837600
Cl 0.77890900 0.90680800 2.23858600
H -0.01559200 6.69590400 -0.00138600
H 2.07555400 5.45653000 -0.52075000
H -2.10023700 5.44590700 0.51878400
H -2.10091900 2.96534000 0.51358300

TS_{1-7}
E (M06-SMD/SDD) = -2453.902857 au
H (M06-SMD/SDD) = -2453.280678 au
G (M06-SMD/SDD) = -2453.404749 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.899859 au

C -1.34597100 1.64986100 0.05074300
H -1.23789800 4.92545900 -0.04376600
N -2.63340300 1.97573700 -0.22417700
C -2.79124700 3.35256900 -0.30585100
C -1.57455400 3.89703100 -0.07359800
N -0.70341000 2.83797100 0.14169600
H -3.75210200 3.80369200 -0.51799000
C -3.71743600 1.49098900 -2.84405300
C 0.00784400 2.61997200 2.91530100
C -3.70812600 1.03244000 -0.35489000
C -4.21259200 0.41500800 0.79709300
C -5.24935700 -0.50499800 0.63820700
C -5.78742600 -0.79987800 -0.61433500
C -5.27039500 -0.14379800 -1.73201900
C -4.23412900 0.78351700 -1.62969700
C -3.67630100 0.71578400 2.16423800
H -5.65399600 -0.99739300 1.52460300
C -6.92319000 -1.76777500 -0.75314400
H -5.68689900 -0.35845300 -2.71791400

C 0.67813600 2.99002400 0.50005500
C 1.61559600 3.25489400 -0.50205900
C 2.94499500 3.43396500 -0.11167400
C 3.34323100 3.33220400 1.21872400
C 2.37421100 3.05375400 2.18682900
C 1.03185900 2.89080100 1.85454000
C 1.23856600 3.30864800 -1.95035700
H 3.68878600 3.66083400 -0.87763000
C 4.77705200 3.51421100 1.61509600
H 2.66978900 2.98564100 3.23592700
H -2.74055900 0.16630300 2.35996800
H -4.39760900 0.41854000 2.93497900
H -3.45369800 1.78378800 2.29567400
H -4.16038000 1.06790100 -3.75332300
H -2.62363300 1.40323400 -2.92567000
H -3.96185200 2.56274000 -2.82483300
H -6.88015000 -2.30394800 -1.70953100
H -7.89165800 -1.24777800 -0.71833900
H -6.92356000 -2.50790900 0.05662100
H 5.21241000 2.57128500 1.97719500
H 4.87740900 4.24184400 2.43206200
H 5.38849500 3.86307100 0.77372000
H -0.35233300 1.57901600 2.86886200
H -0.87455100 3.26709600 2.80959900
H 0.43114100 2.78130500 3.91368800
H 1.22115400 2.29464500 -2.38218300
H 1.96237300 3.90467200 -2.52047100
H 0.23920500 3.73108300 -2.11407900
C -0.04452400 -1.84326200 1.82668300
C 1.04381200 -1.73421700 2.70360300
C -0.78947800 -3.02993400 1.83664700
Au -0.58379900 -0.21605200 0.67104800
Cl 3.04023100 -4.03172500 -1.61430000
C 2.84580000 -0.66347000 -1.14098200
C 3.11122100 0.11922800 -2.25803400
C 4.74166700 0.18432100 0.02564800
C 5.04011000 0.97517400 -1.08218400
C 4.22834500 0.94867000 -2.21435700
C 3.62705300 -0.64829200 0.01049500
I 1.25021300 -2.06070100 -1.22773000
H 4.46150800 1.57616500 -3.07309900
H 5.91515300 1.62326400 -1.06093500
H 3.38478300 -1.28428900 0.86074800
H 2.45557900 0.09082600 -3.12692900
H 5.37989800 0.20762700 0.90721700
Cl -0.38555900 -0.01953900 -2.88800100
C 1.38113500 -2.78187200 3.56215700
C -0.45560500 -4.07708500 2.69689000
C 0.63345100 -3.95731900 3.55779900
H -1.63895600 -3.14847800 1.15980500
H -1.04784800 -4.99241000 2.68985700
H 0.89948400 -4.77859700 4.22214900
H 2.23137700 -2.67768500 4.23659500
H 1.64368700 -0.81930500 2.71973100

7

E (M06-SMD/SDD) = -2453.969924 au
H (M06-SMD/SDD) = -2453.347248 au
G (M06-SMD/SDD) = -2453.468215 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.957631 au

C -1.78531500 1.26132900 0.06721100
H -3.13702200 4.08789800 0.96819400
N -3.07731900 0.90529600 0.21365300
C -3.83277700 2.00350800 0.59962500
C -2.98181900 3.05079600 0.69914500
N -1.72350300 2.57547600 0.36861500
H -4.89992300 1.92002300 0.76051300
C -3.72588000 -0.01402300 -2.44517000
C -0.34097300 2.81445800 2.87016700
C -3.62166300 -0.41662600 0.05190100
C -3.85592400 -1.17601700 1.20383000
C -4.37570700 -2.45829800 1.03278400
C -4.66589600 -2.97106800 -0.23220500
C -4.43604500 -2.16640900 -1.34995100
C -3.92318400 -0.87432500 -1.23552900
C -3.55503800 -0.64292700 2.57099200
H -4.55272000 -3.07522400 1.91586300
C -5.24968400 -4.34206100 -0.38878600
H -4.67737900 -2.54889600 -2.34336700
C -0.51565200 3.35451000 0.40448600
C -0.13153500 4.06541500 -0.73725200
C 1.09498900 4.72798700 -0.69314900
C 1.90076900 4.71324200 0.44673700
C 1.43268200 4.06147200 1.58993800
C 0.21188900 3.38782000 1.60025500
C -1.02898500 4.18566100 -1.92973100
H 1.42612000 5.27736100 -1.57615900
C 3.23746200 5.38980500 0.44430600
H 2.02464600 4.09308500 2.50650700
H -2.53439600 -0.23779600 2.63412900
H -3.64970800 -1.43410800 3.32398900
H -4.24302100 0.16733200 2.85192600
H -4.25774600 -0.43370100 -3.30678400
H -2.66410400 0.07323300 -2.71961500
H -4.09428900 1.00905000 -2.28237400
H -4.88271600 -4.83451900 -1.29799400
H -6.34544700 -4.29567800 -0.46806700
H -5.01229700 -4.98186900 0.46995700
H 3.53164200 5.70717700 1.45241100
H 3.24233700 6.26977500 -0.21110700
H 4.01939400 4.71024300 0.07572100
H -0.86991800 1.86500600 2.71886500
H -1.06330500 3.51401500 3.31727300
H 0.45296900 2.64911800 3.60857400
H -0.45591100 4.45409500 -2.82480600
H -1.77589900 4.97705900 -1.76448300
H -1.57081600 3.25717000 -2.14466100
C -0.15020200 -0.89618800 1.21901800
C 0.53110000 -0.39166000 2.31991200
C -0.77817100 -2.13741700 1.26464400
Au -0.17569100 0.10612000 -0.57626400
Cl 4.64957500 -3.00643000 -2.44029700
C 3.07013200 -1.41355900 0.49612600
C 3.71737000 -0.26652800 0.93764600
C 3.74437900 -2.62975000 2.43390700
C 4.39616100 -1.49264700 2.90514000
C 4.38470700 -0.31640800 2.16017700
C 3.07235600 -2.60141600 1.21387300
I 2.03604200 -1.32822900 -1.36803400
H 4.90036200 0.57051600 2.52447600
H 4.92113600 -1.52521100 3.85814700
H 2.55839200 -3.48436600 0.83814100
H 3.70177400 0.64813400 0.34642600
H 3.75645600 -3.55028800 3.01496400
Cl -0.14964600 0.99652500 -2.88146200
C 0.56705600 -1.13931000 3.49869300
C -0.73299600 -2.87723800 2.44740300
C -0.06854200 -2.37643300 3.56444400
H -1.29573200 -2.53711600 0.39191500
H -1.22513300 -3.84876800 2.48804900
H -0.03805000 -2.95641500 4.48549700
H 1.10521200 -0.74932000 4.36232700
H 1.05104200 0.56446600 2.26671500

10

E (M06-SMD/SDD) = -2453.980886 au
H (M06-SMD/SDD) = -2453.356558 au
G (M06-SMD/SDD) = -2453.481694 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.970314 au

C -0.51280300 1.85237600 -0.14575200
H 0.33557600 4.98422600 0.11097400
N -1.71887900 2.44361000 -0.04648500

C -1.56168700 3.81685600 0.06765700
C -0.23136700 4.06428300 0.04684500
N 0.40448900 2.83933400 -0.08305700
H -2.41859400 4.47300000 0.14898000
C -3.00285100 1.57365600 -2.50946500
C 1.64934200 2.61868100 2.49079300
C -2.98817400 1.76629600 0.02198200
C -3.56216800 1.58765200 1.28648600
C -4.77038400 0.89560900 1.35114000
C -5.39354000 0.39766200 0.20584400
C -4.80219000 0.63632900 -1.03512400
C -3.59784300 1.32768200 -1.15833400
C -2.90558500 2.10526000 2.53021400
H -5.22904800 0.72945600 2.32773000
C -6.66591000 -0.38766800 0.29468600
H -5.29012000 0.27035500 -1.94040000
C 1.83158200 2.65581900 -0.03677300
C 2.57059600 2.73123300 -1.22061000
C 3.94104000 2.47555700 -1.13473000
C 4.56392300 2.19627900 0.08081500
C 3.79493200 2.20760500 1.24785800
C 2.42595400 2.46114600 1.21846600
C 1.95181400 3.15931800 -2.51471300
H 4.53807900 2.50930500 -2.04777400
C 6.03726300 1.93328700 0.15152100
H 4.27894000 2.03307400 2.21104800
H -1.85626600 1.78165700 2.60399500
H -3.43027600 1.74159500 3.42151200
H -2.90904100 3.20408500 2.56731700
H -3.78949200 1.60896500 -3.27254400
H -2.30675000 0.76984200 -2.79044300
H -2.43824800 2.51508600 -2.55395100
H -6.48299900 -1.44794300 0.06901800
H -7.40873500 -0.03169500 -0.43146800
H -7.10933200 -0.33087600 1.29606400
H 6.56926800 2.78668200 0.59605300
H 6.46615500 1.75822500 -0.84274000
H 6.25799400 1.06097700 0.78155300
H 0.63536600 2.20370400 2.43333600
H 1.54489700 3.68583300 2.73883000
H 2.16610800 2.13709900 3.32986500
H 1.91736700 4.25817800 -2.57006300
H 0.92925000 2.78559500 -2.63815400
H 2.54336500 2.80569100 -3.36739200
C -0.51666300 -0.54836500 1.51163200
C 0.51708200 -0.44565300 2.43342900
C -1.77403500 -1.01820500 1.87290800
Au -0.15347500 -0.14605300 -0.47442400
Cl -2.67494700 -3.00108400 -1.35132200
C 2.39278700 -2.47638200 -0.01626700
C 3.24433200 -1.67520400 -0.77132800
C 4.04824500 -2.68612900 1.70721000
C 4.91121100 -1.88309900 0.96657100
C 4.51056700 -1.37921800 -0.26913000
C 2.77641600 -2.98491500 1.21989000
I 0.38572400 -2.84904100 -0.70893400
H 5.18532500 -0.75221100 -0.85187300
H 5.90325700 -1.65242300 1.35220300
H 2.08976500 -3.59549200 1.80525400
H 2.92541400 -1.28199300 -1.73648600
H 4.36007800 -3.08186800 2.67255500
Cl 0.32483500 0.14487000 -2.88138800
C 0.27317800 -0.79732500 3.76305000
C -2.00367200 -1.36644000 3.20418000
C -0.98634100 -1.24731400 4.14895400
H -2.56008600 -1.14103400 1.12710100
H -2.98709800 -1.73478200 3.49560300
H -1.17316800 -1.51720400 5.18725000
H 1.07792100 -0.71622300 4.49340100
H 1.50862100 -0.10650100 2.13005200

9
E (M06-SMD/SDD) = -2211.144490 au
H (M06-SMD/SDD) = -2210.618502 au
G (M06-SMD/SDD) = -2210.723389 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2211.655142 au

