

“Supporting Information”

A mechanistic investigation of the gold(III)-catalyzed hydrofurylation of C-C multiple bonds

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Contents:

Figure S1. A calculated energy profile for AuCl₃-catalyzed hydroarylation where allenyl ketone is activated by a second AuCl₃ (page S3).

Figure S2. A calculated energy profile a pathway in which the deauration occurs directly from 3-furyl complex **3** with a pathway in which **3** is initially isomerized to 2-furyl complex **5** and then the deauration takes place (page S4).

Figure S3. A calculated energy profile comparing the energetics of the ring closure process and the nucleophilic attack of the 2-furyl complex **5** on the π -complex **1** (page S5).

Figure S4. A calculated energy profile comparing the energetics of the direct substitution reaction and the solvent-assisted substitution reaction (page S6).

Figure S5. A calculated energy profile comparing the energetics of the nucleophilic attack on the central and terminal carbons of the allenyl ketone with the ring closure process (page S7).

Table S1. Cartesian coordinates and total energies for all of the calculated structures (page S8)

Table S2. Cartesian coordinates and total energies for the structures optimized by inclusion of dispersion (page S54)

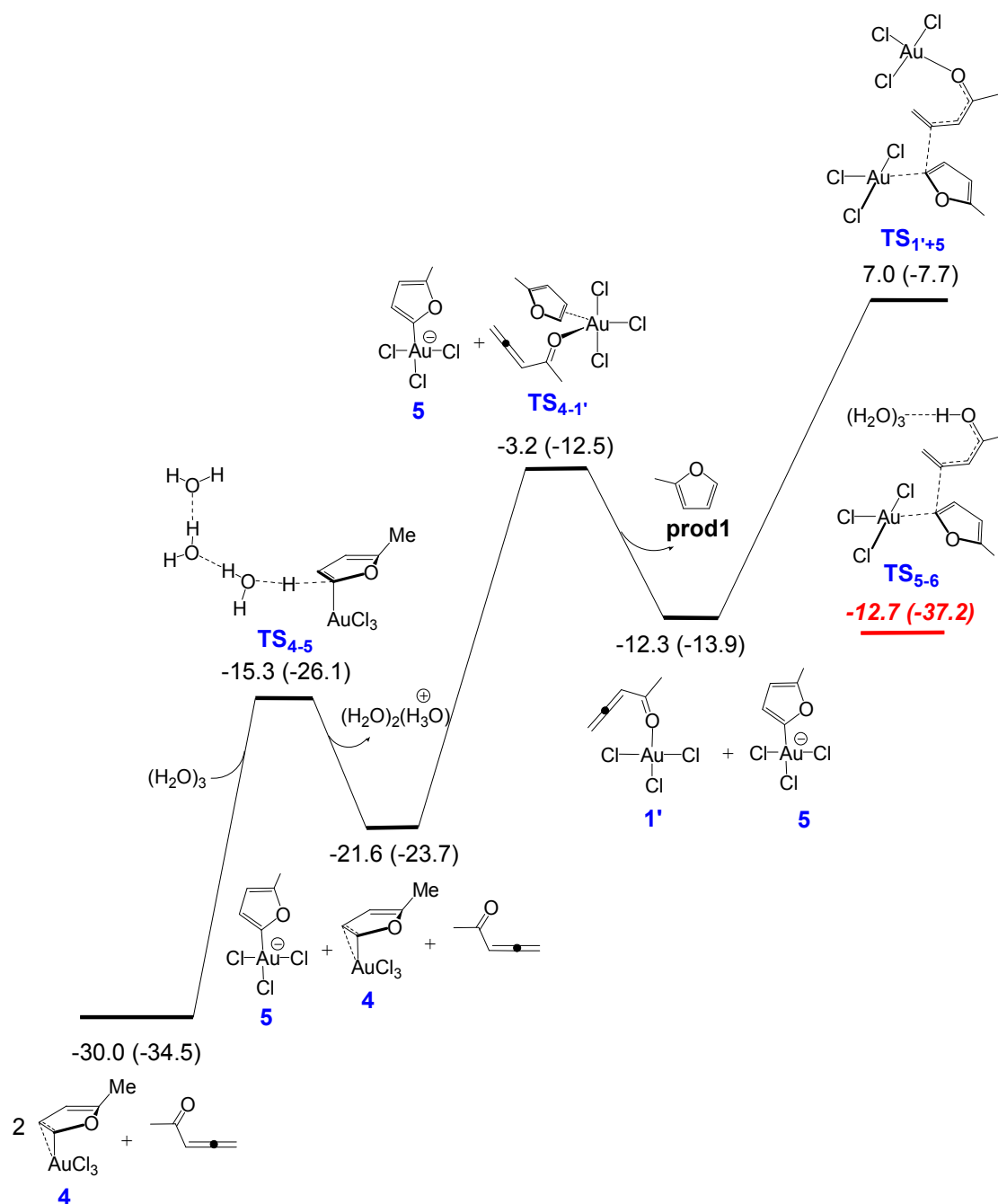


Figure S1. A calculated energy profile for AuCl₃-catalyzed hydroarylation where allenyl ketone is activated by a second AuCl₃. This alternative pathway was found to be about 19.7 kcal/mol higher in energy than the one activated by the proton (see TS₅₋₆). The relative Gibbs and potential energies (in parentheses) obtained from the M06/BS2//B3LYP/BS1 calculations in acetonitrile are given in kcal/mol.

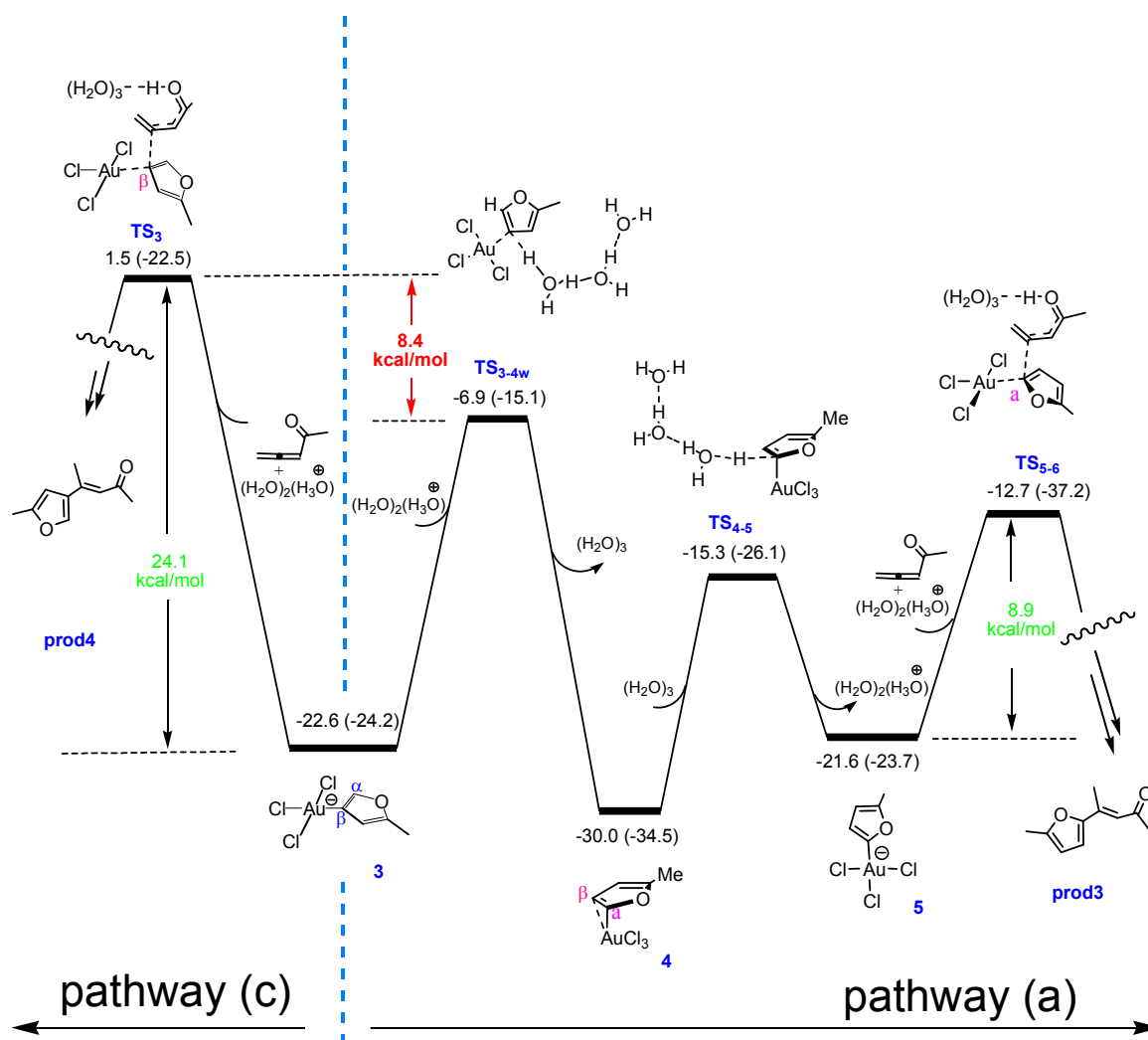


Figure S2. A calculated energy profile comparing pathways (c) and (a). In pathway (c), the deauration occurs directly from 3-furyl complex **3** while in pathway (a), **3** is initially isomerized to 2-furyl complex **5** and subsequently the deauration takes place from **5**. The relative Gibbs and potential energies (in parentheses) obtained from the M06/BS2//B3LYP/BS1 calculations in acetonitrile are given in kcal/mol.

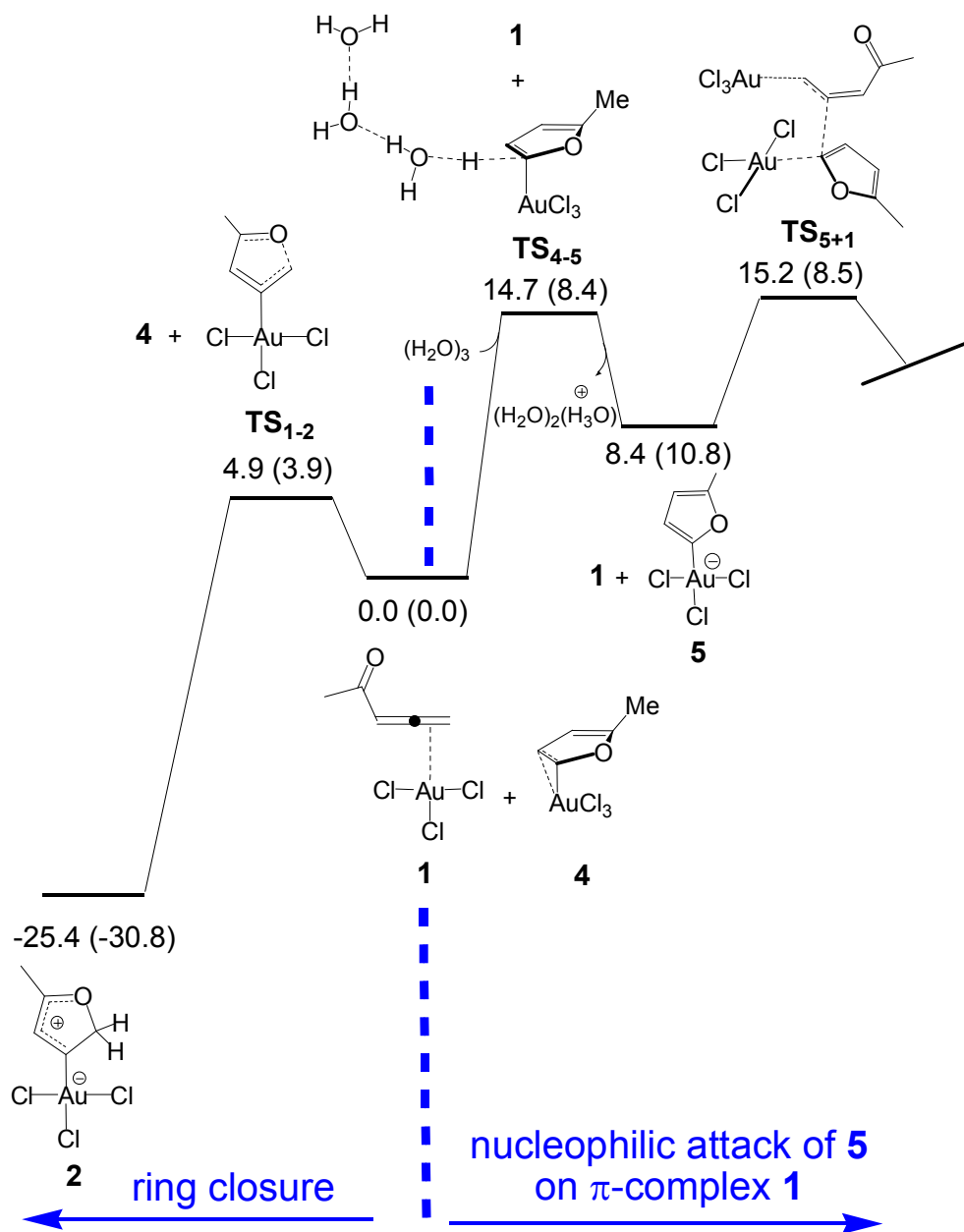


Figure S3. A calculated energy profile comparing the energetics of the ring closure process and the nucleophilic attack of the 2-furyl complex **5** on the π -complex **1**. The relative Gibbs and potential energies (in parentheses) obtained from the M06/BS2//B3LYP/BS1 calculations in acetonitrile are given in kcal/mol.