C -0.15099300 -0.72010200 -0.78761600
H -1.65829000 -1.73528400 -3.49342100
N 0.89389400 -1.11795300 -1.54455400
C 0.44114700 -1.60277400 -2.76364700
C -0.90545100 -1.48740800 -2.75628900
N -1.25748300 -0.94061800 -1.53046800
H 1.13283400 -1.97717100 -3.50734800
C 2.20336100 1.18415500 -2.61083400
C -3.20248600 -2.82483000 -0.36287100
C 2.29131200 -0.94277100 -1.23928600
C 2.96296500 -1.91435900 -0.49015000
C 4.31264700 -1.69045000 -0.21497200
C 4.98416700 -0.55918200 -0.68031400
C 4.28284100 0.35832500 -1.46413000
C 2.93228300 0.18751400 -1.76267900
C 2.28265900 -3.16349100 -0.02523700
H 4.85797000 -2.43430300 0.36857500
C 6.42579700 -0.33206300 -0.34123900
H 4.79921500 1.23817400 -1.85279500
C -2.59546500 -0.50378000 -1.22038900
C -2.94976000 0.79806900 -1.61174300
C -4.22719300 1.24570100 -1.28970800
C -5.15069300 0.42351800 -0.63731600
C -4.78343500 -0.88759700 -0.34794100
C -3.51001100 -1.38580100 -0.63918200
C -2.02967200 1.65124600 -2.43179700
H -4.51890500 2.25767800 -1.57684500
C -6.50811500 0.94274600 -0.27443000
H -5.51108100 -1.55907000 0.11195400
H 1.57172000 -2.96502100 0.78986000
H 3.01870100 -3.88873500 0.34039200
H 1.70885300 -3.63795300 -0.83385300
H 2.85580900 2.02921800 -2.85991100
H 1.31988500 1.58514100 -2.09299200
H 1.85318700 0.74203600 -3.55447700
H 6.52428000 0.22559400 0.60127200
H 6.93547900 0.25205900 -1.11759600
H 6.96344200 -1.27970700 -0.21219600
H -6.47174800 1.51033900 0.66643700
H -7.22836000 0.12728400 -0.13560300
H -6.89847200 1.62185600 -1.04327600
H -3.02954800 -2.99355600 0.70720900
H -2.30861400 -3.17683400 -0.89046900
H -4.04996400 -3.45291400 -0.66666600
H -2.34664700 2.70095000 -2.41004600
H -2.03904300 1.32606400 -3.48309800
H -0.98725600 1.60742900 -2.09240600
Au -0.08006200 -0.08210900 1.16370000
H 2.61892300 1.30253900 0.96419400
C 0.54503200 1.78533400 0.58544900
C -0.37539400 2.76024500 0.22181800
C 1.90603500 2.06531000 0.64989000
C 0.08454700 4.03356800 -0.12090700
C 2.35371000 3.34113700 0.30713500
C 1.44594300 4.32164200 -0.08649800
Cl 0.00330500 0.73239100 3.40708000
Cl -0.69629000 -2.33549600 1.97260600
H 1.79971200 5.31511300 -0.35793800
H 3.42016900 3.56211100 0.34865800
H -0.63256100 4.80001700 -0.41367400
H -1.44361900 2.54294900 0.20356100

TS_{1-19}

E (M06-SMD/SDD) = -2453.914548 au
H (M06-SMD/SDD) = -2453.291871 au
G (M06-SMD/SDD) = -2453.415215 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.916013 au

C 1.25125500 -1.63816600 -0.40613300
H 3.59308200 -3.92206100 -0.16374500
N 0.55581400 -2.79082600 -0.56733000
C 1.39203700 -3.89636700 -0.49510700
C 2.64111900 -3.42050400 -0.28233200
N 2.53358000 -2.03892700 -0.23040500
H 1.01235600 -4.90444200 -0.60240200
C -1.14882100 -3.44405700 1.63848500
C 3.63636700 -0.74537800 -2.54836700
C -0.85714900 -2.85957600 -0.80303000
C -1.34110200 -2.61130700 -2.09117000
C -2.72285300 -2.67666600 -2.28648700
C -3.59913000 -2.97987300 -1.24517600
C -3.07017200 -3.23159400 0.02396800
C -1.70002400 -3.17932000 0.27053400
C -0.42243500 -2.26130500 -3.22190300
H -3.12223900 -2.48243700 -3.28377600
C -5.08171500 -3.01111200 -1.46095500
H -3.74648100 -3.46596000 0.84845000
C 3.63747000 -1.13967500 -0.04893500
C 4.12472700 -0.92839800 1.24462800
C 5.18646700 -0.03771500 1.39750200
C 5.75309000 0.62423600 0.30769200
C 5.24393100 0.37147400 -0.96731700
C 4.18146300 -0.50717700 -1.17287400
C 3.52877800 -1.62992300 2.42570000
H 5.57851100 0.14661400 2.39940100
C 6.87300000 1.60104400 0.50185300
H 5.68695900 0.87250600 -1.83016100
H -0.06992000 -1.22024300 -3.13947800
H -0.93451800 -2.36369300 -4.18583300
H 0.47280000 -2.89853000 -3.23895300
H -1.95749800 -3.54890300 2.37100800
H -0.48668400 -2.63214100 1.97518400
H -0.55298500 -4.36746400 1.66624300
H -5.58704200 -2.27631400 -0.81799000
H -5.50315100 -3.99394600 -1.20874600
H -5.34471500 -2.78718300 -2.50198600
H 6.48678500 2.62422300 0.61490200
H 7.55560400 1.60780400 -0.35749500
H 7.45546500 1.37333800 1.40331600
H 2.68206900 -0.21320700 -2.69145100
H 3.44072400 -1.81007900 -2.73901400
H 4.33477700 -0.38283300 -3.31173700
H 3.90924000 -1.20443600 3.36159200
H 3.76602400 -2.70378200 2.42551100
H 2.43391100 -1.53840700 2.43726400
Au 0.60429400 0.35366600 -0.64114400
H -0.98936900 1.70294600 -2.92915100
C 0.09404200 2.29639400 -1.14621800
C 0.50179400 3.41720000 -0.40321500
C -0.63498400 2.54234900 -2.32413700
C 0.19955300 4.71625700 -0.81416300
C -0.93745300 3.83820100 -2.74288100
C -0.52246900 4.93157000 -1.98576200
C -2.66503700 1.34091800 0.51087800
C -3.08305600 0.46765400 -0.48567500
C -3.97388400 0.94924800 -1.43822100
C -4.40455200 2.27552600 -1.38931200
C -3.95998700 3.12807900 -0.38231600
C -3.07644300 2.66465400 0.59074900
H -2.73707200 -0.56459200 -0.51557200
H -4.32810800 0.28213200 -2.22341300
H -5.09388400 2.64722100 -2.14509700
H -4.29744500 4.16209500 -0.34830200
H -2.71702500 3.32077000 1.38107400
I -1.36589700 0.60455300 2.04513800
Cl 1.31966800 1.40417900 2.58129600
Cl -3.52568500 -0.47505900 3.19694500
H -0.76176200 5.94525500 -2.30643500
H -1.50270900 3.99372600 -3.66264600
H 0.52992700 5.56479900 -0.21383800
H 1.06128100 3.26938200 0.52357100

19
E (M06-SMD/SDD) = -2453.933685 au
H (M06-SMD/SDD) = -2453.310002 au
G (M06-SMD/SDD) = -2453.436783 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.928479 au

C 1.12667000 -1.79600500 -0.36835700
H 3.38635700 -4.16287700 -0.26360400
N 0.36920200 -2.91274000 -0.40550800
C 1.16523000 -4.04876900 -0.36738300
C 2.44995100 -3.62200000 -0.30677600
N 2.40336800 -2.23788200 -0.30773200
H 0.73533300 -5.04208000 -0.38879500
C -1.18980700 -2.97016100 2.01401300
C 3.18784700 -0.81833200 -2.69309700
C -1.06282100 -2.92271700 -0.51235900
C -1.63291200 -2.91137000 -1.78956700
C -3.02589900 -2.92836100 -1.87605700
C -3.83035500 -2.93711800 -0.73599100
C -3.21652800 -2.94728400 0.51907900
C -1.82908900 -2.94800200 0.65998700
C -0.78340900 -2.84894500 -3.02246200
H -3.49300600 -2.92119200 -2.86288900
C -5.32284900 -2.88021900 -0.84902100
H -3.83620300 -2.95571900 1.41771500
C 3.52338100 -1.34245100 -0.23439800
C 4.15061600 -1.15881600 1.00519500
C 5.18188700 -0.22476200 1.07056700
C 5.58618100 0.50774300 -0.04845800
C 4.93410100 0.28991700 -1.26202800
C 3.89447600 -0.63352200 -1.38270200
C 3.72045000 -1.92510000 2.21800300
H 5.68064700 -0.05839000 2.02708400
C 6.71676200 1.48566400 0.05442800
H 5.24183200 0.85329000 -2.14483700
H -0.30877200 -1.86119600 -3.12952100
H -1.38709700 -3.02358700 -3.92039800
H 0.02740900 -3.59035500 -3.00756900
H -1.95395400 -2.98916900 2.80013700
H -0.55703500 -2.08657300 2.19519400
H -0.54663000 -3.85239000 2.14445100
H -5.68654800 -1.86026200 -0.65388900
H -5.80944600 -3.53672100 -0.11628300
H -5.66472100 -3.16688400 -1.85116200
H 6.67407000 2.04976000 0.99494700
H 6.70903000 2.20121000 -0.77668300
H 7.68736300 0.96922400 0.03505600
H 2.24078300 -0.25372100 -2.71781400
H 2.93709600 -1.87030800 -2.88730900
H 3.80633000 -0.45321900 -3.52157400
H 4.23740000 -1.55427500 3.11059700
H 3.94323400 -2.99740700 2.12421100
H 2.63925900 -1.82634800 2.39709000
Au 0.66719600 0.26734600 -0.40473600
H -0.89191900 2.30034500 -2.21674700
C 0.55410200 2.31494800 -0.60057800
C 1.45150900 3.08273000 0.14876400
C -0.14965100 2.88177800 -1.66639000
C 1.70442200 4.40173900 -0.22789700
C 0.10886800 4.20109800 -2.03367800
C 1.03274400 4.95814600 -1.31444200
C -2.79268600 1.50574100 -0.17911700
C -3.21963100 0.54321100 -1.08542100
C -4.09489200 0.92096100 -2.10134300
C -4.53116000 2.24085500 -2.19032000
C -4.09867100 3.18957800 -1.26529900
C -3.21856800 2.82759000 -0.24863000

H -2.87605900 -0.48755500 -1.00961700
H -4.43655700 0.17501900 -2.81859900
H -5.21493800 2.53335900 -2.98518500
H -4.44334800 4.21972100 -1.33585600
H -2.86104300 3.56572100 0.46857700
I -1.40701500 0.93432600 1.35691200
Cl 0.73940000 0.18650000 3.43146300
Cl -3.54153700 0.86552600 3.10317400
H 1.21684600 5.99486900 -1.59231200
H -0.42122100 4.64056300 -2.87785900
H 2.41550200 4.99827300 0.34200100
H 1.96008900 2.65264100 1.01353300

TS_{19-7}

E (M06-SMD/SDD) = -2453.922916 au
H (M06-SMD/SDD) = -2453.302607 au
G (M06-SMD/SDD) = -2453.426115 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.915388 au