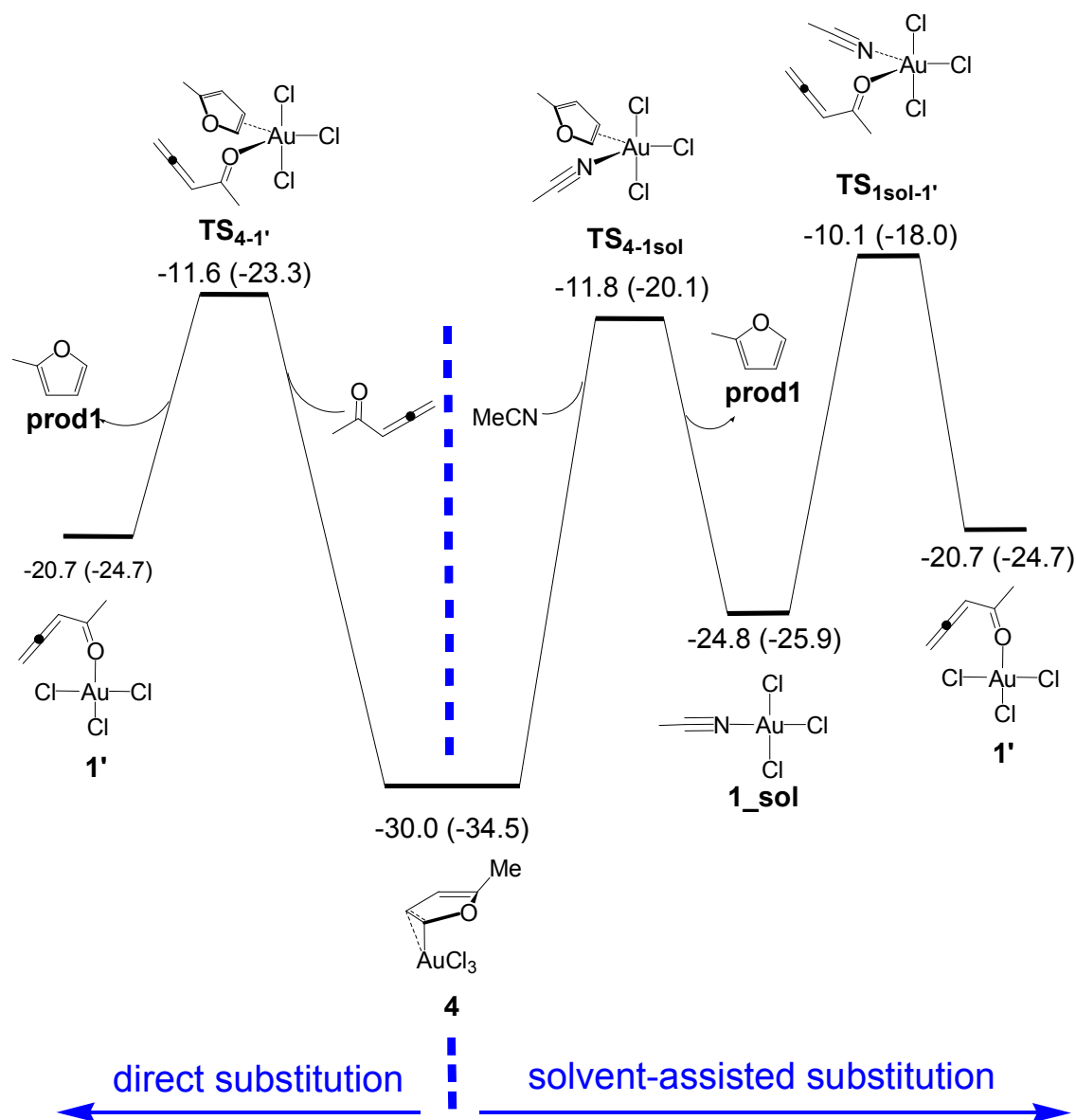


Figure S4. A calculated energy profile comparing the energetics of the direct substitution reaction and the solvent-assisted substitution reaction. The relative Gibbs and potential energies (in parentheses) obtained from the M06/BS2//B3LYP/BS1 calculations in acetonitrile are given in kcal/mol.

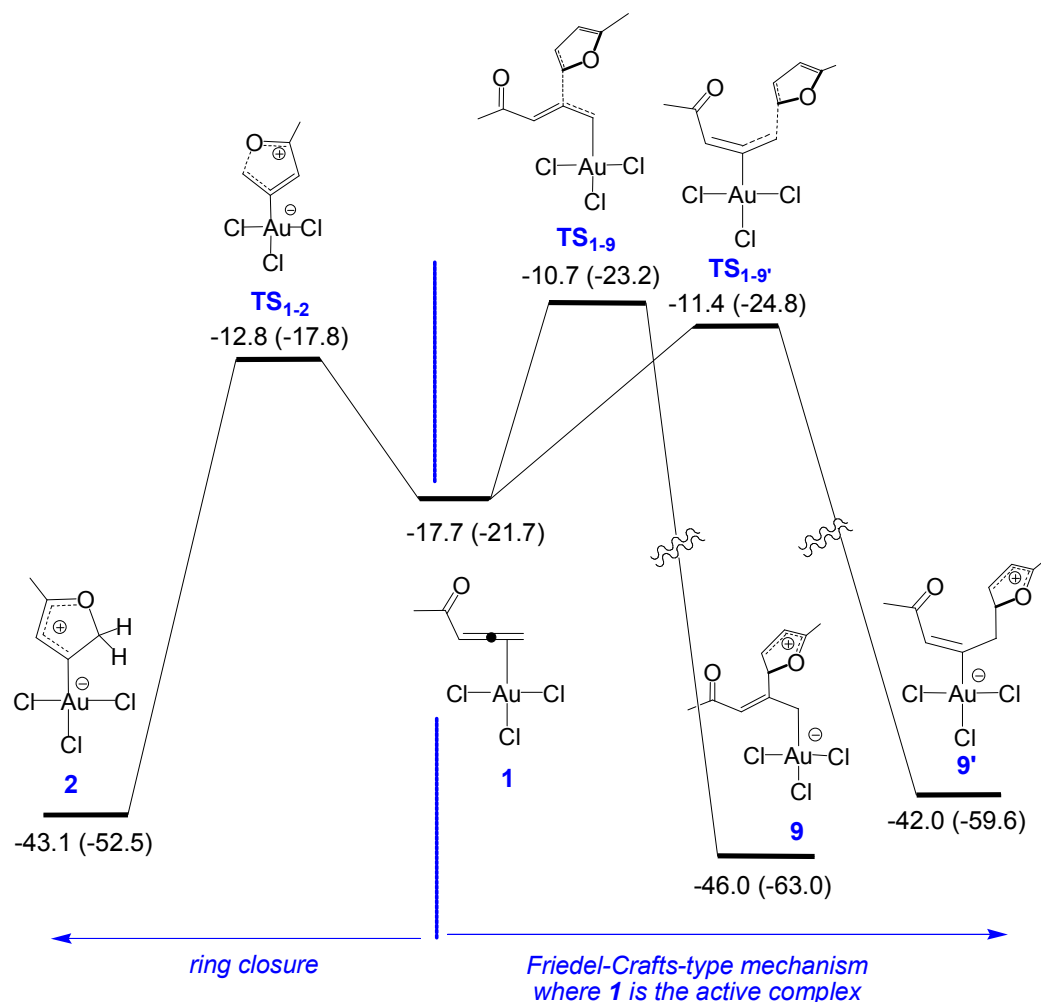


Figure S5. A calculated energy profile comparing the energetics of the nucleophilic attack on the central and terminal carbons of the allenyl ketone with the ring closure process. As illustrated, $\text{TS}_{1,9'}$ is 0.7 kcal/mol lower in energy than $\text{TS}_{1,9}$, indicating that the nucleophilic attack on the terminal carbon atom is slightly more favorable than that on the central carbon atom. The nucleophilic attack on the terminal carbon of allenyl ketone leads to a product that was not being detected experimentally. This result suggests that once **1** is formed, it is involved immediately in the ring closure and not the *Friedel-Crafts-type* process.

Table S1. Cartesian coordinates and total energies for all of the calculated structures**1**

E (B3LYP/BS1) = -1785.370950 au

H(B3LYP/BS1) = -1785.256949 au

G(B3LYP/BS1) = -1785.317474 au

E(M06/BS2//B3LYP/BS1) = -1785.613840 au

C	-1.58622700	0.00034100	-0.49202600
C	-2.41367100	-0.00009800	0.51786000
C	-0.93217200	0.00094200	-1.67142000
C	-3.91560100	0.00015300	0.25584700
C	-4.77509100	-0.00113300	1.49983600
O	-4.35758100	0.00134100	-0.87211200
H	-5.82831000	-0.00101900	1.21487200
H	-4.55551400	-0.88464400	2.11246500
H	-4.55577500	0.88135100	2.11404200
H	-0.75741500	0.93933800	-2.19485900
H	-0.75766800	-0.93684200	-2.19601300
H	-2.05582900	-0.00071500	1.54346900
Au	0.78567700	0.00002700	-0.11360900
Cl	0.72913800	-2.37112300	-0.12986700
Cl	2.83719700	-0.00076000	1.00525800
Cl	0.73009100	2.37120400	-0.12848300

Sub1

E (B3LYP/BS1) = -269.298094 au

H(B3LYP/BS1) = -269.196433 au

G(B3LYP/BS1) = -269.235010 au

E(M06/BS2//B3LYP/BS1) = -269.198739 au

C	-1.49404400	-0.34405800	-0.00003300
C	-0.24620500	-0.76017800	-0.00020800
C	-2.72657600	0.07690700	0.00013000
C	0.91762000	0.18413100	-0.00008900
C	2.28702400	-0.47577600	0.00015000
O	0.78231100	1.39443600	-0.00005700
H	3.06376200	0.29101200	-0.00009000
H	2.40370500	-1.11798800	0.88262300
H	2.40375700	-1.11862600	-0.88185500
H	-3.26156800	0.26663100	-0.92824000
H	-3.26140900	0.26628700	0.92866300
H	-0.03364900	-1.82896100	-0.00033700

TS1-2

E (B3LYP/BS1) = -1785.366027 au

H(B3LYP/BS1) = -1785.253014 au

G(B3LYP/BS1) = -1785.311002 au

E(M06/BS2//B3LYP/BS1) = -1785.607630 au

C	1.39610900	0.00041500	0.13869400
C	2.34064600	0.00026500	-0.78307000
C	1.32391600	0.00025600	1.50598900
C	3.72089800	0.00030500	-0.17658300
C	4.88849800	-0.00026300	-1.13233200
O	3.85945400	0.00042200	1.03754500
H	5.82812300	0.00374900	-0.57840700
H	4.84042000	-0.88529800	-1.77879200

H	4.83647700	0.87939800	-1.78569600
H	1.23240400	0.93728700	2.05305500
H	1.23272700	-0.93686800	2.05294700
H	2.18548100	0.00010500	-1.85484900
Au	-0.74129800	0.00004200	0.03346100
Cl	-0.67603200	-2.37294400	0.06617700
Cl	-3.02852200	-0.00072200	-0.50656500
Cl	-0.67715900	2.37302300	0.06578500

2

E (B3LYP/BS1) = -1785.415083 au

H(B3LYP/BS1) = -1785.300157 au

G(B3LYP/BS1) = -1785.352905 au

E(M06/BS2//B3LYP/BS1) = -1785.662981 au

C	-1.26399700	-0.00002000	0.10206000
C	-2.21492700	-0.00049300	-0.89142100
C	-1.98931900	0.00058000	1.39365200
C	-3.47962200	-0.00020200	-0.27191000
C	-4.82971900	-0.00029900	-0.88868400
O	-3.40877300	0.00039500	1.03851100
H	-5.61009700	-0.00193400	-0.12608700
H	-4.94232900	0.88239700	-1.52922700
H	-4.94109800	-0.88107700	-1.53202400
H	-1.80148200	-0.89519700	1.99402000
H	-1.80149300	0.89693900	1.99315300
H	-2.04986000	-0.00100600	-1.96007300
Au	0.73632700	-0.00000900	-0.01994000
Cl	0.59577900	2.37619600	0.02488900
Cl	3.09729900	0.00001100	-0.18167900
Cl	0.59587800	-2.37620300	0.02533500

TS2-3w

E (B3LYP/BS1) = -2014.698191 au

H(B3LYP/BS1) = -2014.503422 au

G(B3LYP/BS1) = -2014.574684 au

E(M06/BS2//B3LYP/BS1) = -2014.952730 au

C	-1.49920200	-0.25128700	0.03209500
C	-2.53044600	-0.44043200	-0.89510100
C	-2.06449900	0.36169600	1.17362700
C	-3.70047900	-0.02522400	-0.27182100
C	-5.10290200	0.04748900	-0.76343300
O	-3.46324800	0.41622800	0.96299700
H	-5.78458200	-0.42611000	-0.04868500
H	-5.41657000	1.09234200	-0.87661200
H	-5.19539800	-0.45131200	-1.73052700
H	-1.81036000	0.11181600	2.20083600
H	-1.50782300	1.64378800	1.06082400
H	-2.44989000	-0.81009900	-1.90717300
Au	0.48300500	-0.51823700	-0.21810300
Cl	0.44803500	1.34055900	-1.75226700
Cl	2.85194800	-0.88916100	-0.53439100
Cl	0.37351500	-2.20136500	1.42560400
O	-0.84221600	2.69094400	0.95959700
H	0.03701500	2.48340000	1.47361800
O	1.38062000	2.07198700	2.08508500

H	2.10733900	2.16604600	1.39465100
H	-0.57040800	2.67871800	0.01415700
H	1.44525700	1.15813300	2.40666000
O	3.16218400	2.22319700	0.10796000
H	3.41451600	1.28423200	-0.01964100
H	2.61052100	2.38691800	-0.67733400

TS2-4

E (B3LYP/BS1) = -1785.371336 au

H(B3LYP/BS1) = -1785.258872 au

G(B3LYP/BS1) = -1785.314473 au

E(M06/BS2//B3LYP/BS1) = -1785.619140 au

C	-1.30264600	0.20796500	-0.01423200
C	-2.34243800	-0.61739100	-0.60160200
C	-2.02352400	1.14465100	0.76628200
C	-3.53839100	-0.16745900	-0.14687200
C	-4.95001100	-0.57210300	-0.36613600
O	-3.34503000	0.93258900	0.67903200
H	-5.43373800	-0.81946700	0.58547800
H	-5.52176400	0.23846300	-0.83219700
H	-4.98780000	-1.44795600	-1.01745800
H	-1.67591700	1.94125300	1.41063800
H	-1.42899300	1.41152300	-0.45048900
H	-2.16978500	-1.45819800	-1.25583200
Au	0.73625500	-0.02661000	-0.01645200
Cl	0.40819600	-2.35965900	0.21367700
Cl	3.08039000	-0.29274800	0.01514100
Cl	0.90883300	2.34663600	-0.25218900

3

E (B3LYP/BS1) = -1784.937784 au

H(B3LYP/BS1) = -1784.833100 au

G(B3LYP/BS1) = -1784.888760 au

E(M06/BS2//B3LYP/BS1) = -1785.234892 au

C	1.31727900	0.18948200	0.08213200
C	2.31775700	-0.69155500	-0.46044900
C	2.00384800	1.20361000	0.67451500
C	3.53088600	-0.14875700	-0.15934200
C	4.93692300	-0.56475900	-0.42511600
O	3.35858800	1.01576700	0.54494600
H	5.48698900	0.19511500	-0.99722800
H	5.49604100	-0.73889000	0.50472600
H	4.94420100	-1.49436700	-1.00239800
H	1.69950700	2.10375200	1.18222400
H	2.13826900	-1.61748000	-0.98627600
Au	-0.69840500	-0.01791100	0.00076600
Cl	-0.43046100	-2.37355900	0.23499400
Cl	-3.13657000	-0.26968300	-0.09475400
Cl	-0.90943300	2.34398100	-0.22209900

TS3-4w

E (B3LYP/BS1) = -2014.667254 au

H(B3LYP/BS1) = -2014.472997 au

G(B3LYP/BS1) = -2014.547970 au

E(M06/BS2//B3LYP/BS1) = -2014.934389 au

C	-0.82601800	-0.83724500	0.10277400
C	-1.45736600	-1.55270200	-1.00745900
C	-1.30975500	-1.49354700	1.22991100
C	-2.27204000	-2.49722100	-0.48331500
C	-3.19063300	-3.52493800	-1.04123500
O	-2.18816900	-2.44442000	0.91098000
H	-2.89830600	-4.53218900	-0.72164300
H	-4.22562900	-3.36144400	-0.71713600
H	-3.16189500	-3.48920400	-2.13322600
H	-1.11488800	-1.35356400	2.28288100
H	-1.30805600	-1.33862800	-2.05592900
Au	1.09413200	-0.00023900	-0.05445000
Cl	0.37963500	1.14823200	-2.04874300
Cl	3.29031600	0.89023100	-0.30978100
Cl	1.74528100	-1.06410300	1.95191000
H	-1.39692800	0.43712700	0.18514800
O	-1.79176100	1.61704400	0.03881300
H	-2.78746200	1.67660100	-0.18822600
O	-4.30821000	2.14620600	-0.21966600
H	-4.17635700	2.87008000	0.44321700
H	-4.94493500	1.53151000	0.17633500
H	-1.26034300	1.85204700	-0.76697400
O	-3.13564000	3.84062700	1.52594500
H	-3.21634400	3.91477000	2.48862500
H	-2.27911900	3.40586900	1.36828300

4

E (B3LYP/BS1) = -1785.426289 au
H(B3LYP/BS1) = -1785.309538 au
G(B3LYP/BS1) = -1785.365764 au
E(M06/BS2//B3LYP/BS1) = -1785.668771 au

C	1.53788500	1.45733600	0.99729700
C	2.71415700	0.75157900	1.19995900
C	1.15166300	1.27051400	-0.36580800
C	3.06842600	0.21207300	-0.04179400
C	4.21324200	-0.63504900	-0.45590500
O	2.19651200	0.56443100	-0.98071400
H	3.84179500	-1.59674500	-0.82542700
H	4.76666100	-0.15470500	-1.27106800
H	4.88730900	-0.81016500	0.38463600
H	0.71852800	2.02548000	-1.01209200
H	3.25291200	0.60711400	2.12519200
Au	-0.61789200	-0.03292300	-0.04854300
Cl	0.71770200	-1.97819800	0.15576700
Cl	-2.58938100	-1.32769700	0.12804000
Cl	-1.85169300	1.99145300	-0.13325200
H	0.95928600	2.02128300	1.71744700

TS4-5

E (B3LYP/BS1) = -2014.696178 au
H(B3LYP/BS1) = -2014.501673 au
G(B3LYP/BS1) = -2014.573040 au
E(M06/BS2//B3LYP/BS1) = -2014.951708 au

C	2.23831900	-0.28734400	1.46187400
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C	3.57704500	-0.32071100	1.05242800
C	1.46111000	0.19840900	0.39546800
C	3.58529400	0.07369900	-0.27685000
C	4.69254200	0.26892800	-1.25051900
O	2.34761200	0.35559900	-0.69388600
H	4.48616100	-0.27322500	-2.17980700
H	4.80096900	1.32999800	-1.50657000
H	5.63647700	-0.08702200	-0.83134500
H	1.06488500	1.51296100	0.74287100
H	1.84258500	-0.54437400	2.43437400
H	4.44341800	-0.58997700	1.64027100
Au	-0.42215400	-0.44971700	-0.18455800
Cl	-0.25477600	-2.27036500	1.29988300
Cl	-2.62174100	-1.20832300	-0.84509200
Cl	-0.59969900	1.42600200	-1.70857200
O	0.68392700	2.66713800	0.86187700
H	-0.16844500	2.60348900	1.45651400
O	-1.44625700	2.30519900	2.21367300
H	-2.16859900	2.05182600	1.56047300
O	-3.23515800	1.71475500	0.34294200
H	-3.38625000	0.74979800	0.27285600
H	0.34440900	2.81112600	-0.05080800
H	-1.80925800	3.02082800	2.75734600
H	-2.76737500	1.89845400	-0.49303500

5

E (B3LYP/BS1) = -1784.935943 au

H(B3LYP/BS1) = -1784.832574 au

G(B3LYP/BS1) = -1784.886045 au

E(M06/BS2//B3LYP/BS1) = -1785.234152 au

C	-2.04469200	0.00062300	1.52360200
C	-3.42267700	0.00047100	1.11593400
C	-1.30701300	0.00019000	0.37749300
C	-3.42921900	-0.00003100	-0.24676200
C	-4.50328800	-0.00044800	-1.27814000
O	-2.13578200	-0.00022500	-0.70768800
H	-4.44511100	0.88314200	-1.92802600
H	-4.44542700	-0.88480800	-1.92701100
H	-5.48410800	0.00000500	-0.79139600
H	-1.65711500	0.00103900	2.53195000
H	-4.29554800	0.00073000	1.75663700
Au	0.66979400	0.00001800	0.02604400
Cl	0.59878500	2.38272900	0.03369600
Cl	3.08167600	-0.00031300	-0.36152500
Cl	0.59842900	-2.38268200	0.03424500

TS5-6

E (B3LYP/BS1) = -2283.996430 au

H(B3LYP/BS1) = -2283.692695 au

G(B3LYP/BS1) = -2283.781745 au

E(M06/BS2//B3LYP/BS1) = -2284.168190 au

C	-0.11826300	-2.37321900	1.20157300
C	1.04339200	-2.58854900	1.97110000
C	-0.03463800	-1.08600800	0.64232000
C	1.78250900	-1.43164600	1.89261700

C	3.05170600	-0.99160300	2.53827200
O	1.12087100	-0.51348600	1.13283500
H	3.79047700	-1.79913900	2.53556300
H	3.45978600	-0.11196700	2.03308700
H	2.86979900	-0.71807800	3.58617600
H	-0.95174800	-3.04390300	1.06357700
H	1.31627100	-3.48363600	2.51285500
Au	-1.51537100	0.18882700	0.00249400
Cl	-3.10233400	-1.54905800	0.27856400
Cl	-3.28530700	1.64176100	-0.68976800
Cl	-0.00202700	2.01197400	-0.32001200
C	0.69511100	-2.20907900	-1.17102600
C	2.08074000	-2.21743200	-1.08071900
C	-0.36148000	-2.55316000	-1.87154200
C	2.85425200	-1.11501500	-1.42722600
C	4.34770100	-1.10283900	-1.26918500
O	2.26778600	-0.05855400	-1.92121800
H	4.64128000	-0.31267800	-0.56723000
H	4.72072600	-2.06124100	-0.90289500
H	4.82683800	-0.87089300	-2.22718200
H	2.58322200	-3.09146800	-0.67867200
H	-0.20409200	-2.96805300	-2.86750800
H	-1.38608600	-2.42929900	-1.53705700
H	2.87936200	0.76175200	-1.99257900
O	3.68776500	2.08206300	-1.81244100
H	3.54863800	2.17860300	-0.82453300
O	3.05900400	1.87652800	0.76921400
H	2.73929000	2.69002300	1.23362400
O	1.60417800	3.96518900	1.81832600
H	0.82015300	3.70752900	1.29707900
H	3.17182600	2.79889100	-2.21608000
H	2.22199300	1.40407100	0.59381300
H	1.32797000	3.84998600	2.74080100

6

E (B3LYP/BS1) = -2054.762334 au

H(B3LYP/BS1) = -2054.538872 au

G(B3LYP/BS1) = -2054.611507 au

E(M06/BS2//B3LYP/BS1) = -2054.907130 au

C	-0.20744800	1.03215700	1.31211600
C	-1.39212500	1.85773900	1.51370700
C	0.61230900	1.79052300	0.41012500
C	-1.28020800	2.93040700	0.70535900
C	-2.14500500	4.08529800	0.36221300
O	-0.04805600	2.88049700	0.03731300
H	-3.04689700	4.06720000	0.97886800
H	-1.62459600	5.03588300	0.52729400
H	-2.44441200	4.04073700	-0.69122500
H	0.22703400	0.42653600	2.09956400
H	-2.22828100	1.61968700	2.15504600
Au	-0.81004500	-0.72856200	0.01063300
Cl	-0.02881700	-2.10982000	1.79249700
Cl	-1.52053500	-2.64699500	-1.19555000
Cl	-1.54856400	0.65969300	-1.76563200
C	1.96127000	1.56116200	-0.08834400

C	2.57978100	0.29464900	0.30689300
C	2.51487500	2.52872200	-0.86870800
C	3.74785000	-0.22865400	-0.12410700
C	4.24962100	-1.57697400	0.30312300
O	4.54577600	0.46114100	-0.98959000
H	5.21137100	-1.48975900	0.82732700
H	3.53659300	-2.07454700	0.96337200
H	4.40399600	-2.22369000	-0.57194600
H	2.02602300	-0.33187100	0.99417500
H	3.51635200	2.42464200	-1.26110000
H	1.95785000	3.42432100	-1.11736800
H	5.29582600	-0.09492100	-1.25239900

TS2-3s

E (B3LYP/BS1) = -2054.706811 au

H(B3LYP/BS1) = -2054.491522 au

G(B3LYP/BS1) = -2054.565344 au

E(M06/BS2//B3LYP/BS1) = -2054.852991 au

C	-1.09403900	-0.91319700	0.04308800
C	-2.05570000	-1.45628300	-0.83805200
C	-1.78255900	-0.53524200	1.19940500
C	-3.25732200	-1.46434700	-0.16182400
C	-4.62709300	-1.88273000	-0.56829500
O	-3.11886700	-0.94860300	1.07258200
H	-5.04701000	-2.59231700	0.15357400
H	-5.30182500	-1.01916400	-0.61365300
H	-4.60186400	-2.35539700	-1.55287600
H	-1.42597800	-0.51759900	2.22132300
H	-1.85934600	0.98384200	0.88045700
H	-1.89444400	-1.78235100	-1.85515500
C	0.40366900	2.13538600	1.94274400
C	0.11052500	2.82855600	0.84836600
C	0.74152800	1.49240500	3.01677200
C	-1.18762700	2.82683500	0.20902800
C	-1.47116300	3.85485600	-0.83698100
O	-2.12158100	2.00675400	0.46924600
H	-2.54333800	3.92534200	-1.02624300
H	-1.05570200	4.83003800	-0.56688300
H	-0.97037900	3.51727100	-1.75597800
H	1.17053900	0.48991100	2.93702900
H	0.60961300	1.92585100	4.00654200
H	0.87159800	3.46437000	0.40112200
Au	0.86415000	-0.54024800	-0.30227600
Cl	3.17729300	-0.00924200	-0.67023300
Cl	1.39141400	-1.80706000	1.63504900
Cl	0.19732700	0.75907600	-2.18891000

TS3-4s

E (B3LYP/BS1) = -2054.698870 au

H(B3LYP/BS1) = -2054.484054 au

G(B3LYP/BS1) = -2054.559805 au

E(M06/BS2//B3LYP/BS1) = -2054.840043 au

C	0.35034200	1.33046000	0.17441800
C	1.04373900	2.10475800	-0.85494100
C	0.39186800	2.16001700	1.29077900

C	1.47547600	3.25421800	-0.28722900
C	2.24667700	4.43519300	-0.75888700
O	1.07849900	3.27812800	1.05036200
H	1.67128400	5.36059500	-0.63619800
H	3.18537600	4.55168500	-0.20367600
H	2.48576500	4.31760700	-1.81894000
H	-0.00509000	2.04364100	2.28758100
H	1.19774700	1.78923800	-1.87549400
Au	-1.15236800	-0.07513300	-0.20701700
Cl	-0.03912000	-0.68163500	-2.21750800
Cl	-2.84925600	-1.69879800	-0.65519500
Cl	-2.15019000	0.38346800	1.90613500
H	1.24844800	0.28942900	0.53691100
C	4.19953700	-2.35915200	0.15120800
C	3.10095000	-2.65928800	0.82535700
C	5.27410200	-2.07136900	-0.51677600
C	2.01657700	-1.69632900	1.01309900
C	0.75430300	-2.17698100	1.65916000
O	2.18190600	-0.51723600	0.61286500
H	0.21338000	-1.37430000	2.16468600
H	0.08858700	-2.57472000	0.87797000
H	0.96304600	-2.99140900	2.35856500
H	6.15650800	-1.66858100	-0.02349300
H	5.32096700	-2.21622200	-1.59442800
H	2.96199700	-3.65933900	1.22954400

TS3

E (B3LYP/BS1) = -2283.980404 au

H(B3LYP/BS1) = -2283.677124 au

G(B3LYP/BS1) = -2283.766445 au

E(M06/BS2//B3LYP/BS1) = -2284.144855 au

C	-1.30383700	-2.53693500	0.06286400
C	-2.43074900	-2.70322200	-0.66437100
C	-0.76604900	-1.20558300	-0.24015600
H	-0.88532600	-3.23284800	0.77298300
Au	1.20826600	-0.57460900	-0.14853600
Cl	1.74964900	-2.43503300	1.21401500
Cl	3.48702500	0.20435100	0.06400800
Cl	0.77631100	1.24255600	-1.65045700
C	-1.71582400	-0.29058300	1.44063200
C	-3.00792200	0.22790900	1.22070000
C	-0.90123400	-0.47614400	2.46009900
C	-3.19453700	1.42906900	0.57281800
C	-4.51211300	2.14061500	0.49619600
O	-2.15404500	1.96214000	-0.03238300
H	-4.84573900	2.20579700	-0.54736000
H	-5.28032000	1.63235200	1.08254400
H	-4.40172500	3.16805300	0.86334400
H	-3.86498900	-0.30879600	1.61638000
H	-1.18636800	-0.01649000	3.40687000
H	0.02325700	-1.03962700	2.43623700
O	-2.61801300	-1.57038500	-1.47129900
C	-1.60855700	-0.73999200	-1.25649300
C	-3.45681700	-3.77105700	-0.79283900
H	-4.45305800	-3.41201600	-0.50714700