C -2.28997000 0.83194000 -0.21046900
H -5.55756600 0.72873300 -0.25542700
N -2.61156500 2.13668000 -0.34454000
C -3.98698700 2.30272400 -0.37781100
C -4.52869000 1.06440600 -0.27016700
N -3.47037100 0.17532400 -0.17041500
H -4.44007600 3.28119100 -0.47358300
C -1.95122800 3.61658600 2.02145900
C -2.98080700 -1.41888000 -2.52604300
C -1.63570900 3.18482100 -0.44818200
C -1.03857300 3.42190400 -1.69080900
C -0.06697400 4.42088200 -1.75918800
C 0.29896000 5.16660200 -0.63778800
C -0.32774600 4.89629700 0.58053800
C -1.30120000 3.90600600 0.70400500
C -1.41248600 2.62691900 -2.90530500
H 0.41102800 4.62597200 -2.71900800
C 1.32031900 6.25838000 -0.74100300
H -0.04729000 5.47038300 1.46552500
C -3.58473500 -1.25275100 -0.06880100
C -3.92321500 -1.81018400 1.17151500
C -3.99778900 -3.19861500 1.25308300
C -3.74893800 -4.01725600 0.14854000
C -3.42436700 -3.41764000 -1.06754400
C -3.33816600 -2.03077900 -1.20471500
C -4.18965400 -0.94758700 2.36621300
H -4.25297400 -3.65598500 2.21086900
C -3.85645500 -5.50685900 0.27265800
H -3.23744200 -4.04391200 -1.94189200
H -0.98436000 1.61274900 -2.87032600
H -1.04072000 3.11071000 -3.81611200
H -2.50067800 2.50794800 -3.00170000
H -1.57057500 4.29441300 2.79427700
H -1.75229200 2.58520100 2.35656200
H -3.04232900 3.74006500 1.97520900
H 1.93875600 6.31655800 0.16363900
H 0.83792100 7.23897200 -0.86345900
H 1.98336300 6.11177300 -1.60247300
H -3.43980900 -6.01705000 -0.60420600
H -4.90530500 -5.82101100 0.37228100
H -3.32967000 -5.87246200 1.16391700
H -1.91960300 -1.12467000 -2.55860800
H -3.57015000 -0.51620500 -2.73888800
H -3.14641600 -2.13434000 -3.34021200
H -4.35940000 -1.56500500 3.25587900
H -5.07831000 -0.31633400 2.22393800
H -3.33942500 -0.28104200 2.57859900
C 1.07861300 -1.09160600 -1.33203200
C 0.95659800 -2.47984800 -1.37010000
C 1.80762200 -0.39248300 -2.29327100
Au -0.37366900 -0.03172000 -0.25178000
Cl 3.59545500 -0.46358200 3.60023200
C 3.76053600 -0.74027600 0.19785400
C 4.20956500 -2.03218800 -0.04756500
C 5.64276800 0.20113600 -0.93664400
C 6.10614800 -1.08494000 -1.20379200
C 5.39622000 -2.19725500 -0.75805100
C 4.46026100 0.38430400 -0.22460700
I 1.95645200 -0.45503000 1.33234100
H 5.76446900 -3.20125700 -0.96195900
H 7.03206800 -1.22186400 -1.75960900
H 4.08788000 1.38511900 -0.00902300
H 3.64440700 -2.89503900 0.30213500
H 6.20389600 1.06889900 -1.27918100
Cl -0.59578700 0.09874400 2.97880200
C 1.52806000 -3.17381200 -2.43756800
C 2.37648600 -1.10067000 -3.35021100
C 2.24155700 -2.48722000 -3.41740700
H 1.92958600 0.68962600 -2.22414200
H 2.93559600 -0.56557600 -4.11675900
H 2.70693600 -3.03688700 -4.23391100
H 1.42730100 -4.25713500 -2.48881800
H 0.41811100 -3.01421200 -0.58660100

TS_{10-9}

E (M06-SMD/SDD) = -2453.973293 au
H (M06-SMD/SDD) = -2453.348875 au
G (M06-SMD/SDD) = -2453.473072 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.958020 au

C 1.17191300 1.54958500 0.53924300
H 3.71843200 3.05514500 1.89349500
N 0.58326700 2.64562800 1.07038100
C 1.53025100 3.43088800 1.70554000
C 2.71961600 2.80133500 1.56234000
N 2.47947400 1.63840100 0.84407600
H 1.25613300 4.35828800 2.19214500
C -0.55116400 4.46003600 -0.89574700
C 3.12878900 -0.19851800 2.93535000
C -0.83573200 2.88327500 1.06104100
C -1.59982900 2.30932800 2.08237200
C -2.98835400 2.35587600 1.94803700
C -3.59669000 2.99444800 0.86639000
C -2.78956100 3.66595600 -0.05600000
C -1.39853300 3.64238000 0.02844300
C -0.95820700 1.74480400 3.31401700
H -3.60804200 1.89141900 2.71756700
C -5.08608800 2.99288300 0.70390600
H -3.25713100 4.22751800 -0.86698500
C 3.48732700 0.64630900 0.57701600
C 4.13225300 0.65289700 -0.66326600
C 5.09538000 -0.32968400 -0.88490900
C 5.41376300 -1.28206900 0.08485800
C 4.76562400 -1.22536600 1.31967900
C 3.79820700 -0.26034800 1.59608300
C 3.79864600 1.66499400 -1.71430900
H 5.60827100 -0.35412900 -1.84786400
C 6.41991300 -2.35317600 -0.20653800
H 5.01680300 -1.95424200 2.09258700
H -0.09465000 1.10357600 3.09583900
H -1.67721200 1.16059300 3.90107600
H -0.59423200 2.56101800 3.95602300
H -1.12080600 4.76573500 -1.78095200
H 0.33783400 3.91936800 -1.23975700
H -0.21129500 5.37423300 -0.38558100
H -5.37879100 2.48155200 -0.22418600
H -5.48363600 4.01500300 0.64069900
H -5.58386600 2.48531500 1.53885600
H 6.83149100 -2.78478900 0.71409700
H 7.25218700 -1.97014000 -0.81084700
H 5.96092600 -3.17304500 -0.77741300
H 2.03261600 -0.19342800 2.84366500
H 3.41193100 0.70826100 3.48926100
H 3.40874300 -1.06350800 3.54805000
H 3.77449500 2.68609200 -1.30698700

H 2.80944200 1.47424100 -2.15833400
H 4.53576800 1.63781200 -2.52502900
C 0.19831200 -1.15342300 0.92580000
C 1.19435200 -2.12423400 0.93476400
C -0.80585600 -1.13389200 1.88575500
Au 0.17930300 0.17472800 -0.64361400
Cl 0.08825800 1.64220100 -2.64021000
C -2.92651000 -2.25658500 -0.34167600
C -2.34833800 -3.51080600 -0.18444000
C -4.44438900 -2.65867100 1.46178100
C -3.88095300 -3.91994700 1.63861500
C -2.83442200 -4.34205900 0.82220100
C -3.96538000 -1.80809400 0.46709400
I -2.15682000 -0.96163400 -1.85033800
H -2.38813300 -5.32480800 0.96472900
H -4.25813800 -4.57730400 2.42007400
H -4.38684600 -0.81222700 0.33439000
H -1.52418400 -3.82838400 -0.82165400
H -5.26067300 -2.32741000 2.10169200
Cl 1.57717500 -1.97829300 -2.47447900
C 1.17496100 -3.09794500 1.93408000
C -0.80757900 -2.10927400 2.88504000
C 0.18394500 -3.08608200 2.91258700
H -1.59404200 -0.38148900 1.86206100
H -1.59274700 -2.09731400 3.64096500
H 0.18056500 -3.84336800 3.69535500
H 1.95031900 -3.86394000 1.94345100
H 1.94941100 -2.13607900 0.15058500

$TS_{TS14-2P}$

E (M06-SMD/SDD) = -3062.224277 au
H (M06-SMD/SDD) = -3061.766697 au
G (M06-SMD/SDD) = -3061.880844 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.367529 au

Au 0.23509800 -0.94123400 -0.14987600
P 2.19122600 0.39382800 0.17781000
C -0.87398800 0.78229300 -0.10988200
C -1.56211000 1.13505000 1.04098300
C -0.97333900 1.63189700 -1.20260200
C -2.38307500 2.25342600 1.09409200
C -1.76974300 2.76977800 -1.16852900
C -2.48817600 3.07309200 -0.02051400
F -3.25899500 4.15078900 0.01713000
C -3.59608100 -1.25161000 0.14076800
C -3.77915900 -0.72059100 -1.13028000
C -4.79402700 0.21885400 -1.30591700
C -5.59581800 0.60271500 -0.23327400
C -5.39164000 0.05000400 1.02863900
C -4.37955100 -0.88736500 1.22963000
H -3.11987700 -1.00815500 -1.95369100
H -4.95118000 0.65400600 -2.29180000
H -6.38458500 1.33827500 -0.38155100
H -6.01680200 0.34969800 1.86804100
H -4.20431200 -1.31470600 2.21532400
I -2.00240500 -2.64938600 0.43777900
Cl 1.56070900 -2.96225600 -0.00182500
Cl -0.82957300 -1.70719000 -3.02917500
C 3.46384000 -0.27372500 -0.91528600
C 4.74883800 -0.54354800 -0.43726800
C 3.13564600 -0.52361000 -2.25391800
C 5.71268900 -1.03648700 -1.31092600
H 4.99984000 -0.37855900 0.60932100
C 4.10779600 -1.01189400 -3.11680600
H 2.11793100 -0.36136400 -2.61371700
C 5.39492800 -1.26575700 -2.64615800
H 6.71420200 -1.24783000 -0.94127800
H 3.85392400 -1.20823900 -4.15638600
H 6.15175600 -1.65625200 -3.32411000
C 1.98669200 2.15808900 -0.16371800
C 1.37516800 2.96455800 0.80716300
C 2.36125400 2.70515600 -1.39420000
C 1.14452300 4.30720300 0.54380300
H 1.07619500 2.54175000 1.76690300
C 2.12162500 4.05125400 -1.65095400
H 2.83512300 2.08755800 -2.15546700
C 1.51156500 4.84935200 -0.68806900
H 0.67199500 4.93168300 1.29976300
H 2.41495700 4.47546600 -2.60899600
H 1.32289000 5.90121900 -0.89497800
C 2.67284000 0.26372500 1.91794300
C 3.70035100 1.09921400 2.38143100
C 2.04598800 -0.62536500 2.79565300
C 4.10695300 1.02132900 3.70730400
H 4.18157700 1.80935700 1.70858700
C 2.45399500 -0.68849700 4.12405400
H 1.23517400 -1.26628600 2.44861200
C 3.48462400 0.12864900 4.57743800
H 4.90859200 1.66554400 4.06288400
H 1.96075900 -1.37942800 4.80469200
H 3.80199300 0.07503600 5.61722900
F -1.84143800 3.57530000 -2.22210400
F -0.27896300 1.40918900 -2.31353100
F -3.05784100 2.54639900 2.20036100
F -1.44818700 0.40901200 2.15978500

TS_{12-1P}

E (M06-SMD/SDD) = -2453.960194 au
H (M06-SMD/SDD) = -2453.337156 au
G (M06-SMD/SDD) = -2453.456204 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.942763 au

C 1.44188300 1.32572300 0.24088300
H 4.04107100 3.32508700 0.25483800
N 0.87490900 2.55075700 0.42391100
C 1.83699800 3.54945700 0.45757200
C 3.03040600 2.93955000 0.29698700
N 2.77166700 1.58251600 0.16603500
H 1.56558300 4.58935000 0.58792900
C -0.30666500 3.36761300 -2.03555000
C 4.35391500 0.57719000 2.35513200
C -0.52806300 2.86718000 0.43592800
C -1.24377500 2.84682500 1.63742900
C -2.60296700 3.16834300 1.58488300
C -3.23131500 3.53082000 0.39498100
C -2.46633100 3.58713000 -0.77292000
C -1.11030500 3.27136600 -0.77464100
C -0.60137100 2.52059500 2.94930300
H -3.18074300 3.14775800 2.51093100
C -4.69299300 3.86174800 0.36426500
H -2.94128100 3.88049200 -1.71147500
C 3.83626900 0.65680200 -0.11839000
C 4.12446200 0.37499900 -1.45712400
C 5.20450700 -0.46291600 -1.72352900
C 5.96824300 -1.02393500 -0.69966200
C 5.65833400 -0.69644400 0.62048500
C 4.60449300 0.16083000 0.93853000
C 3.29245900 0.93159100 -2.56959300
H 5.44609500 -0.69661500 -2.76227800
C 7.09161300 -1.96510400 -1.01314900
H 6.26563000 -1.10470600 1.43053200
H -0.58208200 1.43767800 3.13403100
H -1.15341500 2.99031900 3.77222700
H 0.44142500 2.86180000 2.99477200
H -0.96450000 3.45726100 -2.90831900
H 0.33928500 2.49093100 -2.18582900
H 0.35232900 4.24826700 -2.02522800
H -6.03421200 0.32064300 0.57698300
H -5.17514900 3.45711000 -0.53597700
H -4.85657800 4.94895600 0.35305300
H 7.58039000 -1.70833100 -1.96178800
H 6.72360500 -2.99675800 -1.10968100
H 7.85231000 -1.96515300 -0.22240100
H 3.29303300 0.49515800 2.62751500