H	-3.51944500	-4.14033800	-1.82345800
H	-3.19485400	-4.61023400	-0.14333400
H	-1.60066500	0.18031500	-1.81670900
H	-2.21635300	2.96639300	-0.25649900
O	-1.85430200	4.46127800	-0.29326300
H	-0.99547400	4.33306400	0.22576700
O	0.25311200	3.60651100	1.03670500
H	1.17658200	3.66538400	0.67077200
O	2.73575400	3.44125800	-0.09016400
H	3.13952000	2.65129900	0.31880200
H	-1.57484600	4.74076400	-1.17950900
H	0.02218000	2.67182400	0.90879800
H	2.46966200	3.08651600	-0.95618600

TS5-6c

E (B3LYP/BS1) = -2054.200227 au

H(B3LYP/BS1) = -2053.993594 au

G(B3LYP/BS1) = -2054.065588 au

E(M06/BS2//B3LYP/BS1) = -2054.408636 au

C	0.93289200	-0.57173500	1.81560500
C	2.09061100	0.08239700	2.20553700
C	0.58777200	-0.08350400	0.52016600
C	2.36334300	1.03331700	1.21062500
C	3.42160700	2.06629900	1.06085500
O	1.37757300	1.05783400	0.31634500
H	3.84878400	2.00828800	0.05112700
H	2.99571500	3.06998800	1.18557900
H	4.21045200	1.92368700	1.80509800
H	0.43185500	-1.39874900	2.29576600
H	2.70355700	-0.10152200	3.07874000
Au	-1.41657600	0.04748600	0.00941000
Cl	-1.67986000	-2.22379100	0.71746800
Cl	-3.79111900	0.15027700	-0.50008800
Cl	-1.19400600	2.31434100	-0.65798400
C	1.64350700	-1.19452000	-0.75000100
C	2.97853200	-1.22976500	-0.35500600
C	0.89817200	-1.63726400	-1.75146200
C	4.05026900	-0.47023100	-0.94924700
C	5.47056000	-0.82429500	-0.47612900
O	3.92666700	0.43082300	-1.79055800
H	5.95789700	0.07738500	-0.08543100
H	5.50098400	-1.60725800	0.28909700
H	6.05927200	-1.15347300	-1.34068900
H	3.24933500	-1.90608300	0.45344000
H	1.35541100	-2.26990300	-2.51050500
H	-0.15654700	-1.42128800	-1.86731600

TS5-6b

E (B3LYP/BS1) = -2054.723637 au

H(B3LYP/BS1) = -2054.503667 au

G(B3LYP/BS1) = -2054.575762 au

E(M06/BS2//B3LYP/BS1) = -2054.850615 au

C	0.97470900	2.15719600	-0.27947700
C	2.18612700	2.30481000	-0.99885600
C	0.56959500	0.82098300	-0.41374300

C	2.46650600	1.07776000	-1.54150100
C	3.54955900	0.57654400	-2.42775300
O	1.47893500	0.18930000	-1.21212600
H	4.04819500	-0.29939100	-1.99876400
H	3.14250800	0.27749100	-3.40114500
H	4.29370100	1.36023800	-2.58771800
H	0.42183500	2.92524700	0.23719500
H	2.78760700	3.19791900	-1.09186800
Au	-1.24134600	-0.07597300	-0.16226100
Cl	-2.15734000	1.98854600	0.61487200
Cl	-3.41604700	-1.10611000	0.15484100
Cl	-0.43505500	-2.15128800	-1.00124700
C	1.60618700	0.75717100	1.71952100
C	2.87389000	0.28016400	1.42990400
C	0.71129900	1.11789800	2.60474000
C	3.13186900	-1.06486200	1.23299300
C	4.48916100	-1.59878900	0.91071100
O	2.13081700	-1.92263000	1.36325700
H	4.46649000	-2.11952200	-0.05582400
H	5.23205400	-0.80156600	0.86309500
H	4.79796600	-2.32827000	1.66950400
H	3.69693300	0.97784700	1.31857100
H	0.95267100	0.98314200	3.66008200
H	-0.26327900	1.52663400	2.36051300
H	2.40176600	-2.83401600	1.15279500

TS5-6a

E (B3LYP/BS1) = -2324.021536 au

H(B3LYP/BS1) = -2323.697936 au

G(B3LYP/BS1) = -2323.791560 au

E(M06/BS2//B3LYP/BS1) = -2324.065017 au

C	-3.20729200	1.17703900	0.02872600
C	-3.42505400	2.42564200	-0.59683400
C	-1.89257700	0.77020400	-0.26176100
C	-2.26520100	2.71752500	-1.27365700
C	-1.86067100	3.84809100	-2.15173300
O	-1.36055000	1.72437600	-1.10228800
H	-0.93220600	4.31076300	-1.79927200
H	-1.67832800	3.49237300	-3.17304600
H	-2.64610200	4.60728400	-2.18084400
H	-3.90904100	0.60460700	0.61463300
H	-4.31613600	3.03616200	-0.55560200
Au	-0.98904000	-1.06853900	-0.30158600
Cl	-2.94595800	-2.03805900	0.65771400
Cl	0.07842900	-3.21778700	-0.28341500
Cl	0.93814700	-0.17432100	-1.37854200
C	-1.42740000	1.49194600	1.75668100
C	-0.59769600	2.59142700	1.53716300
C	-1.89834400	0.66876700	2.66633600
C	0.77348900	2.41272200	1.43920100
C	1.71223400	3.50858300	1.03115200
O	1.28223800	1.24015900	1.73675900
H	2.22729500	3.21405100	0.10818300
H	1.18550600	4.45003200	0.86164300
H	2.48351100	3.65955400	1.79556400
H	-1.01750300	3.57284000	1.34126000

H	-1.64242000	0.86315100	3.70789300
H	-2.48583000	-0.21599000	2.44576400
H	2.24780900	1.12565600	1.45923100
C	5.88936100	0.06622100	-0.76038400
C	5.12785100	-0.81929100	-0.15008600
C	6.64257500	0.93891100	-1.36348400
C	3.97791500	-0.42866800	0.70004700
C	3.16303400	-1.54797400	1.28806100
O	3.70972000	0.76413200	0.89149400
H	2.46546500	-1.92829700	0.52690800
H	3.80049300	-2.38265300	1.59818500
H	2.56995600	-1.19597700	2.13460500
H	5.31987600	-1.88256100	-0.28045100
H	7.53556200	1.34171000	-0.88976800
H	6.40115400	1.29853800	-2.36172000

1'

E (B3LYP/BS1) = -1785.381290 au

H(B3LYP/BS1) = -1785.267065 au

G(B3LYP/BS1) = -1785.327844 au

E(M06/BS2//B3LYP/BS1) = -1785.618583 au

C	-4.18076600	0.00027100	-0.47700500
C	-3.59805000	0.00030700	0.71157600
C	-4.75109200	0.00019600	-1.64231300
C	-2.14300500	0.00025100	0.86454500
C	-1.54854700	-0.00019900	2.24134000
O	-1.42752700	0.00052100	-0.16201900
H	-0.90799200	0.88420100	2.35093900
H	-2.30886800	-0.00022000	3.02439900
H	-0.90847800	-0.88501800	2.35045300
H	-4.99265900	-0.93063600	-2.15187000
H	-4.99273000	0.93098300	-2.15192300
H	-4.19813900	0.00030900	1.61821400
Au	0.69584300	-0.00001200	-0.11638000
Cl	3.00202600	-0.00046400	-0.18363500
Cl	0.61852300	-2.36657400	-0.04761600
Cl	0.61981700	2.36657900	-0.04750800

TS1'-1

E (B3LYP/BS1) = -1785.368296 au

H(B3LYP/BS1) = -1785.255201 au

G(B3LYP/BS1) = -1785.312915 au

E(M06/BS2//B3LYP/BS1) = -1785.605672 au

Au	0.52976200	0.00000000	0.02148100
Cl	2.74289400	0.00005700	-0.75446200
Cl	0.47425500	2.36291600	0.07752600
C	-1.82497200	-0.00004600	1.61022900
C	-2.89279800	-0.00002200	0.85476400
C	-0.70533400	-0.00006700	2.31008100
C	-2.77011000	-0.00001400	-0.63977400
O	-1.68537900	-0.00004100	-1.20304600
H	-3.88904900	-0.00001000	1.29019000
H	-0.26774200	-0.93515700	2.65604900
H	-0.26771800	0.93500600	2.65606400
C	-4.06224800	0.00003400	-1.41727600

H	-4.65598500	-0.88361200	-1.15203600
H	-4.65584100	0.88380900	-1.15214000
H	-3.85436000	-0.00004200	-2.48780700
Cl	0.47433700	-2.36291300	0.07746000

TS1-9

E (B3LYP/BS1) = -2054.710983 au

H(B3LYP/BS1) = -2054.491675 au

G(B3LYP/BS1) = -2054.568110 au

E(M06/BS2//B3LYP/BS1) = -2054.849530 au

C	-1.15464300	0.76330600	0.18586500
C	-1.17246200	2.02266000	-0.17355000
C	-0.64456400	-0.44718700	0.59028500
C	-2.32011100	2.97726600	-0.39405200
C	-1.88949400	4.37453400	-0.78188100
O	-3.48863000	2.66229800	-0.27463300
H	-2.76885300	5.00494000	-0.92081200
H	-1.24374100	4.80184100	-0.00430600
H	-1.30117000	4.34628400	-1.70786500
H	-0.90804600	-1.31447200	-0.01814500
H	-0.61832200	-0.61398400	1.66761100
H	-0.17978500	2.45116900	-0.32528500
Au	1.48107300	-0.19982200	0.04585500
Cl	1.78980400	0.95505100	2.09522700
Cl	3.79242700	-0.08638800	-0.45817800
Cl	1.01330500	-1.31628500	-1.99519100
C	-3.64531900	-0.07367000	0.54230000
H	-3.86703300	0.79814800	1.13398200
C	-3.68677400	-0.32245500	-0.81369900
H	-3.86491600	0.41450400	-1.58185100
C	-3.46401200	-1.71691400	-0.97079600
C	-3.31828700	-2.23942100	0.29154400
H	-3.40906200	-2.27229400	-1.89636700
O	-3.44300200	-1.24049700	1.21936100
C	-3.10054200	-3.61601400	0.81067600
H	-2.21088000	-3.66765000	1.44888800
H	-3.95554900	-3.94723100	1.41287000
H	-2.97123100	-4.31281100	-0.02085800

9

E (B3LYP/BS1) = -2054.762202 au

H(B3LYP/BS1) = -2054.539513 au

G(B3LYP/BS1) = -2054.612088 au

E(M06/BS2//B3LYP/BS1) = -2054.913016 au

C	1.30027600	0.85800300	-0.44202700
C	1.20046000	2.19786900	-0.23951300
C	0.36961400	0.10975500	-1.30349600
C	2.07771100	3.04751800	0.59487800
C	1.71424000	4.51384300	0.65090300
O	3.05608100	2.62185600	1.21831200
H	2.42836900	5.05253900	1.27577500
H	1.70379800	4.94350300	-0.35858800
H	0.70128100	4.63242300	1.05602400
H	0.73118600	-0.87068800	-1.61032200
H	0.00685700	0.69210400	-2.14824500

H	0.36479300	2.70260500	-0.71697700
Au	-1.40179200	-0.28305700	-0.17998900
Cl	-2.29802000	1.72098200	-1.06242900
Cl	-3.40336500	-0.72078600	1.10778600
Cl	-0.35821000	-2.27701300	0.63302700
C	2.41607800	0.09045600	0.25283700
H	3.02520600	0.86201500	0.78656800
C	2.15391800	-1.00679500	1.20154500
H	1.54142200	-0.89041100	2.08435100
C	2.97237700	-2.06674700	0.87994000
C	3.63134500	-1.72336100	-0.30848100
H	3.06563400	-3.00885600	1.40099300
O	3.31560600	-0.51644500	-0.72711300
C	4.60569800	-2.49508800	-1.11975800
H	5.55396200	-1.94927000	-1.18920700
H	4.78423600	-3.47937600	-0.68378700
H	4.22413400	-2.61520500	-2.14051300

TS4-1

E (B3LYP/BS1) = -2054.709680 au

H(B3LYP/BS1) = -2054.490419 au

G(B3LYP/BS1) = -2054.568478 au

E(M06/BS2//B3LYP/BS1) = -2054.843584 au

C	-3.10461400	-0.37614500	-0.62008400
C	-3.79979100	0.49675600	0.25333900
C	-2.26393300	0.42141100	-1.37930700
C	-3.36292000	1.76892000	-0.02656800
C	-3.67510800	3.10268200	0.54792300
O	-2.44524500	1.73380600	-1.03627600
H	-2.78523500	3.54056500	1.01438600
H	-4.02257100	3.79554400	-0.22778500
H	-4.45342500	3.00953800	1.30893600
H	-1.71427000	0.23174200	-2.28771700
H	-3.19238800	-1.45085700	-0.69869600
H	-4.51331500	0.22548800	1.01785400
Au	-0.15897900	-0.59902900	0.03085100
Cl	-0.54828800	0.87442100	1.83377700
Cl	-0.01563700	-2.48140400	1.51116800
Cl	0.15713600	-1.97491900	-1.86831900
C	2.08610500	0.91545100	-0.52131400
C	3.17640500	0.56648400	0.10902800
C	1.01227800	1.31302000	-1.19638700
C	4.47233400	1.32457200	-0.08586400
C	5.64606700	0.79484500	0.71148800
O	4.54990900	2.28212700	-0.82849000
H	6.53079700	1.39974400	0.50610000
H	5.41922200	0.82035200	1.78484600
H	5.84285000	-0.25240500	0.44926000
H	0.85922900	0.96942400	-2.21721500
H	0.38138100	2.11302900	-0.81559900
H	3.16418800	-0.28195500	0.79037700