H 4.65240500 1.62323000 2.52072500
H 4.93185200 -0.04413400 3.04928200
H 3.08462900 2.00365300 -2.44195200
H 2.32663000 0.40572100 -2.62006600
H 3.79272900 0.79548300 -3.53579200
Au 0.36120100 -0.57438400 0.45189100
H -2.21271100 -0.81192400 1.93310300
C -0.89039700 -2.17856700 0.89377700
C -0.64229800 -3.49197000 0.51858300
C -2.02953500 -1.84302200 1.62310000
C -1.56605300 -4.48143400 0.86869700
C -2.94503600 -2.83805800 1.96371900
C -2.71278900 -4.15902700 1.58705600
C -3.36313100 -0.79621600 -1.16652900
C -4.15189800 0.07949200 -0.42899500
C -5.40441400 -0.35401600 -0.00137600
C -5.84421000 -1.63928300 -0.30903800
C -5.03344000 -2.50021800 -1.04453700
C -3.77791100 -2.08427200 -1.48383600
H -3.79235400 1.07832200 -0.18223500
H -5.21447500 3.46064000 1.24248400
H -6.82314400 -1.97364300 0.02978000
H -5.37277300 -3.50792900 -1.27838300
H -3.13323800 -2.75679600 -2.04672400
I -1.44591400 -0.13365000 -1.82501000
Cl 0.91276600 -0.68415800 2.77227200
Cl 1.90573600 -2.12623000 -1.14286400
H -3.42558200 -4.93697800 1.85750900
H -3.83798400 -2.57307500 2.52956200
H -1.37645000 -5.51282500 0.57196200
H 0.25353500 -3.74211500 -0.04713300

TS_{16-17}

E (M06-SMD/SDD) = -3062.207940 au
H (M06-SMD/SDD) = -3061.750632 au
G (M06-SMD/SDD) = -3061.867101 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -3349.349811 au

Au 0.01480300 -0.87808500 0.00983800
P 2.29406100 -0.01351600 -0.23321200
C -2.12237400 2.36717300 0.57663200
C -1.62374400 3.28729900 -0.33828900
C -4.35173800 2.67969500 -0.22192000
C -3.87613300 3.59771500 -1.15461200
C -2.51816200 3.90231900 -1.21058900
C -3.47315700 2.04966600 0.65796000
I -0.74700000 1.35546300 1.85492600
H -2.14288700 4.61910600 -1.93988200
H -4.56871700 4.07813000 -1.84310800
H -3.83507400 1.31730800 1.37878800
H -0.55859900 3.51379900 -0.38429700
H -5.41307600 2.44039800 -0.17892200
Cl 0.15814000 -1.80221100 -2.25613000
C -2.04074900 -1.29631200 -0.07331200
C -2.76583100 -0.57383600 -1.01371400
C -2.75589700 -2.17690700 0.72266900
C -4.13734400 -0.71685200 -1.17177000
C -4.13253200 -2.33680700 0.59107600
C -4.82601000 -1.60459600 -0.35942500
Cl 0.86192100 -2.32416900 2.03405500
C 2.04916300 1.59983200 -1.04512600
C 1.33055000 1.65650000 -2.24900700
C 2.48450700 2.78630100 -0.44415100
C 1.07809700 2.88324700 -2.85228900
H 0.97048500 0.73824100 -2.71513800
C 2.22081700 4.01118200 -1.05130600
H 3.03284200 2.76020100 0.49672300
C 1.52198800 4.06139700 -2.25476900
H 0.52584600 2.91718800 -3.78965400
H 2.56866200 4.92901000 -0.58068600
H 1.31963800 5.02132000 -2.72723000
C 3.31226200 -1.06681100 -1.30283100
C 3.89916200 -0.60408800 -2.48151200
C 3.51648100 -2.38710000 -0.88399200
C 4.69261500 -1.46293600 -3.23786400
H 3.74672600 0.42365700 -2.80949600
C 4.30942400 -3.23633300 -1.64431300
H 3.04447700 -2.74738500 0.03253300
C 4.89633600 -2.77495700 -2.82174400
H 5.15317600 -1.10150700 -4.15558700
H 4.46534200 -4.26363000 -1.32021500
H 5.51499000 -3.44368400 -3.41789100
C 3.34486700 0.30873400 1.22098800
C 4.70643400 0.55458900 0.99619700
C 2.83620900 0.38315400 2.51917800
C 5.53988800 0.88286400 2.05859100
H 5.11699000 0.49755300 -0.01200300
C 3.67631300 0.70899900 3.57970700
H 1.79256900 0.14667600 2.70967200
C 5.02541100 0.96100400 3.35058400
H 6.59569700 1.07397400 1.87565500
H 3.27371800 0.75415000 4.58997400
H 5.68080900 1.21226600 4.18279200
F -6.13917200 -1.74858300 -0.48829500
F -4.79753000 0.00810900 -2.07069300
F -2.16609800 0.32348500 -1.80511500
F -2.16439000 -2.91366800 1.66020300
F -4.79004700 -3.18837200 1.37355100

(i)

E (M06-SMD/SDD) = -942.687456 au
H (M06-SMD/SDD) = -942.433509au
G (M06-SMD/SDD) = -942.498177au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -942.912337au

C -3.87392600 -1.24630600 -1.16869900
C -3.92070300 1.52214800 -0.42989800
C -3.88920800 -0.50192800 1.59920200
Au -0.74796900 0.00291500 -0.00036300
P -3.12148900 -0.06259200 0.00121700
H -5.01446700 1.42159200 -0.40777600
H -3.61474000 2.29690700 0.28376300
C 1.32604800 0.09449900 -0.00072500
C 2.13704500 -1.05129400 -0.00074700
C 2.01234400 1.32676900 -0.00013500
C 3.53395500 -0.99640000 -0.00034300
C 3.39861300 1.40937300 0.00029400
C 4.17103900 0.24413100 0.00022700
H 1.44719700 2.26139400 0.00008600

H 3.91112100 2.37157600 0.00084700
H 4.10830300 -1.92112000 -0.00037300
H 1.67483400 -2.04109200 -0.00102400
H -3.53864700 -2.26382200 -0.93357000
H -4.97002900 -1.20382600 -1.10780700
H -3.55956900 -1.00526300 -2.19151900
H -3.58149900 0.21823100 2.36718200
H -4.98462000 -0.49598900 1.51547500
H -3.55613500 -1.50054000 1.90742600
H -3.60689000 1.83266200 -1.43406500
O 5.51801200 0.42191300 0.00078500
C 6.33114200 -0.72913400 0.00112400
H 7.36679500 -0.37655900 0.00174600
H 6.16350100 -1.34609700 0.89668800
H 6.16450300 -1.34593000 -0.89474200

(ii)

E (M06-SMD/SDD) = -927.437667 au
H (M06-SMD/SDD) = -927.226269 au
G (M06-SMD/SDD) = -927.287502 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -927.660090 au

C 3.58273600 -0.69986800 1.50147700
C 3.58094400 1.65025500 -0.13999300
C 3.58805800 -0.94673100 -1.35421700
Au 0.43897000 -0.00051600 -0.00136700
P 2.81202800 -0.00004500 0.00100300
H 4.67627600 1.56581600 -0.13225800
H 3.26219200 2.12860100 -1.07413200
C -1.63920300 -0.00021000 -0.00116200
C -2.38234700 -1.19550600 -0.00050600
C -2.38195700 1.19536200 -0.00062700
C -3.77696300 -1.21047000 0.00071300
C -3.77652400 1.21078200 0.00057300
C -4.44814300 0.00025900 0.00123500
H 3.26599600 -1.74228600 1.62847500
H 4.67801300 -0.66117700 1.42502200
H 3.26178900 -0.13006600 2.38204600
H 3.27141300 -0.53627200 -2.32080200
H 4.68302000 -0.89614400 -1.28085000
H 3.27060000 -1.99532100 -1.30190700
H 3.26143900 2.28021200 0.69916200
H -1.86406200 -2.15622100 -0.00085800
H -1.86340000 2.15593000 -0.00109600
H -4.34354700 -2.14040800 0.00130900
H -4.34281300 2.14090000 0.00104200
F -5.79506300 0.00051400 0.00253400

(iii)

E (M06-SMD/SDD) = -1287.796878 au
H (M06-SMD/SDD) = -1287.586649 au
G (M06-SMD/SDD) = -1287.649216 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -1288.004629 au

C 3.88215600 -0.70154000 1.50110300
C 3.88077700 1.65070100 -0.13843200
C 3.88759700 -0.94575500 -1.35525800
Au 0.74033300 -0.00047500 -0.00131200
P 3.11286700 0.00005100 0.00100900
H 4.97611400 1.56655600 -0.13018400
H 3.56234300 2.12950700 -1.07242700
C -1.33802700 -0.00023200 -0.00116700
C -2.08098600 -1.19473500 -0.00066800
C -2.08070300 1.19448000 -0.00077100
C -3.47529100 -1.21091100 0.00019500
C -3.47496000 1.21099100 0.00009100
C -4.15394700 0.00011400 0.00057000
H 3.56515900 -1.74404000 1.62665200
H 4.97744700 -0.66294900 1.42503000
H 3.56100100 -0.13260500 2.38213300

H 3.57043300 -0.53476100 -2.32142300
H 4.98256800 -0.89505500 -1.28235200
H 3.57026000 -1.99438100 -1.30319000
H 3.56063700 2.27984900 0.70107200
H -1.56431500 -2.15632700 -0.00089500
H -1.56383400 2.15596900 -0.00108300
H -4.02621800 -2.15029500 0.00060400
H -4.02567000 2.15050400 0.00041900
Cl -5.91793800 0.00035900 0.00177600

(iv)

E (M06-SMD/SDD) = -920.419111 au
H (M06-SMD/SDD) = -920.199912 au
G (M06-SMD/SDD) = -920.263508 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -920.633367 au

C 3.76508900 -0.70194700 1.50212300
C 3.76692800 1.65050400 -0.13900000
C 3.77117800 -0.94742600 -1.35514200
Au 0.62715200 -0.00018000 -0.00137900
P 2.99933100 0.00021000 0.00097300
H 4.86217200 1.56565100 -0.13029700
H 3.44911800 2.12881500 -1.07343300
C -1.45153000 -0.00024600 -0.00107100
C -2.19162600 -1.19885300 -0.00060500
C -2.19138600 1.19855600 -0.00065900
C -3.58032000 -1.21242300 0.00025100
C -3.58002800 1.21242100 0.00018700
C -4.28212900 0.00006400 0.00065900
H 3.44679500 -1.74406300 1.62732500
H 4.86045000 -0.66450200 1.42695900
H 3.44376200 -0.13233000 2.38261600
H 3.45459900 -0.53621400 -2.32137200
H 4.86618700 -0.89825900 -1.28224100
H 3.45224700 -1.99550100 -1.30232700
H 3.44678800 2.28007200 0.70015100
H -1.67009900 -2.15710000 -0.00083000
H -1.66967500 2.15670400 -0.00093100
C -5.70934100 0.00023800 0.00163600
N -6.87397500 0.00034300 0.00246300
H -4.13049300 -2.15250800 0.00066200
H -4.13001200 2.15261800 0.00053300

(v)

E (M06-SMD/SDD) = -1104.788022 au
H (M06-SMD/SDD) = -1104.568020 au
G (M06-SMD/SDD) = -1104.640224 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -1105.074987 au

C 4.31781200 -0.70583200 1.50202600
C 4.32099800 1.65186800 -0.13735300
C 4.32216600 -0.94725300 -1.35872300
Au 1.19518900 0.00015700 -0.00101100
P 3.55930300 0.00021800 0.00073000
H 5.41621600 1.56774200 -0.12887100
H 4.00256600 2.13038400 -1.07137300
C -0.88779600 -0.00010900 -0.00091200
C -1.62787100 -1.19277400 -0.00068700
C -1.62784400 1.19261400 -0.00058200
C -3.02655700 -1.20569700 -0.00009600
C -3.02649900 1.20557900 -0.00004700
C -3.74864300 -0.00005800 0.00024100
H 3.99812700 -1.74782300 1.62394200
H 5.41320100 -0.66929300 1.42817200
H 3.99583200 -0.13704000 2.38271200
H 4.00434500 -0.53342800 -2.32333100
H 5.41730800 -0.90011100 -1.28781900
H 4.00123800 -1.99462700 -1.30592400
H 4.00029600 2.27941600 0.70298500
H -1.11858400 -2.15622100 -0.00092100
H -1.11856300 2.15606700 -0.00069200
C -3.72176700 -2.45473600 0.00023700

C -5.17450300 -0.00001200 0.00096800
C -3.72167800 2.45463600 0.00024000
N -4.27469300 3.47736200 0.00047100
N -6.33738400 0.00005500 0.00157000
N -4.27483400 -3.47743200 0.00055500

(vi)

E (M06-SMD/SDD) = -1324.268920 au
H (M06-SMD/SDD) = -1324.085534 au
G (M06-SMD/SDD) = -1324.154939 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -1324.667120 au

C -4.04843500 -0.42552200 1.60522300
C -4.05696400 -1.17206300 -1.16743000
C -4.04798300 1.60310300 -0.42816200
Au -0.93851000 -0.00103300 -0.00168900
P -3.29138800 0.00026800 0.00137400
H -3.72110800 0.28916900 2.36994600
H -5.14399200 -0.39951400 1.52919700
H -3.73053800 -1.43033600 1.90880400
H -3.73093100 1.90384000 -1.43409700
H -5.14354300 1.52755200 -0.40098800
H -3.71990300 2.36994500 0.28392900
H -3.73723200 -2.19389200 -0.93001300
H -5.15198900 -1.11131400 -1.10532500
H -3.73887300 -0.93618700 -2.19011300
C 1.14807400 -0.00043700 -0.00130400
C 1.88730400 1.17090300 -0.00056000
C 1.88827700 -1.17114100 -0.00069200
C 3.27553600 1.19999400 0.00065800
C 3.27655000 -1.19902200 0.00051700
C 3.97392600 0.00077500 0.00122100
F 1.26608600 -2.36508800 -0.00121900
F 3.94816000 -2.35055900 0.00111200
F 5.30368000 0.00134200 0.00241300
F 3.94615900 2.35210400 0.00138600
F 1.26408000 2.36428900 -0.00095500

Iodonium ion (i)

E (M06-SMD/SDD) = -2105.850076au
H (M06-SMD/SDD) = -2105.493795au
G (M06-SMD/SDD) = -2105.586547au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2392.622507au

C 3.97078300 -2.64793100 0.08539400
C 3.60031600 -1.34361400 2.62406000
C 4.01760800 0.23065300 0.25019300
Au 0.77775300 -1.10606500 0.41320200
P 3.12865700 -1.23428900 0.86614100
H 4.69409700 -1.37272800 2.71914900
H 3.21548200 -0.47048100 3.16547400
C -1.26121300 -1.12446300 0.05567400
C -1.74714700 -1.72357900 -1.11186200
C -2.14629400 -0.82548400 1.10349400
C -3.06737300 -2.15776800 -1.18490700
C -3.46020200 -1.25130200 1.03725300
C -3.92677400 -1.92660100 -0.10370700
H -1.80465900 -0.28131600 1.98560500
H -4.15683200 -1.07055000 1.85446900
H -3.41893900 -2.65676200 -2.08459400
H -1.08994500 -1.87939700 -1.96802300
H 3.82358800 -2.61194300 -1.00073700
H 5.04629500 -2.61498100 0.30583700
H 3.55138000 -3.58676500 0.46648500
H 3.65709600 1.12742500 0.77135900
H 5.09729000 0.12387800 0.42225200
H 3.81743200 0.34389600 -0.82437200
H 3.17468000 -2.24911000 3.07292900
C -0.87514200 2.20715900 0.72221100
C -0.20628600 2.45113800 1.91650100
C -0.92665500 2.97176900 2.98945900
C -2.28506700 3.24656300 2.85025500
C -2.93358800 3.00678500 1.64021600

C -2.22913500 2.47878400 0.56193600
H 0.85854200 2.23686100 2.01328400
H -0.42112800 3.16684400 3.93363600
H -2.84324000 3.65340500 3.69151300
H -3.99465200 3.22554300 1.53394500
H -2.73054300 2.26819900 -0.38225700
I 0.21985300 1.33665000 -0.90588900
Cl 1.92917900 -0.20208900 -2.94434500
Cl 0.33107800 3.82649100 -2.09647100
O -5.21850600 -2.29272800 -0.07124900
C -5.76012700 -2.95627100 -1.20068000
H -6.80695600 -3.15793300 -0.96008300
H -5.70962100 -2.32425500 -2.09769900
H -5.24243000 -3.90685700 -1.39024400

Iodonium ion (vi)
E (M06-SMD/SDD) = -2487.417444 au
H (M06-SMD/SDD) = -2487.129234 au
G (M06-SMD/SDD) = -2487.225393 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2774.369695 au
C 4.24774400 -1.94612400 -0.33903700
C 3.43780500 -2.16615200 2.42812900
C 3.86876300 0.43387600 1.24268100
Au 0.84765700 -1.22480200 0.27539600
P 3.15256500 -1.20420800 0.90713400
H 4.50830500 -2.16696500 2.67449100
H 2.87636600 -1.72466100 3.26034400
C -1.17000700 -1.30631700 -0.21886700
C -1.61590800 -1.39396500 -1.52875800
C -2.14439100 -1.23406500 0.76478200
C -2.96425500 -1.42976600 -1.85910800
C -3.50106100 -1.26246400 0.48020900
C -3.90980600 -1.35963500 -0.84402600
F -1.79497800 -1.10431000 2.05361100
F -4.41113000 -1.17541300 1.44603700
F -5.20234100 -1.38750000 -1.13832600
F -3.36323100 -1.52424700 -3.12368900
F -0.73765400 -1.43977000 -2.53996100
H 4.17771500 -1.35755700 -1.26381000
H 5.28434300 -1.93908500 0.02441400
H 3.93985100 -2.97896300 -0.54141600
H 3.28858000 0.95168500 2.01695400
H 4.90570700 0.31789800 1.58591600
H 3.85558700 1.02471100 0.31613400
H 3.10035600 -3.19965600 2.28412700
C -0.97263500 1.94278600 0.82585300
C -0.68515900 2.08434600 2.18027800
C -1.73916400 2.30112200 3.06327000
C -3.04557900 2.37265200 2.58489900
C -3.31147100 2.23381300 1.22306100
C -2.26978700 2.01438900 0.32706500
H 0.34114100 2.02264700 2.54167600
H -1.53705900 2.41325600 4.12681800
H -3.86627200 2.53908700 3.28005400
H -4.33485900 2.28942600 0.85593500
H -2.46563200 1.88728100 -0.73747200
I 0.64159200 1.54392100 -0.52320100
Cl 2.96715800 0.92470000 -2.35177800
Cl 0.67411200 4.06881700 -1.19642600

Iodonium ion (iii)
E (M06-SMD/SDD) = -2450.954260 au
H (M06-SMD/SDD) = -2450.639602 au
G (M06-SMD/SDD) = -2450.732745 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2737.712189 au
C 4.13748300 -2.20643400 -0.19110400
C 3.58771500 -1.59977200 2.57154300

C 3.93202200 0.53267300 0.66538700
Au 0.79881900 -1.11526900 0.35710800
P 3.15493300 -1.10172700 0.87070300
H 4.67660600 -1.56311900 2.71094400
H 3.11080300 -0.92430400 3.29227700
C -1.22016300 -1.26802400 -0.07583500
C -1.64072100 -1.67402900 -1.34600800
C -2.14820100 -1.15834100 0.96445800
C -2.96618500 -2.04485100 -1.56096900
C -3.47419200 -1.53137700 0.76332100
C -3.86142000 -1.96860500 -0.49988200
H 3.99421000 -1.90749900 -1.23719700
H 5.20154000 -2.13348800 0.07175900
H 3.80249400 -3.24321900 -0.06609000
H 3.45639700 1.26384000 1.33168600
H 5.00282300 0.47165300 0.90268100
H 3.80456900 0.85691900 -0.37603700
H 3.23583200 -2.62089000 2.76209600
C -1.03544600 2.04572100 0.76454300
C -0.51606100 2.28476600 2.03224700
C -1.39375600 2.65474100 3.04886600
C -2.75485200 2.78613300 2.78286200
C -3.25142100 2.55195100 1.50198100
C -2.38956000 2.17217000 0.47698500
H 0.55083500 2.17991000 2.22849800
H -1.00953700 2.84299300 4.04979600
H -3.43553600 3.07447700 3.58174700
H -4.31549100 2.65700400 1.29826300
H -2.76881500 1.96185700 -0.52298400
I 0.29405900 1.39395200 -0.78577200
Cl 2.26523300 -0.03445000 -2.68647700
Cl 0.26658800 3.90270500 -1.83143000
H -0.93857800 -1.70918300 -2.17988900
H -1.84754600 -0.78466300 1.94493100
H -4.19955500 -1.47162500 1.57263700
H -3.30002800 -2.37462200 -2.54287800
Cl -5.53583800 -2.41435100 -0.76672600

Iodonium ion (iv)
E (M06-SMD/SDD) = -2083.574013 au
H (M06-SMD/SDD) = -2083.251430 au
G (M06-SMD/SDD) = -2083.342639 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2370.339475 au
C 4.16360600 -1.97917200 -0.32436200
C 3.54006900 -1.77864300 2.48565600
C 3.78587600 0.60489600 0.88792300
Au 0.76191000 -1.18055600 0.28556300
P 3.10655200 -1.08395700 0.85582100
H 4.62365300 -1.70246000 2.64872900
H 3.01854200 -1.22858800 3.27838500
C -1.24453500 -1.38131200 -0.18701200
C -1.65330200 -1.64645200 -1.49843400
C -2.17663700 -1.41353800 0.85700800
C -2.97314200 -1.99475100 -1.76156700
C -3.49570600 -1.76773500 0.60603400
C -3.89268900 -2.05587600 -0.70691100
H 4.00367400 -1.55556100 -1.32455400
H 5.21984900 -1.87317300 -0.04208200
H 3.89555200 -3.04251300 -0.33621600
H 3.24565500 1.21645100 1.62210400
H 4.85042100 0.57461800 1.15712200
H 3.67335700 1.05091000 -0.10917100
H 3.24265800 -2.83297700 2.53557400
C -1.21705200 1.88165200 0.81918700
C -0.79508900 2.10987800 2.12516800
C -1.75888100 2.36491100 3.09774600
C -3.10809300 2.39368300 2.75206200
C -3.50758100 2.16975400 1.43569300
C -2.55825000 1.90580800 0.45284500
H 0.26405500 2.08805900 2.38142100
H -1.45178500 2.54626800 4.12610600
H -3.85670000 2.59423700 3.51618800
H -4.56309600 2.19353500 1.17103400

H -2.85897500 1.70727900 -0.57599600
I 0.25911000 1.42866700 -0.66681700
Cl 2.41719000 0.46211900 -2.63104500
Cl 0.16685200 3.98084600 -1.51112600
H -0.94214500 -1.58134700 -2.32308900
H -1.88058300 -1.15928600 1.87627300
H -4.22379000 -1.81143300 1.41443600
H -3.29853000 -2.20959900 -2.77782900
C -5.25386600 -2.40100300 -0.97204700
N -6.36298800 -2.68193300 -1.18442100

Iodonium ion (v)
E (M06-SMD/SDD) = -2267.936109 au
H (M06-SMD/SDD) = -2267.612576 au
G (M06-SMD/SDD) = -2267.712782 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2554.778273 au
C -4.15345200 -2.44778900 0.27570800
C -3.55833400 -2.17149000 -2.53899000
C -4.16245600 0.16134400 -0.94973900
Au -0.90432000 -1.22321300 -0.39519000
P -3.24824900 -1.41064800 -0.91168700
H -4.63963000 -2.25988200 -2.71041800
H -3.11820100 -1.55385900 -3.33121700
C 1.13340400 -1.15392000 0.02054700
C 1.62112400 -1.34104100 1.31648600
C 2.05166900 -0.97866700 -1.01861200
C 2.99647800 -1.37961400 1.57111900
C 3.42848500 -1.01996700 -0.78181300
C 3.91688100 -1.21892500 0.52125900
H -4.06242300 -1.99595700 1.27219000
H -5.21303200 -2.50611700 -0.00763800
H -3.72568900 -3.45737800 0.29465000
H -3.71232300 0.84607800 -1.67971200
H -5.20774800 -0.02717100 -1.22954700
H -4.12941700 0.61710100 0.04922600
H -3.10591700 -3.16971600 -2.57833200
C 0.57909000 2.12289800 -0.73590600
C 0.19815300 2.27099000 -2.06639500
C 1.16309400 2.66026600 -2.99182300
C 2.47119800 2.90107400 -2.57641800
C 2.82770600 2.76004000 -1.23596300
C 1.87883700 2.36095400 -0.29959800
H -0.82954800 2.08208200 -2.37650600
H 0.88935300 2.77952100 -4.03843100
H 3.22107700 3.20496100 -3.30425300
H 3.85088400 2.95234700 -0.91816900
H 2.14856300 2.23062700 0.74841300
I -0.87480200 1.43432400 0.67560800
Cl -2.93681500 0.27137000 2.59555600
Cl -1.12960100 3.87787900 1.60496200
H 0.93703400 -1.45311000 2.15808000
H 1.71288900 -0.79675000 -2.03914800
C 5.32146900 -1.24413500 0.77234700
N 6.46608500 -1.26276500 0.97374000
C 4.33587400 -0.82481500 -1.86941200
C 3.46547300 -1.57356700 2.90791800
N 3.83997900 -1.73263300 3.99652100
N 5.05887100 -0.65565800 -2.76371200