TS4-1'

E (B3LYP/BS1) = -2054.719500 au

H(B3LYP/BS1) = -2054.499959 au

G(B3LYP/BS1) = -2054.577881 au
E(M06/BS2//B3LYP/BS1) = -2054.849664 au

C	-1.37317200	1.83940900	-1.56081600
C	-1.90304100	2.86900500	-0.73859000
C	-0.02499700	1.75916100	-1.26108800
C	-0.85497200	3.36231300	-0.00174600
C	-0.74880100	4.41560100	1.04125800
O	0.29325200	2.70431100	-0.32859200
H	-0.42026900	3.98425600	1.99357400
H	-0.02234500	5.18559600	0.75398700
H	-1.72034700	4.89219900	1.19304000
H	0.80298000	1.23992900	-1.71591300
H	-1.89389300	1.22699400	-2.28349100
H	-2.93202600	3.19275100	-0.67601900
Au	-0.61619100	-0.65254000	-0.02659900
Cl	-0.82724000	0.41698200	2.06868800
Cl	-2.49539900	-2.02598800	0.40743700
Cl	-0.30405700	-1.61988100	-2.15913300
C	4.51365900	0.25027300	-0.15776900
C	3.99368200	-0.66446500	0.63878100
C	5.02259400	1.14855900	-0.94760100
C	2.53924400	-0.92468700	0.69642300
C	2.04834100	-2.02565000	1.60062100
O	1.76010600	-0.25150900	0.01010200
H	1.53892300	-2.78290000	0.99187100
H	2.85392700	-2.49983500	2.16534000
H	1.30293200	-1.61258800	2.29007800
H	5.15912500	2.17731300	-0.62036500
H	5.32166700	0.90233900	-1.96457100
H	4.64016200	-1.26387500	1.27600700

TS1'-8

E (B3LYP/BS1) = -2054.707301 au
H(B3LYP/BS1) = -2054.487385 au
G(B3LYP/BS1) = -2054.560522 au
E(M06/BS2//B3LYP/BS1) = -2054.840626 au

C	-2.79513000	1.82624000	0.10233200
C	-1.77040300	2.28929700	0.91350400
C	-3.51674000	2.07595000	-0.96757600
C	-0.47334100	1.75151500	0.86645100
C	0.61856200	2.28939200	1.74801200
O	-0.24134100	0.78198900	0.05151100
H	1.45358800	2.63277200	1.12580700
H	0.26934600	3.11751400	2.36898900
H	0.99658300	1.48831300	2.39568900
H	-4.36506200	1.48149700	-1.28278300
H	-3.24683100	2.93232900	-1.58332000
H	-1.98823700	3.05052800	1.65837100
Au	1.59585900	-0.16919800	-0.10003200
Cl	3.59513500	-1.32232000	-0.36000200
Cl	0.85487900	-1.68948800	1.57691000
Cl	2.25740000	1.45605700	-1.68513600
C	-2.68771400	-0.88292700	0.62142300
C	-4.56565500	-1.25406300	-0.53495700
C	-3.27397600	-1.70615600	-0.35475400

H	-1.68148500	-0.96219500	1.00997200
H	-2.80765600	-2.52805600	-0.87913600
O	-4.81553100	-0.20536900	0.28312600
C	-3.63836300	0.09760500	0.95583200
H	-3.80789600	0.57643100	1.90900800
C	-5.66522700	-1.68649800	-1.43718200
H	-6.58669200	-1.86165400	-0.87030200
H	-5.88434000	-0.92044500	-2.19137800
H	-5.38729200	-2.60774900	-1.95413400

8

E (B3LYP/BS1) = -2054.743250 au

H(B3LYP/BS1) = -2054.519487 au

G(B3LYP/BS1) = -2054.589443 au

E(M06/BS2//B3LYP/BS1) = -2054.874551 au

C	-3.51904900	-1.35741900	0.12498100
C	-2.48354800	-1.92765100	0.96573200
C	-4.77602500	-1.83059600	0.07936700
C	-1.21737100	-1.47748200	1.04075900
C	-0.15702900	-2.02407000	1.94021900
O	-0.80492300	-0.36845600	0.29906100
H	0.26003600	-1.23597100	2.57815800
H	-0.57656300	-2.80480000	2.57966700
H	0.66431100	-2.46322300	1.35844700
H	-5.52700300	-1.38981600	-0.56922300
H	-5.09166600	-2.66208700	0.70314300
H	-2.74781400	-2.76861500	1.59872100
C	-1.62693300	0.04598000	-0.93888600
C	-2.69867700	2.02374600	-0.52364700
C	-1.55848000	1.51963300	-1.04346800
H	-1.19577400	-0.55900000	-1.73562400
H	-0.70120400	2.08973400	-1.37235500
O	-3.61602900	1.07491300	-0.18263100
C	-3.12175400	-0.18112700	-0.72685000
H	-3.56160200	-0.26920200	-1.72844400
Au	1.32943600	-0.00749600	-0.01708300
Cl	1.32171000	-1.69447200	-1.68284900
Cl	3.57041100	0.43851800	-0.37691600
Cl	1.23233900	1.62682100	1.68932100
C	-3.11149400	3.43111300	-0.26964600
H	-2.31868500	4.12480400	-0.55738700
H	-4.02417500	3.67306800	-0.82631100
H	-3.33138900	3.56815200	0.79547400

Cl⁻

E (B3LYP/BS1) = -460.248731 au

H(B3LYP/BS1) = -460.246371 au

G(B3LYP/BS1) = -460.263754 au

E(M06/BS2//B3LYP/BS1) = -460.371685 au

Cl	0.00000000	0.00000000	0.00000000
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H₃O-Cl

E (B3LYP/BS1) = -690.074880 au

H(B3LYP/BS1) = -689.982625 au

G(B3LYP/BS1) = -690.025539 au

E(M06/BS2//B3LYP/BS1) = -690.105280 au

O	0.91392500	1.94174800	-0.06078000
H	1.83002800	0.49120500	0.05780900
H	0.88567500	2.40764600	0.78945500
H	-0.00300200	1.61632400	-0.18627200
O	2.22747000	-0.42187600	0.07436300
H	2.76516400	-0.47437300	-0.73076200
H	0.93584900	-1.41804800	-0.03186200
O	0.05828900	-1.91782300	-0.06719200
H	-0.00662400	-2.39746600	0.77499700
H	-0.94023600	-0.88225400	-0.05198900
Cl	-1.82731300	0.22591600	-0.01132400

Furan

E (B3LYP/BS1) = -269.338773 au
H(B3LYP/BS1) = -269.234381 au
G(B3LYP/BS1) = -269.269342 au
E(M06/BS2//B3LYP/BS1) = -269.233335 au

C	-1.55030300	0.61662200	0.00004500
C	-0.22276200	1.16415100	-0.00005200
C	-1.39778600	-0.73448000	0.00008100
C	0.63906400	0.10637600	-0.00022400
C	2.12375100	-0.01348100	0.00014900
O	-0.07256400	-1.06437900	-0.00017500
H	2.48488100	-0.55318700	0.88464700
H	2.48538700	-0.55412800	-0.88355000
H	2.57681300	0.98188600	-0.00024800
H	-2.08677100	-1.56537500	0.00043200
H	-2.48459100	1.16083900	0.00034000
H	0.05301100	2.20986900	-0.00021500

Prod3(Z-isomers)

E (B3LYP/BS1) = -538.698216 au
H(B3LYP/BS1) = -538.487524 au
G(B3LYP/BS1) = -538.541329 au
E(M06/BS2//B3LYP/BS1) = -538.493802 au

C	0.73185000	1.31736900	-0.07473900
C	1.89281600	0.60767900	-0.09228700
C	0.79979600	2.82632600	-0.21074600
C	2.14876600	-0.82431500	0.20068200
C	3.50181200	-1.34037200	-0.28176000
O	1.39045300	-1.55189300	0.82418500
H	3.59691300	-1.22306800	-1.36894500
H	4.32127500	-0.76991500	0.17449600
H	3.60484500	-2.39444600	-0.01642900
H	2.79542300	1.17964600	-0.30319600
C	-1.80523500	1.42707800	0.32545500
C	-2.21182700	-0.72732400	-0.11388700
C	-2.82882700	0.44190700	0.24735200
H	-1.92826700	2.46913700	0.58429200
H	-3.88543100	0.57590900	0.43326900
O	-0.87814900	-0.51961900	-0.25510700
C	-0.61694800	0.79582200	0.02513500
H	1.83444000	3.16833900	-0.29327200
C	-2.70323000	-2.10938600	-0.36613000

H	-3.78549200	-2.15576900	-0.21766900
H	-2.48032700	-2.43134200	-1.39093800
H	-2.22606100	-2.82601900	0.31272100
H	0.24298800	3.17606700	-1.08807000
H	0.35741900	3.31484500	0.66666700

MeCN

E (B3LYP/BS1) = -132.751485 au
 H(B3LYP/BS1) = -132.701304 au
 G(B3LYP/BS1) = -132.728818 au
 E(M06/BS2//B3LYP/BS1) = -132.704026 au

N	0.00000000	0.00000000	1.44082600
C	0.00000000	0.00000000	0.28063900
C	0.00000000	0.00000000	-1.18100300
H	0.00000000	1.02650000	-1.56120000
H	0.88897500	-0.51325000	-1.56120000
H	-0.88897500	-0.51325000	-1.56120000

AuCl₃

E (B3LYP/BS1) = -1516.027068 au
 H(B3LYP/BS1) = -1516.017010 au
 G(B3LYP/BS1) = -1516.058409 au
 E(M06/BS2//B3LYP/BS1) = -1516.367073 au

Au	-0.00000100	-0.23420400	-0.00024500
Cl	-2.30782700	-0.48990900	0.00051300
Cl	2.30782500	-0.48991500	0.00051300
Cl	0.00000600	2.06818300	0.00011400

Au₂Cl₆

E (B3LYP/BS1) = -3032.135799 au
 H(B3LYP/BS1) = -3032.113502 au
 G(B3LYP/BS1) = -3032.172478 au
 E(M06/BS2//B3LYP/BS1) = -3032.812406 au

Au	0.00000000	0.00000000	1.80204700
Cl	0.00000000	1.66899600	0.00000000
Cl	0.00000000	-1.66899600	0.00000000
Cl	0.00000000	1.64793400	3.43694300
Cl	0.00000000	-1.64793400	3.43694300
Au	0.00000000	0.00000000	-1.80204700
Cl	0.00000000	1.64793400	-3.43694300
Cl	0.00000000	-1.64793400	-3.43694300

(H₂O)₃

E (B3LYP/BS1) = -229.262781 au
 H(B3LYP/BS1) = -229.180933 au
 G(B3LYP/BS1) = -229.216770 au
 E(M06/BS2//B3LYP/BS1) = -229.296345 au

O	-0.10375900	1.57225000	0.12212800
H	-0.06458800	2.05672400	-0.71669700
H	0.66404900	0.94986300	0.08382700
O	1.42317000	-0.69036100	-0.09919900
H	0.50543900	-1.05520600	-0.14339300
H	1.78092200	-1.01492600	0.74098400
O	-1.31894200	-0.87409900	-0.10492200

H	-1.72974700	-1.09933500	0.74343300
H	-1.15983200	0.10055900	-0.05219900

(H₃O) , (H₂O)₂

E (B3LYP/BS1) = -229.612162 au
 H(B3LYP/BS1) = -229.520545 au
 G(B3LYP/BS1) = -229.559145 au
 E(M06/BS2//B3LYP/BS1) = -229.713823 au

O	-2.09503500	-0.47416100	0.01066100
H	-0.89471800	0.36243400	0.00022100
H	-2.67714400	-0.39346300	0.78581600
H	-2.67336900	-0.53282500	-0.76864500
O	0.00469400	0.90516500	0.06948700
H	0.04819500	1.61514200	-0.59858300
H	0.87637300	0.30609900	0.02692400
O	2.13855600	-0.39911400	-0.05815600
H	2.77163400	-0.26976600	0.66887900
H	2.16331500	-1.34273800	-0.29054500

(sub1-(H₃O) , (H₂O)₂)

E (B3LYP/BS1) = -498.954407 au
 H(B3LYP/BS1) = -498.758766 au
 G(B3LYP/BS1) = -498.820388 au
 E(M06/BS2//B3LYP/BS1) = -498.928127 au

C	-3.58249900	-0.28231600	0.23912700
C	-2.51083800	-1.02903700	-0.01828500
C	-4.63433600	0.43063900	0.48517000
C	-1.21303500	-0.44914900	-0.26083400
C	-0.03720900	-1.32158400	-0.56809300
O	-1.08186600	0.81624300	-0.21142200
H	0.76458500	-1.13610500	0.15944200
H	-0.30144800	-2.37947800	-0.56229700
H	0.36476800	-1.05345300	-1.55355600
H	-2.59656800	-2.11189300	-0.05830400
H	-5.27592300	0.78583700	-0.32012400
H	-4.91085600	0.69776500	1.50413300
H	-0.07767100	1.18496400	-0.41861800
O	1.19619000	1.61314400	-0.71073100
H	1.86186700	1.22850600	-0.05613500
O	2.70260200	0.30302600	0.96505800
H	3.57113200	-0.02611800	0.61607600
O	5.06061400	-0.61137600	-0.01410100
H	5.80207400	-0.03282300	-0.24904900
H	1.30186900	2.57786900	-0.73251200
H	2.88115400	0.63366100	1.85876500
H	5.46218900	-1.42834400	0.31923300

sub1-H

E (B3LYP/BS1) = -269.640063 au
 H(B3LYP/BS1) = -269.525792 au
 G(B3LYP/BS1) = -269.566911 au
 E(M06/BS2//B3LYP/BS1) = -269.609218 au

C	-1.51160900	-0.35579000	0.00051500
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C	-0.25669600	-0.83062500	-0.00090300
C	-2.71831100	0.10067000	0.00036500
C	0.87275100	0.02933000	-0.00109000
C	2.26869900	-0.48468300	0.00032600
O	0.65668700	1.31433200	-0.00016800
H	2.79248300	-0.13361200	0.90083600
H	2.30173300	-1.57432700	-0.02267400
H	2.81289000	-0.09345200	-0.87056300
H	-0.07512900	-1.90223800	-0.00169900
H	-3.24801300	0.29762500	-0.93240400
H	-3.24789700	0.29790600	0.93318400
H	1.48143900	1.84003300	-0.00061500