Iodonium ion (ii)
E (M06-SMD/SDD) = -2090.596623 au
H (M06-SMD/SDD) = -2090.280834 au
G (M06-SMD/SDD) = -2090.373070 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2377.368015 au
C 4.49272100 -1.12960600 -0.17143700
C 3.71622000 -0.99557900 2.59912000
C 3.53899000 1.35289300 0.93461600
Au 0.96997200 -0.98140600 0.27130100
P 3.22089200 -0.44059300 0.93368000
H 4.75422500 -0.69963100 2.80266800

H 3.05973700 -0.54569200 3.35385500
C -0.92775700 -1.59348400 -0.28870500
C -1.17683900 -1.99494400 -1.60618200
C -1.87329900 -1.84118900 0.71332900
C -2.32368000 -2.72408100 -1.90717800
C -3.01933400 -2.57405600 0.42323100
C -3.21821300 -2.99973800 -0.88331400
F -4.32924400 -3.68701300 -1.16936200
H 4.30820800 -0.76909100 -1.19140900
H 5.49128500 -0.81121700 0.15748400
H 4.44071000 -2.22511800 -0.16432100
H 2.85518300 1.85530400 1.63108800
H 4.57574500 1.55396100 1.23666200
H 3.36794700 1.73989000 -0.07924700
H 3.63359200 -2.08696700 2.66882200
C -1.82405800 1.47591200 0.77540000
C -1.49223000 1.76084400 2.09522400
C -2.51359900 1.79696300 3.04228200
C -3.83077200 1.55862200 2.65766300
C -4.14106800 1.28358500 1.32695300
C -3.13209800 1.23587200 0.36973300
H -0.45777900 1.94917900 2.38247500
H -2.27656200 2.01657100 4.08175900
H -4.62458500 1.58952800 3.40179600
H -5.17234700 1.10017800 1.03097200
H -3.35757800 1.00007200 -0.67032300
I -0.25076600 1.36942800 -0.67693100
Cl 2.16606300 0.82835500 -2.52447900
Cl -0.89771200 3.90641800 -1.46109500
H -0.47503800 -1.74847900 -2.40342400
H -1.72350400 -1.46910200 1.72819000
H -3.76116400 -2.80464300 1.18507100
H -2.53727900 -3.06456200 -2.91816600

TS_{CIS}-(i)
E (M06-SMD/SDD) = -2105.844865 au
H (M06-SMD/SDD) = -2105.489779au
G (M06-SMD/SDD) = -2105.580035au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2392.614677au
C 4.77523700 -1.23403100 -0.94780500
C 4.03402000 -2.51083000 1.52374200
C 4.60476200 0.30782700 1.48121200
Au 1.44175600 -0.47374300 0.02764100
P 3.75231600 -1.00024600 0.54081200
H 5.10946900 -2.66033200 1.69167000
H 3.52687300 -2.42238200 2.49208600
C -0.51566700 -1.24509800 -0.14155400
C -1.02842700 -1.54313900 -1.40215100
C -1.16833500 -1.67947600 1.01718700
C -2.15121700 -2.36215000 -1.51919100
C -2.28577100 -2.48675800 0.90321900
C -2.79395700 -2.81838100 -0.36391400
H 4.71590200 -0.33229900 -1.56937400
H 5.82007900 -1.41924400 -0.66319300
H 4.39998900 -2.08712700 -1.52600100
H 4.10797300 0.45548700 2.44772100
H 5.65343600 0.02633000 1.65011000
H 4.56000200 1.24485400 0.91349900
H 3.62714600 -3.38071100 0.99416500
C -2.37095000 1.18961200 0.57019500
C -2.53464700 1.33078500 1.94311600
C -3.78379400 1.04657900 2.48884800
C -4.83164700 0.63836400 1.66659100
C -4.64452300 0.51807900 0.29183800
C -3.40248800 0.79734100 -0.27373400
H -1.70732300 1.64948900 2.57544000
H -3.93591400 1.14792600 3.56195000
H -5.80432600 0.41564700 2.10139300
H -5.46686700 0.20453200 -0.34929200
H -3.24414200 0.70544400 -1.34682400
I -0.45133500 1.62426800 -0.27646700
Cl 2.60485600 1.88016100 -1.34749400
Cl -1.41095200 4.26466000 -0.57953300

H -0.80411000 -1.39617200 2.00450900
H -0.56088600 -1.14479400 -2.30239100
H -2.80231300 -2.86128300 1.78569900
H -2.52778900 -2.60877200 -2.50908500
O -3.91307200 -3.56516000 -0.36148000
C -4.53386000 -3.84223800 -1.60352800
H -3.88181700 -4.44126800 -2.25461500
H -5.43448500 -4.41691100 -1.37263200
H -4.81780600 -2.91480100 -2.12100300

TS_{CIS}-(ii)
E (M06-SMD/SDD) = -2090.591735 au
H (M06-SMD/SDD) = -2090.277079 au
G (M06-SMD/SDD) = -2090.368453 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2377.359494 au
C -4.76933600 0.60636300 -0.73192100
C -4.07580100 1.99415800 1.69509500
C -4.23719300 -0.88013600 1.67866700
Au -1.32549900 0.34076700 0.03540700
P -3.64088700 0.53353600 0.69485600
H -5.15033400 1.98764800 1.92372000
H -3.50692200 1.98586100 2.63256800
C 0.46641100 1.37027300 -0.41159900
C 0.73394900 1.65092400 -1.75103400
C 1.08157800 2.07897600 0.62058300
C 1.57516100 2.71669300 -2.06681200
C 1.92364400 3.14047100 0.30716200
C 2.15160800 3.43555200 -1.03115200
H -4.61696500 -0.28255600 -1.35589800
H -5.81179300 0.64225400 -0.38740400
H -4.55320700 1.49925100 -1.33100100
H -3.67189900 -0.94733600 2.61589800
H -5.30487600 -0.75396600 1.90568200
H -4.08958700 -1.80557500 1.10933500
H -3.82950300 2.90938500 1.14352100
C 2.58732600 -0.68788000 0.64233800
C 2.65632000 -0.67070700 2.02975800
C 3.78976100 -0.12005300 2.62380900
C 4.81890200 0.38505800 1.83350000
C 4.73175100 0.33853100 0.44355200
C 3.60500200 -0.20192700 -0.16962400
H 1.84304900 -1.06680700 2.63606000
H 3.86562500 -0.08974100 3.70921700
H 5.70032600 0.81567900 2.30505200
H 5.54188600 0.72764900 -0.17050100
H 3.51881100 -0.23235900 -1.25469900
I 0.82575500 -1.47311300 -0.28353900
Cl -2.12910900 -2.14670500 -1.41687900
Cl 2.20143800 -3.89935900 -0.52825100
H 0.90716400 1.81898800 1.66396000
H 0.29155400 1.05385000 -2.54809400
H 2.40484500 3.73424200 1.08154000
H 1.79801600 2.97907400 -3.09882900
F 2.97360100 4.44679800 -1.33102500

TS_{CIS}-(iii)
E (M06-SMD/SDD) = -2450.949381 au
H (M06-SMD/SDD) = -2450.636005 au
G (M06-SMD/SDD) = -2450.729008 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2737.703511 au
C 4.64651100 -1.50378800 -0.67049700
C 3.75543200 -2.44017900 1.90390400
C 4.40852000 0.33876600 1.53163600
Au 1.29009900 -0.54916800 0.04981700
P 3.56480600 -1.06178100 0.72541600
H 4.81799000 -2.59326300 2.13711600
H 3.21137000 -2.21642400 2.82942900
C -0.66114200 -1.24052400 -0.28045500
C -1.05045000 -1.50501400 -1.59170400
C -1.38755700 -1.72538200 0.80524300

C -2.15057200 -2.33094300 -1.82331900
C -2.48591700 -2.54964700 0.57724100
C -2.85041600 -2.83800900 -0.73517800
Cl -4.24800000 -3.85646100 -1.02114600
H 4.64584000 -0.68149600 -1.39617000
H 5.66984000 -1.68160100 -0.31276500
H 4.27039600 -2.40931900 -1.16162500
H 3.87355100 0.61986400 2.44670700
H 5.44044400 0.05836400 1.78439800
H 4.41802900 1.19685300 0.84898100
H 3.34562700 -3.35992100 1.46959300
C -2.12678100 1.40429000 0.72564000
C -2.07898800 1.46893500 2.11280400
C -3.24980200 1.21362500 2.82323900
C -4.42775500 0.91124700 2.14493900
C -4.45179400 0.86818200 0.75220900
C -3.29144000 1.11445500 0.02413000
H -1.15049500 1.70340900 2.63132700
H -3.23722700 1.25373500 3.91094000
H -5.33805200 0.71010600 2.70674300
H -5.37634200 0.63736500 0.22611400
H -3.29289300 1.06901300 -1.06398200
I -0.32071600 1.72958300 -0.37090100
Cl 2.58615500 1.52526100 -1.72710200
Cl -1.17008300 4.34867600 -0.77986500
H -1.10777200 -1.47781000 1.82878600
H -0.50811300 -1.08073500 -2.43663800
H -3.05397800 -2.95837800 1.41073000
H -2.46445800 -2.55987900 -2.83982300

TS_{CIS}-(iv)
E (M06-SMD/SDD) = -2083.569074 au
H (M06-SMD/SDD) = -2083.246762 au
G (M06-SMD/SDD) = -2083.339269 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2370.330624 au
C 4.62457300 -1.32657000 -0.78026100
C 3.82445300 -2.46712300 1.74093400
C 4.32125700 0.36078400 1.53868700
Au 1.22391200 -0.62444000 0.05086600
P 3.54360200 -1.02946100 0.65414900
H 4.89678700 -2.57580200 1.95339300
H 3.28246700 -2.33150000 2.68467600
C -0.70269700 -1.34753600 -0.29793400
C -1.08344100 -1.59674300 -1.61632300
C -1.43607000 -1.84459700 0.77948300
C -2.18798800 -2.40604200 -1.86249100
C -2.53874500 -2.65277200 0.53485300
C -2.91307900 -2.93261900 -0.78717000
C -4.05697300 -3.75181500 -1.03851300
H 4.56487800 -0.46418100 -1.45561900
H 5.66181200 -1.46635100 -0.44650300
H 4.29230400 -2.22304900 -1.31759400
H 3.78577100 0.55346100 2.47611900
H 5.37047100 0.12194600 1.76089200
H 4.27079900 1.25675100 0.90841500
H 3.45951600 -3.37966800 1.25448400
C -2.18498100 1.31765200 0.68771300
C -2.18751600 1.33767700 2.07773100
C -3.38004500 1.05256500 2.73825600
C -4.53157500 0.76531400 2.00940500
C -4.50679100 0.76700500 0.61592100
C -3.32328000 1.04362400 -0.06194400
H -1.27955300 1.56254900 2.63560200
H -3.40616000 1.05818500 3.82642500
H -5.45959200 0.54158100 2.53233600
H -5.41102800 0.54814200 0.05095300
H -3.28720600 1.03487600 -1.15041200
I -0.34699600 1.69952300 -0.33325300
Cl 2.56421500 1.70128500 -1.53222700
Cl -1.17599300 4.29555400 -0.74398200
H -1.15457200 -1.61434800 1.80637900
H -0.52888400 -1.16897500 -2.45094300
H -3.11401900 -3.06639700 1.36114000