7

E (B3LYP/BS1) = -1593.902580 au

H(B3LYP/BS1) = -1593.696896 au

G(B3LYP/BS1) = -1593.767687 au

E(M06/BS2//B3LYP/BS1) = -1594.034016 au

C	0.90111800	1.39940900	-0.17501100
C	1.71160400	2.16788100	-0.95700200
C	1.30807800	3.52654800	-0.74080900
Cl	2.82004600	-0.94018300	-0.84794700
H	2.50115200	1.80929000	-1.59825500
Cl	0.39724500	-2.97720500	0.47730800
C	-1.57964600	-0.38189100	0.37257600
C	-2.38960600	-0.43940200	-0.65482400
C	-1.04025700	-0.30449300	1.60982000
C	-3.88514300	-0.33078500	-0.42302200
O	-4.34132000	-0.10379000	0.67821800
H	-2.01792100	-0.58354200	-1.66442300
H	-0.83820100	0.66774400	2.05207200
H	-0.95966600	-1.20292700	2.21869900
C	-4.73779100	-0.53021100	-1.65729600
H	-4.46837900	0.20064900	-2.43017600
H	-4.56211300	-1.52714800	-2.08106300
H	-5.79151000	-0.42134900	-1.39573900
Au	0.71482500	-0.59536500	0.12584400
O	0.02260500	2.20225900	0.51457100
C	0.28528000	3.50498100	0.16004900
C	-0.55524200	4.55300100	0.80082300
H	-0.26164000	5.53848800	0.42887000
H	-1.62045900	4.40785800	0.58136600
H	-0.44040900	4.55285700	1.89209500
H	1.73339700	4.40951800	-1.19837700

10

E (B3LYP/BS1) = -2055.973535 au

H(B3LYP/BS1) = -2055.726787 au

G(B3LYP/BS1) = -2055.802606 au

E(M06/BS2//B3LYP/BS1) = -2056.128512 au

C	-0.80661000	1.69246600	-0.94834300
C	-1.17147900	2.66212000	-0.03583600
C	-0.85696100	0.39605000	-0.31244200
C	-1.48910800	1.98064200	1.14770100
C	-1.87647100	2.48630100	2.48817000
O	-1.34627300	0.68131700	1.00870400

H	-2.22406900	3.52004900	2.43039700
H	-2.65343300	1.85256400	2.92600400
H	-1.00637300	2.44664700	3.15712900
H	-0.51203300	1.84543300	-1.97548300
H	-1.19309800	3.73374900	-0.17519700
Au	1.28768200	-0.13043300	0.02189600
Cl	2.08095300	1.27911200	-1.74501000
Cl	3.54237200	-0.75417600	0.46610400
Cl	0.56671200	-1.63887300	1.70084200
C	-1.60433900	-0.80573400	-0.92901300
C	-3.05294300	-0.43711200	-1.15882500
C	-4.07671600	-0.83740900	-0.38901500
C	-5.51950000	-0.51767100	-0.66184100
O	-3.83078200	-1.58450000	0.73383000
H	-5.96652000	0.03257900	0.17756700
H	-5.63061500	0.08573300	-1.56571400
H	-6.10457900	-1.43841400	-0.79832600
H	-3.28004900	0.17604700	-2.02752800
H	-4.66599000	-1.92394800	1.08875900
H	-1.54866700	-1.60212500	-0.18249800
C	-0.94486900	-1.28742100	-2.23328500
H	-0.90803200	-0.49743300	-2.99247000
H	0.07741300	-1.64150500	-2.06758600
H	-1.53101000	-2.11619400	-2.64163900

11

E (B3LYP/BS1) = -2016.669567 au

H(B3LYP/BS1) = -2016.451987 au

G(B3LYP/BS1) = -2016.524371 au

E(M06/BS2//B3LYP/BS1) = -2016.834652 au

C	-0.48370000	-0.27765100	1.40000900
C	-0.54026100	-1.67927500	1.76239800
C	-1.34659900	-0.14778400	0.27540900
C	-1.31592100	-2.29585600	0.84383200
C	-1.72357600	-3.69918800	0.59078100
O	-1.80110400	-1.34971200	-0.06683800
H	-1.33933400	-4.34473000	1.38422500
H	-2.81503800	-3.79462100	0.55465900
H	-1.32118400	-4.04813900	-0.36659300
H	-0.27292000	0.53987300	2.07800400
H	-0.01526300	-2.15202600	2.57939200
Au	1.35881700	0.16555900	0.03943400
Cl	1.32490200	2.31831000	1.05197300
Cl	3.41628200	0.65950400	-1.02199700
Cl	1.30338000	-1.92629000	-1.06234100
C	-1.90149300	1.04684700	-0.43156300
C	-3.26926300	1.37886000	0.12616500
C	-4.41901900	1.07304600	-0.49581200
C	-5.78328300	1.43133800	0.01859000
O	-4.37999700	0.39098700	-1.68234500
H	-6.39050900	0.52975900	0.17707500
H	-5.72214700	1.97394500	0.96445900
H	-6.31705600	2.06717400	-0.70168800
H	-3.31332300	1.89383300	1.07971300
H	-5.26759000	0.35746000	-2.06971800
H	-1.21225000	1.88469300	-0.28903100

H	-1.97001500	0.82546600	-1.50098700
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12

E (B3LYP/BS1) = -2324.119850 au

H(B3LYP/BS1) = -2323.788966 au

G(B3LYP/BS1) = -2323.875545 au

E(M06/BS2//B3LYP/BS1) = -2324.171888 au

C	-0.59615000	-0.72986300	1.09919100
C	-0.73913900	-2.17420400	1.29268500
C	-1.48180100	-0.43200600	0.01630800
C	-1.52981100	-2.63754400	0.30534300
C	-1.97279500	-3.97581900	-0.15556500
O	-1.98054700	-1.55207100	-0.47028000
H	-1.64761500	-4.73806000	0.55696900
H	-3.06383000	-4.02332500	-0.25027300
H	-1.53697200	-4.20825000	-1.13414900
H	-0.44514600	-0.01656000	1.90192400
H	-0.23280300	-2.76360000	2.04355800
Au	1.46739400	-0.53272700	0.20495200
Cl	2.06186900	0.51396200	2.25791200
Cl	3.71277600	-0.34391400	-0.54995600
Cl	0.89007400	-1.62208200	-1.83151100
C	-2.04883800	0.87710700	-0.49129100
C	-3.27269800	1.05170500	0.41248700
C	-4.49658800	0.50349700	0.28901300
C	-5.60763500	0.75962400	1.26978400
O	-4.80477600	-0.33453100	-0.74307000
H	-5.94842300	-0.17995300	1.72594500
H	-5.29170200	1.43229600	2.06954100
H	-6.47120200	1.21552200	0.76558200
H	-3.10234500	1.63193400	1.31091400
H	-5.74754900	-0.55856100	-0.70806400
C	-2.36072100	0.80261300	-2.00823800
H	-1.42548900	0.69932200	-2.56358900
H	-3.01392000	-0.03588100	-2.24477300
H	-2.85298400	1.73214200	-2.30725900
C	-1.18253200	3.18915400	0.47941500
C	0.78468400	3.13371800	-0.60693300
C	0.03738000	3.90181800	0.23529500
H	-2.00746800	3.52424900	1.09103100
H	0.32255400	4.86142500	0.64312300
C	-1.10347800	2.02588300	-0.22959200
O	0.08939100	1.98811500	-0.90469100
C	2.13068500	3.27711500	-1.22384100
H	2.58524000	4.21743100	-0.90026700
H	2.78993900	2.45138200	-0.93194600
H	2.06940900	3.27957300	-2.31911100

13

E (B3LYP/BS1) = -2168.086672 au

H(B3LYP/BS1) = -2167.851024 au

G(B3LYP/BS1) = -2167.925841 au

E(M06/BS2//B3LYP/BS1) = -2168.216863 au

C	1.03394400	1.60281500	-1.44422000
C	2.38010900	1.68973900	-1.74116100
C	0.87991800	1.27352700	-0.04754400

C	3.06014000	1.46746700	-0.53500000
C	4.51002600	1.38251400	-0.23323600
O	2.22074300	1.26618000	0.46012300
H	5.10285800	1.81728800	-1.04070200
H	4.73495800	1.88737100	0.71122400
H	4.79566700	0.32844900	-0.11675500
H	0.20095200	1.74957800	-2.11524100
H	2.83914900	1.87891100	-2.70124300
Au	0.23831500	-0.86857900	-0.06827300
Cl	-0.70160100	-0.73953200	-2.26237200
Cl	-0.39158000	-3.16226700	-0.02332400
Cl	1.10261600	-1.12096900	2.13332400
C	-0.04668600	2.14725500	0.86082500
C	-2.34420500	2.93267800	-0.13863900
C	-3.39180800	0.96872700	0.17687300
C	-3.58441800	2.23224700	-0.30220300
H	-2.13349500	3.96086100	-0.40104000
H	-4.50169700	2.61852300	-0.72421900
C	-1.47570400	2.04891200	0.42906300
O	-2.10515200	0.85093400	0.63426200
C	-4.24725800	-0.24392800	0.27866400
H	-5.24754400	-0.02588500	-0.10512600
H	-3.82298800	-1.07135500	-0.30234700
H	-4.34013300	-0.58195500	1.31764600
O	0.17671000	1.91862200	2.22398200
H	0.13905600	0.95919700	2.40706200
H	0.26318400	3.18621500	0.68717100

14

E (B3LYP/BS1) = -881.427116 au

H(B3LYP/BS1) = -881.352302 au

G(B3LYP/BS1) = -881.6701609 au

E(M06/BS2//B3LYP/BS1) = -881.5178759 au

C	0.28820100	-1.67030000	0.79336900
C	1.52086100	-2.35453500	1.03423800
C	0.49208400	-0.88728400	-0.31547700
C	2.39648900	-1.95072600	0.06321700
C	3.80567800	-2.30066000	-0.26063300
O	1.77817200	-1.05030100	-0.76038100
H	4.19773800	-2.99693100	0.48453900
H	3.87755000	-2.77497100	-1.24638000
H	4.44561500	-1.41068700	-0.27732000
H	-0.64278000	-1.78352900	1.33029500
H	1.72268100	-3.07599100	1.81346900
C	-0.33908700	0.05496400	-1.10035000
O	2.42170100	2.08508400	-1.40407600
H	2.82825300	2.30957300	-0.50988300
O	3.06741900	2.68307600	1.07122800
H	2.35599300	2.29573400	1.61856900
O	0.58801000	1.49129200	1.86416600
H	-0.02510600	1.85105800	2.52799600
H	2.49794900	2.88138300	-1.95700200
H	3.90714900	2.48058000	1.51101100
H	0.56987900	0.51957400	1.97160100
C	-2.83995100	-0.07458400	-1.77100300

C	-3.63267300	-0.07471000	0.33095900
C	-4.02598800	-0.11738600	-0.97659400
H	-2.77563300	-0.08922900	-2.85052900
H	-5.04508500	-0.17246100	-1.33210800
C	-1.79319900	-0.02110200	-0.89773600
O	-2.26169900	-0.01436500	0.39668000
C	-4.37039000	-0.07940200	1.62286700
H	-5.44492900	-0.13646900	1.43351500
H	-4.08799800	-0.93743600	2.24481300
H	-4.17556100	0.83190600	2.20143100
O	0.11077900	1.51721000	-0.79280900
H	1.14013400	1.75406300	-1.13717400
H	-0.11118600	-0.01547500	-2.16460000
H	0.11814100	1.62769700	0.20214900

15

E (B3LYP/BS1) = -575.9798109 au

H(B3LYP/BS1) = -575.772627 au

G(B3LYP/BS1) = -575.824815 au

E(M06/BS2//B3LYP/BS1) = -575.7959549 au

C	0.07055800	-1.14079900	0.00011300
C	-2.40237800	-1.70073400	-0.00001000
C	-3.08629700	0.42885100	-0.00025200
C	-3.53822200	-0.88549100	-0.00018500
H	-2.36647700	-2.78219400	0.00006400
H	-4.57347100	-1.19548000	-0.00030800
C	-1.28918900	-0.85086200	0.00005900
O	-1.73530300	0.45661800	-0.00015200
C	-3.79547000	1.72936100	0.00023300
H	-4.87580000	1.57266800	-0.00612300
H	-3.52882300	2.31568200	0.88818400
H	-3.51884700	2.32195500	-0.88035800
C	1.27599000	1.14689100	-0.00011600
C	3.29869200	0.18588000	0.00005000
C	2.64288800	1.41850000	-0.00014600
H	0.46050100	1.85549000	-0.00017200
H	3.12336100	2.38661000	-0.00020700
H	0.32855800	-2.19680500	0.00019600
C	1.13581300	-0.25106200	0.00003700
O	2.40466500	-0.81289500	0.00016900
C	4.73468300	-0.17803200	0.00001600
H	5.35649300	0.71909700	0.00142900
H	4.97833400	-0.78221400	0.88239700
H	4.97886000	-0.77961400	-0.88403400

16

E (B3LYP/BS1) = -2360.797288 au

H(B3LYP/BS1) = -2360.710152 au

G(B3LYP/BS1) = -2361.024469 au

E(M06/BS2//B3LYP/BS1) = -2361.049257 au

C	-0.72639000	-0.22309800	1.75081700
C	-1.13748100	-1.39009500	2.35880000
C	-0.58341400	-0.45469900	0.32892200
C	-1.29532400	-2.33199200	1.33103500
C	-1.65651700	-3.77008100	1.37890800
O	-1.02138900	-1.81646300	0.15239500