H -2.49709400 -2.61971200 -2.88397600
N -4.98877000 -4.41837300 -1.24122200

TS_{CIS}-(vi)
E (M06-SMD/SDD) = -2267.928762 au
H (M06-SMD/SDD) = -2267.605307 au
G (M06-SMD/SDD) = -2267.705485 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2554.766701 au
C -4.47864900 -2.22526600 0.81193800
C -3.47419200 -3.13758900 -1.72556800
C -4.63869100 -0.51469000 -1.50890200
Au -1.34619900 -0.77225600 -0.09872500
P -3.53180400 -1.67202100 -0.64067900
H -4.49168500 -3.50074200 -1.92446200
H -2.99211800 -2.87917000 -2.67619400
C 0.70412600 -1.00772000 0.16801500
C 1.20242500 -1.22924200 1.45049600
C 1.51738200 -1.23395100 -0.94206300
C 2.50367500 -1.71483600 1.62536800
C 2.81658400 -1.71871500 -0.77562400
C 3.32421200 -1.96624200 0.51310500
C 4.65298900 -2.45642700 0.68424600
H -4.61929100 -1.37886200 1.49458800
H -5.45679600 -2.61232300 0.49554800
H -3.92772200 -3.01690900 1.33414700
H -4.17960100 -0.19484600 -2.45212900
H -5.59750900 -1.00763600 -1.72036900
H -4.80481700 0.36544500 -0.87619400
H -2.89528000 -3.93506800 -1.24432200
C 1.55510700 1.97521500 -0.60463800
C 1.62689400 2.03714700 -1.99284600
C 2.88590300 2.08477900 -2.58550000
C 4.03205000 2.07848500 -1.79313800
C 3.93398400 2.02206000 -0.40363100
C 2.68477500 1.96791000 0.20770500
H 0.72215700 2.04436200 -2.59919900
H 2.96899800 2.13196800 -3.66954100
H 5.01287900 2.11691900 -2.26300100
H 4.83299600 2.02054000 0.20983900
H 2.59397500 1.92125800 1.29199800
I -0.37297500 1.89854900 0.31357500
Cl -3.19525200 1.25419300 1.42849300
Cl -0.25633700 4.55203900 0.70702700
H 1.15851800 -1.04265900 -1.95259200
H 0.59506400 -1.03045800 2.33279700
C 3.63271000 -1.94651200 -1.92704100
C 3.00126300 -1.94036400 2.94669800
N 5.73615700 -2.85520700 0.82113800
N 3.39905800 -2.12107000 4.02349400
N 4.28712300 -2.12180400 -2.87127200

TS_{CIS}-(v)
E (M06-SMD/SDD) = -2487.408905 au
H (M06-SMD/SDD) = -2487.121791 au
G (M06-SMD/SDD) = -2487.218811 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2774.356567 au
C -4.90640500 -0.75787700 1.11248200
C -4.24089000 -2.56390200 -1.02492200
C -4.70490700 0.21674900 -1.59661300
Au -1.56704100 -0.42434200 -0.04019500
P -3.89438700 -0.88767600 -0.39598400
H -5.32229200 -2.70392100 -1.15927800
H -3.73550900 -2.70960100 -1.98732500
C 0.41653100 -1.11630100 0.14756600
C 0.90316500 -1.50883400 1.38779600
C 1.13872600 -1.50369300 -0.97277500
C 2.05337100 -2.27334700 1.51781900
C 2.30019500 -2.25319900 -0.87858400
C 2.75665100 -2.63885600 0.37632300
F 0.74492500 -1.12374900 -2.19233300

F 2.98627600 -2.59421500 -1.96269200
F 3.86830700 -3.34875600 0.48412800
F 2.49952400 -2.64458900 2.71189400
F 0.27822100 -1.13310900 2.50798700
H -4.82926700 0.25802000 1.51742700
H -5.95651900 -0.98280700 0.88082500
H -4.54089900 -1.46661200 1.86539700
H -4.21402700 0.12686600 -2.57318800
H -5.76557700 -0.05219700 -1.69611900
H -4.61577000 1.25314500 -1.24995900
H -3.86484000 -3.31124500 -0.31587800
C 2.47221100 1.21823100 -0.30692600
C 2.86271200 1.22707000 -1.64259500
C 4.17245200 0.86849000 -1.94579400
C 5.05797000 0.52207200 -0.92643500
C 4.64709300 0.53441000 0.40431500
C 3.33845600 0.88422300 0.72877500
H 2.16140400 1.50062000 -2.42886900
H 4.50117600 0.86383400 -2.98318200
H 6.08073500 0.24294000 -1.17244800
H 5.34373700 0.26892800 1.19727400
H 3.00305300 0.89517200 1.76481600
I 0.45394300 1.75278400 0.16470400
Cl -2.56794600 2.30795900 0.67732900
Cl 1.20961800 4.29355800 0.29342900

TS_{TRANS}-(i)

E (M06-SMD/SDD) = -2105.850850au

H (M06-SMD/SDD) = -2105.493646au

G (M06-SMD/SDD) = -2105.589039au

E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2392.617037au

C -4.18591300 -2.33369600 -0.54434600
C -3.68646300 -0.35802300 -2.57786600
C -4.05396700 0.45517400 0.15463700
Au -0.89243800 -0.97391100 -0.35754600
P -3.23682400 -0.81345300 -0.86887500
H -4.77748400 -0.27796900 -2.67828100
H -3.23007300 0.60564500 -2.83695100
C 1.16455000 -1.13771200 -0.13798500
C 1.70584100 -1.94202300 0.86904600
C 1.96474500 -0.69882800 -1.20342400
C 2.99480400 -2.44453800 0.73538200
C 3.24662200 -1.20131800 -1.34165300
C 3.76789100 -2.07821700 -0.37557400
H 1.58212300 0.00967300 -1.94005200
H 3.87679200 -0.92033400 -2.18394800
H 3.39075300 -3.10858600 1.49995100
H 1.09987300 -2.20265200 1.73802500
H -4.04559400 -2.62861000 0.50274600
H -5.25357000 -2.16443500 -0.73957000
H -3.82336900 -3.14395700 -1.18853100
H -3.62115100 1.44102000 -0.05943600
H -5.13223800 0.48160100 -0.05384200
H -3.89374200 0.22574500 1.21556100
H -3.31556300 -1.11813200 -3.27604900
C 0.85751400 2.36052900 -0.49245200
C 0.01178000 2.73424600 -1.52909600
C 0.56674800 3.40337100 -2.61765600
C 1.93038800 3.68517800 -2.64639300
C 2.75229500 3.30591600 -1.58783100
C 2.21963200 2.63157800 -0.49215900
H -1.05347000 2.50933500 -1.49576400
H -0.07470300 3.70637800 -3.44309200
H 2.35634300 4.20677100 -3.50131300
H 3.81707200 3.52978400 -1.61117000
H 2.85362800 2.31755100 0.33528600
I 0.03936900 1.26531200 1.14575800
Cl -1.56368500 -1.87593200 2.30452700
Cl 0.23114500 3.71246000 2.62592200
O 5.02496400 -2.49569400 -0.59225800
C 5.62319800 -3.36225900 0.35727500
H 6.62729500 -3.57507900 -0.01791300
H 5.69859900 -2.88328700 1.34286700
H 5.06237000 -4.30286600 0.44652600

TS_{TRANS}-(ii)
E (M06-SMD/SDD) = -2090.596698 au
H (M06-SMD/SDD) = -2090.281867 au
G (M06-SMD/SDD) = -2090.371428 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2377.362590 au

```
C 4.58623900 -0.73226800 0.55316500
C 3.38102100 0.76671900 2.69691800
C 3.43016500 1.85396100 0.03591400
Au 1.03578200 -0.71305600 0.35669600
P 3.14121300 0.30297500 0.94889000
H 4.35997400 1.24632000 2.83245200
H 2.59309600 1.46415800 3.00798800
C -0.75630000 -1.69648300 0.01821400
C -0.87131000 -2.57046400 -1.06714500
C -1.69262000 -1.71104700 1.05632800
C -1.86402600 -3.54485800 -1.05753200
C -2.68442400 -2.68775000 1.07245500
C -2.74468900 -3.58457000 0.01488000
H -1.65068100 -0.97734100 1.86319500
H -3.41202700 -2.75284700 1.87882300
F -3.70707600 -4.51272700 0.01915900
H -1.97024900 -4.26125700 -1.86955600
H -0.17165900 -2.49817200 -1.90114900
H 4.56578700 -0.98181800 -0.51474200
H 5.51474600 -0.19487500 0.78897600
H 4.54847900 -1.66257700 1.13278700
H 2.66806800 2.59568200 0.30779700
H 4.42423200 2.25643300 0.27373200
H 3.36382700 1.65859000 -1.04166300
H 3.32741200 -0.12628100 3.33126800
C -1.80213900 1.64780200 0.53903400
C -1.23313100 2.24292800 1.65788400
C -2.06330500 2.53671900 2.73706400
C -3.42284300 2.24038000 2.67573600
C -3.96704800 1.65127700 1.53688000
C -3.15423700 1.34336500 0.44881200
H -0.16830300 2.47058200 1.69401900
H -1.64157100 3.00316200 3.62541500
H -4.06468200 2.47285800 3.52332600
H -5.03023800 1.42345000 1.49089300
H -3.56461300 0.86976000 -0.44146500
I -0.52345600 1.12326100 -1.08934000
Cl 2.07459700 -0.94701500 -2.38559000
Cl -1.62623500 3.31927400 -2.45814300
```

TS_{TRANS}-(iii)
E (M06-SMD/SDD) = -2450.954264 au
H (M06-SMD/SDD) = -2450.640694 au
G (M06-SMD/SDD) = -2450.731704 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2737.707164 au

```
C 4.08972300 -2.40811000 0.53687900
C 3.54103200 -0.58724200 2.69900900
C 4.03577400 0.42849700 0.05425700
Au 0.81290000 -1.01857500 0.36850200
P 3.15664000 -0.89745200 0.94240800
H 4.62790800 -0.53361600 2.84883500
H 3.08727000 0.35983200 3.01729100
C -1.22498300 -1.19633500 0.04352100
C -1.69824300 -1.90660100 -1.06219100
C -2.08762100 -0.83447000 1.08105200
C -3.01948500 -2.34559000 -1.08553400
C -3.40926400 -1.27305500 1.06661200
C -3.85206200 -2.02396100 -0.01782200
H -1.74157300 -0.21797600 1.91270300
H -4.08792200 -1.02351500 1.87988400
Cl -5.52135600 -2.55627800 -0.05157500
```

H -3.39981600 -2.91897600 -1.92883900
H -1.03020200 -2.12605100 -1.89677800
H 3.99022200 -2.61607600 -0.53527600
H 5.15085900 -2.27766100 0.78895200
H 3.68569100 -3.25885800 1.09878600
H 3.62569600 1.40663700 0.33661800
H 5.10554700 0.40331400 0.30269300
H 3.90944200 0.28933000 -1.02661800
H 3.13247200 -1.39532400 3.31791900
C -0.81211200 2.27528600 0.54593100
C -0.07737200 2.59682800 1.68096300
C -0.74854700 3.18330100 2.75130500
C -2.11540200 3.43804500 2.66591000
C -2.82464700 3.11282300 1.51196600
C -2.17508000 2.51877300 0.43301400
H 0.99176200 2.39430000 1.73470500
H -0.19594900 3.44448200 3.65190100
H -2.63254100 3.89648100 3.50659700
H -3.89188400 3.31599700 1.44754200
H -2.72153900 2.24488500 -0.46805400
I 0.18297700 1.29494900 -1.07047800
Cl 1.66072700 -1.51766700 -2.44079900
Cl 0.06049700 3.72339000 -2.44471700

TS_{TRANS}-(iv)

E (M06-SMD/SDD) = -2083.573782 au

H (M06-SMD/SDD) = -2083.251438 au

G (M06-SMD/SDD) = -2083.344340 au

E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2370.333709 au

C 4.04954900 -2.34411300 0.57656400
C 3.48583700 -0.46335000 2.68457000
C 3.94956800 0.47632400 0.00668700
Au 0.75008200 -1.02993100 0.38691100
P 3.09765400 -0.83494300 0.94094300
H 4.57277700 -0.38980400 2.82532700
H 3.02130600 0.48763700 2.97418300
C -1.27718500 -1.30636100 0.06844400
C -1.72105300 -2.01055800 -1.05371300
C -2.15233500 -0.99934800 1.11458800
C -3.02669500 -2.48492300 -1.09349000
C -3.45782500 -1.47435300 1.08172900
C -3.89100600 -2.21939200 -0.02303400
H -1.82322300 -0.39758900 1.96343000
H -4.14553500 -1.26505900 1.89902400
C -5.23823900 -2.69589600 -0.06499700
H -3.38467600 -3.05117600 -1.95141800
H -1.03997300 -2.19408100 -1.88615300
H 3.94521600 -2.58841900 -0.48744500
H 5.11044400 -2.18891300 0.81527700
H 3.66397300 -3.18200100 1.16989300
H 3.52478800 1.45601600 0.26060600
H 5.02055100 0.47614800 0.25087700
H 3.82017200 0.30063800 -1.06855000
H 3.09239900 -1.25590000 3.33255000
C -0.89322900 2.26136700 0.53363200
C -0.16010900 2.65679200 1.64655400
C -0.84266600 3.26235800 2.69848500
C -2.21906800 3.46178100 2.61749200
C -2.92723200 3.06037900 1.48711100
C -2.26608700 2.44672400 0.42646000
H 0.91648700 2.49718500 1.69528800
H -0.29206200 3.58246100 3.58102800
H -2.74488000 3.93668900 3.44347900
H -4.00193900 3.22063400 1.42656800
H -2.80960500 2.11686200 -0.45750900
I 0.12505700 1.27363600 -1.06325000
Cl 1.62607700 -1.48908800 -2.43399600
Cl -0.03335700 3.64439700 -2.48854700
N -6.33502100 -3.08288100 -0.09623000

TS_{TRANS}-(v)

E (M06-SMD/SDD) = -2267.935882 au
H (M06-SMD/SDD) = -2267.612422 au
G (M06-SMD/SDD) = -2267.712743 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2554.771252 au

C -3.85129300 -2.76419000 -1.18374000
C -3.66150300 -0.40340400 -2.83030100
C -4.30752300 -0.15818600 -0.03726800
Au -0.87168800 -0.96352600 -0.64955200
P -3.22011100 -1.05760400 -1.18639800
H -4.73962600 -0.51971900 -3.00614600
H -3.40081900 0.66066700 -2.89097100
C 1.18049000 -0.93087100 -0.33026100
C 1.76503200 -1.73996100 0.64487500
C 1.99964100 -0.19044000 -1.18375300
C 3.15645100 -1.85464300 0.73260100
C 3.39212200 -0.29541100 -1.10483900
C 3.98531500 -1.13521700 -0.14642400
H 1.57451200 0.48585500 -1.92686100
C 4.20387600 0.47608200 -1.99270500
C 5.40545700 -1.24579000 -0.06112800
C 3.73748100 -2.70232800 1.72688600
H 1.13702000 -2.29089000 1.34800500
H -3.69784800 -3.20131600 -0.18982200
H -4.92168700 -2.76858400 -1.43021600
H -3.30684100 -3.36473200 -1.92264500
H -4.07992900 0.91519600 -0.06099800
H -5.35602500 -0.30750400 -0.32878000
H -4.15713800 -0.53474300 0.98186700
H -3.11035400 -0.94434400 -3.60898000
C 0.10591100 2.47942200 0.00655400
C -0.61792200 2.99838800 -1.06054900
C 0.03546400 3.86923100 -1.92859500
C 1.37145900 4.20189800 -1.71360700
C 2.06808200 3.67364900 -0.62894300
C 1.43811700 2.79349000 0.24730500
H -1.66261900 2.73120800 -1.21546800
H -0.50655800 4.29061400 -2.77289500
H 1.87457400 4.88200700 -2.39796300
H 3.11075400 3.93827600 -0.46391300
H 1.97455900 2.36156300 1.09093500
I -0.84525300 1.06922600 1.29416400
Cl -1.64081700 -2.32023800 1.86922500
Cl -1.09524500 3.01554700 3.16735800
N 6.56248800 -1.33430800 0.00563500
N 4.20612200 -3.39325400 2.53531800
N 4.84632900 1.11749400 -2.71864400

TS_{TRANS}-(vi)
E (M06-SMD/SDD) = -2487.411831 au
H (M06-SMD/SDD) = -2487.124866 au
G (M06-SMD/SDD) = -2487.219461 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2774.357184 au

C 4.14930300 -2.05239400 1.22669300
C 3.12674800 0.06519900 2.89719500
C 4.09818200 0.67468000 0.25781700
Au 0.88279600 -0.99824700 0.44969100
P 3.12477100 -0.55131600 1.18035700
H 4.15585400 0.23847900 3.24077500
H 2.56432600 1.00592400 2.95478900
C -1.15847000 -1.29570400 0.14835000
C -1.74853300 -1.80619400 -0.99923900
C -2.02401300 -0.88598600 1.15440000
C -3.12517500 -1.94020100 -1.13491600
C -3.40280600 -0.99495900 1.05604700
C -3.95489200 -1.52742000 -0.10163500
F -1.54360700 -0.33656500 2.28181600
F -4.19837000 -0.57837500 2.03726500
F -5.27038000 -1.64225900 -0.21890800
F -3.65894300 -2.44566700 -2.24267100
F -1.00311800 -2.18247100 -2.03998300
H 4.28660300 -2.42299000 0.20442300

H 5.12481200 -1.82318500 1.67703600
H 3.64840900 -2.82553600 1.82197500
H 3.63737800 1.66674600 0.34550600
H 5.11491600 0.71629700 0.67144800
H 4.14127900 0.38452900 -0.79869600
H 2.64636700 -0.66905400 3.55555800
C -0.74715200 2.23429100 0.24128400
C -0.19420900 2.88649700 1.33752000
C -1.06644200 3.44508300 2.26772700
C -2.44413200 3.33886600 2.08845500
C -2.96760200 2.68398800 0.97538500
C -2.11591000 2.12023900 0.02970900
H 0.88502400 2.95572500 1.46620400
H -0.66368300 3.96300200 3.13584100
H -3.11831600 3.77232300 2.82443000
H -4.04465500 2.60322800 0.83993700
H -2.50961600 1.59734300 -0.84093100
I 0.56771600 1.29326900 -1.14745600
Cl 2.47542900 -1.70223700 -2.02289200
Cl 0.46282600 3.49148700 -2.71478400

8
E (M06-SMD/SDD) = -1750.772620 au
H (M06-SMD/SDD) = -1750.250016au
G (M06-SMD/SDD) = -1750.343422 au
E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -1751.249765au
C -0.16875800 -0.88878400 0.56902500
H -1.68645000 -2.60123600 2.87821400
N 0.87544300 -1.45243100 1.20172400
C 0.41870500 -2.24291600 2.24290400
C -0.93398800 -2.14833300 2.24576900
N -1.27993100 -1.30058400 1.20645800
H 1.10402100 -2.79574100 2.87224800
C 1.84993100 -2.83917300 -1.11387900
C -2.63329300 0.51563200 2.97260600
C 2.25443200 -1.27615600 0.83303200
C 3.04794200 -0.42251200 1.60639700
C 4.37361200 -0.24890300 1.21046500
C 4.89998000 -0.89824200 0.09240000
C 4.06620800 -1.73760800 -0.64960200
C 2.73379100 -1.94696800 -0.29741300
C 2.49668100 0.30147900 2.79608900
H 5.01059900 0.42119300 1.79057100
C 6.33639900 -0.71874600 -0.29224900
H 4.46488200 -2.25062900 -1.52647600
C -2.61940200 -0.89908700 0.86764700
C -3.21052700 -1.41093200 -0.29538600
C -4.51108900 -1.00368600 -0.58515100
C -5.20742200 -0.11626100 0.23851500
C -4.57616600 0.36771400 1.38405200
C -3.27753000 -0.01000200 1.72530600
C -2.48485800 -2.34811300 -1.21296200
H -4.99718800 -1.39718500 -1.47950700
C -6.59662500 0.31807700 -0.11450800
H -5.10976300 1.05935700 2.03798300
H 1.55293500 0.81515500 2.55859200
H 3.20976300 1.05336600 3.15329900
H 2.28996400 -0.38191800 3.63191300
H 2.44233000 -3.44682000 -1.80705200
H 1.13988500 -2.25079100 -1.71857500
H 1.25448100 -3.51700400 -0.48646800
H 6.47673500 -0.80621900 -1.37672600
H 6.96636800 -1.48741800 0.17813300
H 6.72139200 0.25664000 0.02959600
H -7.14103000 0.68172200 0.76529700
H -7.17135000 -0.50249800 -0.56219300
H -6.57804800 1.13521600 -0.84970100
H -1.57110200 0.75622100 2.82501600
H -2.68405200 -0.21580100 3.79198000
H -3.14298600 1.42371700 3.31499100
H -3.19109700 -2.88083900 -1.86014200
H -1.88889100 -3.09284600 -0.66818300

H -1.79536900 -1.80393600 -1.88541800
C 0.57792200 1.80292800 -0.04933400
C -0.31691700 2.49630000 0.74109000
C 1.91353600 2.10925300 -0.21670900
Au -0.14063700 0.21164700 -1.13584200
Cl -0.17686300 1.33967200 -3.19321900
C 0.18956500 3.60932000 1.41957500
C 2.38354200 3.22610300 0.47954800
C 1.52854800 3.96629600 1.29115400
H 2.57028000 1.52995200 -0.86250400
H 3.42986800 3.50770600 0.37171200
H 1.90954400 4.83314400 1.82729800
H -0.48091300 4.18901200 2.05153300
H -1.36171200 2.20496300 0.83327100

TS_{7-10}

E (M06-SMD/SDD) = -2453.967803au

H (M06-SMD/SDD) = -2453.345224au

G (M06-SMD/SDD) = -2453.462227au

E (M06-SMD/DEF2TZVP//M06-SMD/SDD) = -2740.954744au

C 0.96633100 -1.83485500 -0.16958500
H 0.79117600 -5.07392100 0.13204500
N 2.26506300 -2.15749800 -0.01024200
C 2.39808300 -3.53083700 0.13273700
C 1.15269400 -4.05556600 0.06771400
N 0.27971500 -2.99564400 -0.11685800
H 3.37068600 -3.98741800 0.26383700
C 3.41037600 -1.15929000 -2.46809500
C -1.23403800 -3.06424200 2.33652100
C 3.36870500 -1.23732500 0.06290400
C 3.86667700 -0.90880600 1.32866200
C 4.92250900 0.00031300 1.38713600
C 5.47724300 0.55745800 0.23458700
C 4.96465300 0.17609700 -1.00740700
C 3.91349500 -0.73267600 -1.12376600
C 3.29413500 -1.50344100 2.57860600
H 5.31628500 0.28559600 2.36444400
C 6.62407900 1.51807800 0.31766000
H 5.40478700 0.58816800 -1.91732700
C -1.15135500 -3.12407000 -0.19565200
C -1.73888700 -3.35514000 -1.44633200
C -3.13032400 -3.38705600 -1.50013300
C -3.91721900 -3.23273600 -0.35548900
C -3.28321600 -3.09226600 0.87887300
C -1.89162000 -3.05780600 0.98930100
C -0.91466200 -3.64787100 -2.66160000
H -3.61532400 -3.54880000 -2.46461200
C -5.41163800 -3.24299300 -0.46331200
H -3.88405600 -3.02703300 1.78801900
H 2.19631000 -1.44302000 2.59509600
H 3.67411300 -0.98175700 3.46468100
H 3.56079900 -2.56545200 2.67971000
H 4.13515300 -0.90153100 -3.24891600
H 2.45811100 -0.67216000 -2.72501800
H 3.23215900 -2.24324900 -2.51228700
H 6.50957900 2.34195400 -0.39830200
H 7.57392300 1.01782200 0.08008900
H 6.72071100 1.94639600 1.32256000
H -5.88957900 -3.21033700 0.52326600
H -5.76762900 -4.14178400 -0.98482800
H -5.77106400 -2.37974300 -1.04102000
H -0.27746600 -2.52757400 2.35414600
H -1.02517100 -4.09989600 2.64483200
H -1.88820400 -2.62465700 3.09972200
H -1.49218400 -3.47151300 -3.57642900
H -0.60508700 -4.70412900 -2.66281200
H -0.00752400 -3.03479100 -2.71547400
C 0.48245900 0.53721000 1.44922200
C -0.43009900 0.16572400 2.42724200
C 1.58538600 1.33084300 1.74951100
Au 0.16419200 0.04112800 -0.52379900
Cl -0.70871800 5.62502100 -2.23825000
C -2.53567900 2.01757900 0.62250100

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C -3.53841200 2.35957100 2.76346600
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C -2.56902900 2.71033600 1.82523300
I -1.01932400 2.53683300 -0.80446100
H -5.09331200 -0.14473800 1.06350600
H -5.19248600 1.06354100 3.22966000
H -1.84570900 3.49617900 2.03768100
H -3.37696100 0.46530600 -0.63031400
H -3.58070500 2.89169900 3.71222900
Cl -0.19512600 -0.31697200 -2.93794800
C -0.21870000 0.57821400 3.74487900
C 1.77988600 1.74608900 3.06692600
C 0.88475700 1.36351600 4.06434900
H 2.28404300 1.63938200 0.97119800
H 2.63972200 2.37071900 3.30771200
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H -0.93299100 0.28915500 4.51560700
H -1.31264500 -0.42181800 2.17551900
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