H	-2.09467800	-4.03062200	2.34456800
H	-2.35383600	-4.01444600	0.57175200
H	-0.75404700	-4.37731700	1.22798100
H	-0.54712000	0.73736700	2.20884900
H	-1.29823200	-1.57217400	3.41189500
Au	1.57373000	-0.52544600	-0.10637500
Cl	2.18012600	0.30659700	2.05669900
Cl	3.88420600	-0.63260000	-0.67000700
Cl	1.03284600	-1.38450600	-2.25436400
C	-1.28163400	0.49355600	-0.68645000
C	0.08640700	2.49619900	-1.66694500
C	0.04760500	3.74226500	0.20344600
C	0.51025700	3.73259100	-1.07855400
H	0.29398000	2.13648100	-2.66501100
H	1.09824100	4.50841200	-1.54850400
C	-0.61730100	1.83360800	-0.70746200
O	-0.65158000	2.58398600	0.44509300
C	0.16295500	4.70106000	1.33571000
H	0.71935800	5.58564500	1.01461700
H	-0.82170000	5.02682400	1.69402200
H	0.69548800	4.25290600	2.18360800
C	-3.59170800	1.50487900	0.12022400
C	-4.80876800	-0.28099800	-0.49536700
C	-4.91467500	0.95536400	0.07106600
H	-3.29429500	2.46997700	0.50233200
H	-5.82849500	1.42605800	0.40690200
H	-1.11734900	0.04251800	-1.66972900
C	-2.76349200	0.56783300	-0.42505400
O	-3.49550500	-0.53219400	-0.79954900
C	-5.79148000	-1.34525900	-0.83967600
H	-6.79763500	-1.02741400	-0.55305900
H	-5.79272100	-1.55823900	-1.91576500
H	-5.57011300	-2.28648800	-0.32041100

TS5-11

E (B3LYP/BS1) = -2245.932199 au

H(B3LYP/BS1) = -2245.633494 au

G(B3LYP/BS1) = -2245.719658 au

E(M06/BS2//B3LYP/BS1) = -2246.120006 au

C	0.14136400	-2.54848000	0.65686700
C	1.29400800	-2.71268900	1.43517300
C	0.06129300	-1.19839500	0.27785500
C	1.86329300	-1.45719700	1.56837800
C	3.03014900	-0.95006100	2.34773400
O	1.10349800	-0.54277900	0.92151300
H	3.98301700	-1.27247300	1.91092700
H	3.01181500	0.14256900	2.38626900
H	2.99656900	-1.34089300	3.37091600
H	-0.57291800	-3.30399400	0.36518800
H	1.67602900	-3.62873100	1.86507200
Au	-1.59231400	-0.04598800	-0.12825100
Cl	-2.98844300	-1.84340400	0.50628600
Cl	-3.52603500	1.31747800	-0.49024400
Cl	-0.21839000	1.77344600	-0.86275000
C	1.01829400	-1.52142100	-1.72695600
C	2.36620400	-1.81506100	-1.50125700

C	3.31954300	-0.80758500	-1.34893700
C	4.76303500	-1.09434500	-1.05447800
O	2.95673300	0.43798400	-1.51107800
H	5.10459900	-0.49187800	-0.20424000
H	4.93220200	-2.15240300	-0.84503100
H	5.38023800	-0.80167100	-1.91353600
H	2.69727000	-2.84200000	-1.39587800
H	3.62476200	1.13188200	-1.15560800
O	4.34959700	2.20775500	-0.31022200
H	3.63391200	2.33985100	0.38817300
O	2.30869100	2.19574900	1.36684500
H	1.70996100	2.97261600	1.51019300
O	0.30207000	4.06418600	1.45111100
H	-0.16951600	3.65154700	0.70169200
H	4.41459100	3.05250300	-0.78294600
H	1.73443000	1.56961900	0.88840800
H	-0.29367800	3.93479000	2.20579800
H	0.33850100	-2.30078300	-2.05087000
H	0.74194500	-0.50708000	-1.99025700

TS1-1s

E (B3LYP/BS1) = -1555.823683 au
 H(B3LYP/BS1) = -1555.624358 au
 G(B3LYP/BS1) = -1555.689528 au
 E(M06/BS2//B3LYP/BS1) = -1555.975179 au

C	1.47651100	-0.23720400	0.38891200
C	2.37671400	-0.79101100	1.26237000
C	3.66784700	-0.37377500	0.81678300
Cl	-0.08850400	-2.59545800	-0.84701300
H	2.14515700	-1.43774400	2.09660000
Cl	-2.91338500	-0.73386100	-0.15219600
C	0.25289300	1.45936300	1.58555100
C	-1.00045000	1.57347600	0.98155100
H	-1.89301400	1.28249100	1.52976600
Au	-0.53037200	-0.48098600	0.10803800
C	-1.14715600	2.53646500	-0.18725200
O	-0.14981600	3.01025100	-0.70075700
C	-2.55241600	2.86688600	-0.61732300
H	-3.08127800	1.94526600	-0.88830100
H	-3.10687800	3.31992000	0.21506300
H	-2.52569900	3.55916300	-1.46048900
O	2.13064400	0.51303500	-0.54402600
C	3.47406300	0.41421000	-0.28572900
H	4.62282200	-0.63444800	1.25192700
C	4.38551000	1.12303100	-1.22296300
H	5.41958100	1.02448200	-0.88190000
H	4.31530000	0.70542400	-2.23483300
H	4.13861500	2.18909700	-1.28969400
H	1.08101100	2.03031000	1.18070700
H	0.36815600	0.99745000	2.55952400

TS1-FC

E (B3LYP/BS1) = -2016.643355 au
 H(B3LYP/BS1) = -2016.428597 au
 G(B3LYP/BS1) = -2016.500145 au
 E(M06/BS2//B3LYP/BS1) = -2016.793835 au

C	2.91439800	1.86134700	0.27129500
C	1.85871500	2.54932800	-0.35193700
C	0.56352800	2.01269300	-0.37999500
C	-0.58234000	2.74475600	-1.01827900
O	0.38577400	0.84422300	0.14273700
H	-1.39321300	2.86260400	-0.28922000
H	-0.28042300	3.73032300	-1.38038900
H	-0.97612100	2.15869500	-1.85825900
H	2.04546700	3.47168000	-0.89176100
Au	-1.42344900	-0.16356000	0.06471000
Cl	-3.38833300	-1.40184900	0.04268900
Cl	-0.78551400	-1.01614500	-2.06796100
Cl	-1.98069500	0.81060100	2.14471900
C	2.74301600	-0.64120400	-0.88846800
C	4.40626400	-1.20160300	0.50131800
C	3.17799000	-1.61919300	0.01675300
H	1.81527900	-0.64333700	-1.44589200
H	2.65632200	-2.52122200	0.30403400
O	4.76504700	-0.03381700	-0.06639600
C	3.69968300	0.39548000	-0.86393400
H	4.01509500	1.01156600	-1.69509300
C	5.33820700	-1.78333400	1.50270400
H	6.34058300	-1.90392800	1.07553300
H	5.43149100	-1.12841700	2.37751700
H	4.97597300	-2.75839600	1.83565000
H	2.66828200	1.18593500	1.08628700
H	3.85761500	2.38858700	0.39140600

TS2-FC

E (B3LYP/BS1) = -2016.644954 au

H(B3LYP/BS1) = -2016.430079 au

G(B3LYP/BS1) = -2016.502275 au

E(M06/BS2//B3LYP/BS1) = -2016.802265 au

C	1.26354900	0.12622000	-0.03199500
C	0.40462200	0.84327000	0.83523100
H	0.32217300	0.48482200	1.86090000
Au	-1.33952200	-0.26308300	-0.02705500
Cl	-1.06193000	-1.81677100	1.75182500
Cl	-3.31783200	-1.34887800	-0.75696900
Cl	-1.47588800	1.29496900	-1.80905900
C	3.41497900	0.83174200	0.17883600
H	3.02992400	1.83302500	0.03337200
C	3.79444300	0.12146800	1.30842400
H	3.51036000	0.35559500	2.32553900
C	4.57661100	-0.96963100	0.86582500
C	4.66737900	-0.85629400	-0.50510000
H	5.01307400	-1.75329600	1.46851900
O	3.98761000	0.23938100	-0.92476300
C	5.32454700	-1.68482500	-1.54956900
H	4.58641800	-2.09221600	-2.25080800
H	6.03474500	-1.08649300	-2.13222800
H	5.86221200	-2.51644600	-1.08837200
H	1.36299000	0.46183400	-1.05893200
C	0.26723600	2.34430700	0.68257300
O	1.11556300	2.96709100	0.06399200
C	-0.89504100	3.01446900	1.37316800

H	-0.67543900	4.07390600	1.52163400
H	-1.77894300	2.92570000	0.72973000
H	-1.13276200	2.53289800	2.32805800
H	1.49822200	-0.91032000	0.18322200

TS2-FC'

E (B3LYP/BS1) = -2016.650853 au

H(B3LYP/BS1) = -2016.437264 au

G(B3LYP/BS1) = -2016.509879 au

E(M06/BS2//B3LYP/BS1) = -2016.798329 au

C	1.98333500	-1.34105500	1.38786400
C	3.09260300	-1.48468700	0.51315800
C	1.70071700	0.01166600	1.43614500
C	3.42890000	-0.22166400	0.09309200
C	4.46397100	0.30043100	-0.83654900
O	2.59810700	0.69547000	0.66650400
H	3.99724400	0.79335200	-1.69701600
H	5.11022000	1.03417000	-0.33951200
H	5.08570100	-0.52005800	-1.20301900
H	1.05531900	0.60604600	2.06254300
H	1.44864600	-2.11461500	1.92140100
H	3.57054100	-2.40429700	0.20759100
Au	-0.57739600	-0.55470000	-0.03490300
Cl	0.54771700	-0.24715200	-2.08610200
Cl	-1.74488900	-2.43382700	-0.87386500
Cl	-1.62816600	-0.74223800	2.07343400
C	0.29022400	4.54144200	0.43981200
C	-0.86680700	4.08273600	-0.05492000
C	-1.14075900	2.63155000	-0.17195600
C	-2.37374800	2.17714300	-0.90759400
O	-0.34789900	1.81795100	0.32009500
H	-2.92881600	1.46791700	-0.28290900
H	-3.02492100	3.00594600	-1.19419800
H	-2.06052200	1.63531900	-1.80945700
H	-1.63722500	4.76135600	-0.41055300
H	0.49579500	5.60517600	0.51156400
H	1.06080900	3.85291600	0.77484100

TS5-10

E (B3LYP/BS1) = -2285.250465 au

H(B3LYP/BS1) = -2284.921980 au

G(B3LYP/BS1) = -2285.011782 au

E(M06/BS2//B3LYP/BS1) = -2285.419109 au

C	0.12976500	-2.31114000	1.11448600
C	1.25696800	-2.32776400	1.93568500
C	0.08350100	-1.06676700	0.45132300
C	1.84049500	-1.07097000	1.83009800
C	3.00951300	-0.44652300	2.51224400
O	1.11473900	-0.29867100	1.00155500
H	3.95832000	-0.79105000	2.08214700
H	2.96155200	0.64208300	2.42074700
H	3.01597100	-0.72318700	3.57196900
H	-0.58182400	-3.10768800	0.95825700
H	1.61789900	-3.14149800	2.55006100
Au	-1.59541500	0.03540400	-0.05331000
Cl	-2.98333400	-1.68142000	0.79211300

Cl	-3.53515000	1.36030100	-0.51717300
Cl	-0.23804300	1.74127300	-1.04022400
C	0.95093800	-1.63575800	-1.42572000
C	2.30915900	-1.93991600	-1.15664800
C	3.29747000	-0.97149800	-1.13690600
C	4.73806100	-1.28328200	-0.84821600
O	2.98628900	0.27393300	-1.42999300
H	5.12225500	-0.61849900	-0.06456500
H	4.87488500	-2.32258900	-0.54243900
H	5.34594100	-1.09583800	-1.74243500
H	2.59990200	-2.96505100	-0.94998200
H	3.69922800	0.95616100	-1.17915400
O	4.49267800	2.13372500	-0.48234800
H	3.75309900	2.40788300	0.14132800
O	2.34618000	2.46168200	1.03954500
H	1.77052100	3.26721800	1.05834000
O	0.39192100	4.38810200	0.85116000
H	-0.10575900	3.88212400	0.18059500
H	4.61752800	2.88495000	-1.08320900
H	1.77370500	1.79540700	0.61600900
H	-0.18694200	4.37935400	1.62973400
H	0.76748500	-0.63064800	-1.79407400
C	0.02625100	-2.69944700	-1.95986600
H	0.23708900	-3.68454800	-1.53199900
H	-1.02697200	-2.45844400	-1.79195600
H	0.17765200	-2.76749200	-3.04626200

TS5-12

E (B3LYP/BS1) = -2553.387299 au

H(B3LYP/BS1) = -2552.974830 au

G(B3LYP/BS1) = -2553.077346 au

E(M06/BS2//B3LYP/BS1) = -2553.462572 au

C	0.22797700	1.05265400	1.98017700
C	-0.91275900	1.18928900	2.74604400
C	-0.11205100	0.42254300	0.74010200
C	-1.94638600	0.58181600	2.02101800
C	-3.38291700	0.38234500	2.34955400
O	-1.48008600	0.07078300	0.88753300
H	-3.92392900	1.33659300	2.31145100
H	-3.84093700	-0.31524500	1.64268900
H	-3.48136200	-0.00063400	3.37186900
H	1.21888800	1.41218700	2.21140600
H	-1.01527400	1.65909300	3.71495700
Au	1.01928500	-1.24976100	0.11756600
Cl	2.90428800	-0.49283500	1.34224200
Cl	2.29101600	-3.17652200	-0.52407100
Cl	-0.82157300	-2.16197700	-1.11888000
C	-0.13479700	1.86861400	-0.63442000
C	-1.26281000	2.70546300	-0.22039000
C	-2.58012300	2.55279400	-0.54641400
C	-3.64162300	3.49803100	-0.04814100
O	-2.99382300	1.57498500	-1.35559800
H	-4.44922700	2.94309800	0.44657400
H	-3.23741400	4.23670300	0.64762000
H	-4.09867000	4.02826300	-0.89330300
H	-1.04274600	3.52005900	0.45978900

H	-3.98947300	1.43562000	-1.33828700
O	-5.46437500	0.72115900	-1.17596100
H	-5.09916300	-0.15639300	-0.87559900
O	-4.02460400	-1.36066200	-0.31195100
H	-3.98785700	-2.34813500	-0.34366000
O	-3.41380800	-4.05145000	-0.32011400
H	-2.50767200	-3.91120000	-0.65423700
H	-5.86433100	0.54735500	-2.04211800
H	-3.11310000	-1.08766800	-0.52099900
H	-3.28057600	-4.31577400	0.60382800
C	-0.25060200	1.11320000	-1.95740400
H	0.66707300	0.56790300	-2.17772400
H	-1.08973800	0.42656300	-1.97045500
H	-0.40448000	1.85875800	-2.74783900
C	1.59471200	3.72601900	0.05708400
C	3.37095400	2.62761100	-0.76151900
C	3.00924900	3.78274700	-0.12238500
H	0.97577500	4.48279100	0.51746500
H	3.67489600	4.57922100	0.17994100
C	1.17304400	2.53892700	-0.48790800
O	2.26054600	1.87523000	-0.99464200
C	4.66896100	2.05800200	-1.21098800
H	5.48358900	2.74604100	-0.96958500
H	4.85906000	1.09793500	-0.71679000
H	4.67390500	1.87997300	-2.29324100

TS5-13

E (B3LYP/BS1) = -2397.364435 au

H(B3LYP/BS1) = -2397.047076 au

G(B3LYP/BS1) = -2397.136468 au

E(M06/BS2//B3LYP/BS1) = -2397.510154 au

C	0.17673700	1.85475800	-1.91845000
C	1.12353100	2.86628100	-2.06243000
C	0.47819800	1.11694200	-0.74447900
C	2.03435700	2.69948400	-1.01519100
C	3.25601700	3.44219400	-0.60956300
O	1.69304200	1.65536700	-0.26980300
H	3.25066600	4.45869500	-1.01065600
H	3.32856300	3.46570000	0.48219700
H	4.14890900	2.92676000	-0.98710900
H	-0.68697500	1.65838500	-2.53891600
H	1.16850600	3.63446400	-2.82238700
Au	0.35988700	-0.95461600	-0.66448800
Cl	-1.81452800	-0.83487200	-1.60797300
Cl	0.09210100	-3.31581200	-0.32221700
Cl	2.67463200	-1.17661900	-0.12989800
C	-0.63203100	1.82508500	0.77405300
O	2.11680000	1.83986300	2.76002700
H	2.41727700	0.87554600	2.89483700
O	2.59368600	-0.70917700	3.11743500
H	1.67844900	-1.09399800	3.09468100
O	0.01217300	-1.59423300	2.72791300
H	-0.40043300	-0.79848000	2.34602800
H	2.01753900	2.18747900	3.66112000
H	2.96739400	-1.01503400	2.27059000
H	-0.01289400	-2.26194800	2.01667100

C	-2.96102800	2.42225700	-0.17512200
C	-4.00016300	0.69424000	0.80081200
C	-4.22024400	1.79101500	0.00307500
H	-2.74940500	3.31201900	-0.75286300
H	-5.17141200	2.09777300	-0.40833600
C	-2.05084700	1.67553100	0.53364400
O	-2.68671300	0.62739400	1.13669300
C	-4.87920300	-0.38522400	1.32134800
H	-5.91515600	-0.20179800	1.02542000
H	-4.56835800	-1.35850200	0.92326700
H	-4.83183700	-0.44322100	2.41515300
O	-0.19201600	1.20162700	1.86451400
H	0.74081800	1.51872700	2.16729600
H	-0.24793300	2.83412900	0.59864800

TS5-16

E (B3LYP/BS1) = -2361.004362 au

H(B3LYP/BS1) = -2360.692009 au

G(B3LYP/BS1) = -2360.776945 au

E(M06/BS2//B3LYP/BS1) = -2361.029953 au

C	-0.52793200	0.43623900	1.90447500
C	-1.53521700	-0.21289200	2.61175000
C	-0.15390500	-0.37930600	0.80991200
C	-1.73451800	-1.43329000	1.97047700
C	-2.70490300	-2.53154600	2.20127000
O	-0.88928700	-1.56428200	0.94195200
H	-3.05946800	-2.52141800	3.23528700
H	-3.57715300	-2.40959000	1.54143700
H	-2.24950800	-3.50134500	1.98043700
H	-0.10262900	1.40829400	2.10203600
H	-2.07353700	0.13878200	3.48122000
Au	1.75052800	-0.57680100	0.02386600
Cl	2.59185000	0.96663500	1.62750500
Cl	3.94257700	-0.79067100	-0.89469200
Cl	0.91767100	-2.07962700	-1.62229700
C	-1.21043900	0.52679900	-0.80151000
C	0.29918300	2.47080200	-1.50311500
C	-0.81746000	4.04834500	-0.36811600
C	0.26262800	3.85620100	-1.18924400
H	1.02674000	1.95148000	-2.11199900
H	0.95264900	4.61875000	-1.52141700
C	-0.77309800	1.89386500	-0.86236300
O	-1.45696500	2.85797500	-0.15855200
C	-1.39682800	5.24727200	0.29357400
H	-0.79440300	6.12841300	0.05936700
H	-2.42458500	5.43203300	-0.04312000
H	-1.42255500	5.12802400	1.38367500
C	-3.66386800	0.70933100	0.06940200
C	-4.29248300	-1.20739700	-0.90758100
C	-4.75968100	-0.16630300	-0.13703300
H	-3.65415900	1.63924200	0.61782400
H	-5.77171900	-0.04657500	0.22394200
H	-0.70295100	-0.12583700	-1.50721400
C	-2.58291600	0.16342700	-0.59744100
O	-2.97837000	-1.02464600	-1.17716900
C	-4.94166700	-2.40642300	-1.50470300

H	-5.97000500	-2.49693900	-1.14573800
H	-4.96284400	-2.33550700	-2.59917200
H	-4.39566100	-3.32138600	-1.24909700

TS6-1'

E (B3LYP/BS1) = -2324.055352 au

H(B3LYP/BS1) = -2323.729177 au

G(B3LYP/BS1) = -2323.824519 au

E(M06/BS2//B3LYP/BS1) = -2324.095247 au

C	0.00525500	1.64680400	-1.14342800
C	1.08902200	2.49371100	-0.76447300
C	-1.12611400	2.12856500	-0.47737200
C	0.58786600	3.40409100	0.11692500
C	1.18212100	4.51620000	0.90250700
O	-0.75857100	3.19098300	0.28744600
H	2.24381200	4.61593200	0.66240500
H	0.68423200	5.46938000	0.68543300
H	1.08684700	4.32907800	1.97861200
H	0.02185700	0.88559300	-1.90986700
H	2.11827200	2.39490800	-1.07434000
Au	0.09363000	-0.77232900	0.41616800
Cl	-0.12241200	-1.97035000	-1.63498500
Cl	-1.43868000	-2.22157500	1.54190600
Cl	0.44549600	0.50881700	2.36778800
C	-2.53296700	1.74673300	-0.48811900
C	-2.85370200	0.52640900	-1.22678000
C	-3.42345900	2.52297400	0.18799000
C	-3.99306500	-0.19885700	-1.18895000
C	-4.15920800	-1.50610800	-1.90679500
O	-5.07557900	0.22683800	-0.47361200
H	-4.96969200	-1.45036300	-2.64715300
H	-3.23719100	-1.80120300	-2.41062400
H	-4.41130500	-2.30175700	-1.19158300
H	-2.06308100	0.09508600	-1.82651200
H	-4.47645400	2.28179600	0.20554800
H	-3.08931400	3.39915600	0.73087000
H	-5.73564300	-0.48297500	-0.44221300
C	4.96229300	0.24538700	-1.34529400
C	4.64746700	-0.84580800	-0.67560000
C	5.27795900	1.32083200	-2.00631500
C	3.28332700	-1.09450400	-0.14964000
C	3.03916500	-2.38456300	0.59265800
O	2.38398800	-0.26802500	-0.32889500
H	2.30058700	-2.97243200	0.03363600
H	3.94776300	-2.97575200	0.72784300
H	2.59796000	-2.15899700	1.57020500
H	5.65181100	2.20799300	-1.49883400
H	5.17947000	1.36840900	-3.08904800
H	5.40401300	-1.60659400	-0.49507200

TS7

E (B3LYP/BS1) = -1593.890238 au

H(B3LYP/BS1) = -1593.686230 au

G(B3LYP/BS1) = -1593.755447 au

E(M06/BS2//B3LYP/BS1) = -1594.025953 au

C	-0.38148500	1.12833600	0.51456600
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C	-0.85637200	1.57000400	1.72894500
C	-1.75372600	2.64045800	1.44475900
Cl	2.45055900	1.51831500	-0.85258200
H	-0.58287200	1.18667500	2.70203100
Cl	2.72527100	-1.91836800	-0.28329800
C	-1.21439500	-1.08415400	0.37279500
C	-0.20557500	-1.68538100	1.08166200
C	-2.28101300	-0.99192300	-0.38848900
H	0.18912700	-2.63153300	0.71243400
H	-2.42082100	-0.15481700	-1.06488100
Au	1.09652100	-0.19548000	0.06961400
C	-3.35324200	-2.05738700	-0.29046200
O	-3.25798100	-2.99699700	0.47233200
C	-4.53396600	-1.85410300	-1.21812400
H	-5.02690100	-0.89753700	-1.00345500
H	-4.19793600	-1.81886300	-2.26198000
H	-5.24392600	-2.67228400	-1.08689900
H	-0.08680400	-1.47640500	2.14374900
O	-0.96025600	1.84333100	-0.49104200
C	-1.79335000	2.77135600	0.08259400
H	-2.29958500	3.24264100	2.15781000
C	-2.49089000	3.70356400	-0.84257600
H	-3.14826900	4.36823400	-0.27595000
H	-1.77052100	4.31851300	-1.39564900
H	-3.09577700	3.16388800	-1.58106700

TS8

E (B3LYP/BS1) = -1593.891094 au

H(B3LYP/BS1) = -1593.687132 au

G(B3LYP/BS1) = -1593.756517 au

E(M06/BS2//B3LYP/BS1) = -1594.027252 au

C	-0.31786100	1.12404300	0.48850200
C	-0.91976300	1.47800500	1.67471100
C	-1.82766000	2.53319600	1.36777700
Cl	2.61234000	1.53357200	-0.54641300
H	-0.72188600	1.04552700	2.64552100
Cl	2.74800700	-1.96033000	-0.32230400
C	-1.38790700	-1.12901700	0.24044100
C	-0.27995900	-1.78615600	0.71474600
C	-2.51754100	-0.78667200	-0.31430400
H	0.10428800	-2.62538000	0.13301900
H	-2.67399600	0.21036900	-0.71982100
Au	1.13788100	-0.22002500	0.06417200
C	-3.72734900	-1.70242400	-0.39822800
O	-4.75323200	-1.24975500	-0.85848200
C	-3.58730100	-3.12811700	0.08473200
H	-2.85973800	-3.66758600	-0.53384300
H	-3.22558700	-3.15564100	1.11923000
H	-4.55605100	-3.62599800	0.01984300
H	-0.12464500	-1.84058400	1.79297500
O	-0.83333600	1.87179300	-0.52620200
C	-1.75078100	2.74055200	0.01590800
H	-2.45595700	3.07811500	2.05875400
C	-2.38084700	3.71222500	-0.91740300
H	-3.14753500	4.28867500	-0.39302200
H	-1.63585400	4.41170500	-1.31656400

H	-2.84720700	3.20755200	-1.77130100
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TS-T1

E (B3LYP/BS1) = -538.6580685 au

H(B3LYP/BS1) = -538.452394 au

G(B3LYP/BS1) = -538.502637 au

E(M06/BS2//B3LYP/BS1) = -538.4533901 au

C	-1.19229700	1.48815500	0.03437700
C	-2.60704600	1.42647200	0.16609900
C	-0.74681700	0.19622100	-0.13099900
C	-2.94955700	0.10189200	0.08022200
C	-4.24805400	-0.62320300	0.14098900
O	-1.83304800	-0.65128400	-0.10083900
H	-5.06580600	0.08652700	0.29177400
H	-4.43893500	-1.17832700	-0.78574000
H	-4.26243900	-1.34700900	0.96513600
H	-0.57238900	2.37218400	0.07842500
H	-3.28946200	2.25246100	0.31204600
C	0.56183100	-0.39202600	-0.32724300
C	1.67136700	0.46980500	-0.53511900
C	0.78121500	-1.78171100	-0.12636700
C	2.91368700	0.09675900	-0.01326900
C	4.02643300	1.09963800	0.15588200
O	3.14998800	-1.09024400	0.45036200
H	3.78136400	2.06469700	-0.29580400
H	4.23077700	1.24415500	1.22353800
H	4.94734300	0.71643700	-0.29764200
H	1.51973100	1.50680100	-0.81153000
H	-0.04998700	-2.36973600	0.25409700
H	1.35518900	-2.29854700	-0.89931200
H	2.04452400	-1.60943800	0.50138900

prod2

E (B3LYP/BS1) = -538.6735322 au

H(B3LYP/BS1) = -538.462581 au

G(B3LYP/BS1) = -538.515266 au

E(M06/BS2//B3LYP/BS1) = -538.4771559 au

C	-1.20355600	1.42865100	-0.16947800
C	-2.63426200	1.42783500	-0.18547900
C	-0.80598400	0.12827700	0.00992800
C	-3.02585500	0.13170700	-0.01630800
C	-4.35094200	-0.54211200	0.06381500
O	-1.92223700	-0.66701300	0.10442100
H	-5.15061800	0.19563400	-0.04736800
H	-4.46834300	-1.29616600	-0.72489400
H	-4.48676800	-1.05243000	1.02592300
H	-0.55820400	2.28516000	-0.30040100
H	-3.28782600	2.28083000	-0.30814900
C	0.50465800	-0.52262200	0.09359500
C	1.64196100	0.40293700	0.20880600
C	0.59782300	-1.87140700	0.06902000
C	2.95259500	0.16046200	0.01270600
C	4.02260400	1.20442600	0.16563900
O	3.39995400	-1.08877000	-0.33614200
H	4.58651300	1.33009300	-0.77072700

H	3.59889100	2.17463800	0.43430500
H	4.74304900	0.91944400	0.94564000
H	1.40007000	1.41969800	0.49967000
H	1.55169300	-2.37433500	0.14531800
H	-0.29274500	-2.48219500	-0.02838600
H	4.34830100	-1.04303400	-0.53061400

Prod3

E (B3LYP/BS1) = -538.7067259 au

H(B3LYP/BS1) = -538.495835 au

G(B3LYP/BS1) = -538.549646 au

E(M06/BS2//B3LYP/BS1) = -538.4995084 au

C	-1.23765800	-1.52743300	-0.00007100
C	-2.65818400	-1.44934400	-0.00003900
C	-0.76295200	-0.23497400	-0.00003000
C	-2.97890100	-0.11760900	0.00003100
C	-4.26840900	0.62567900	0.00004700
O	-1.83923800	0.62599200	0.00002700
H	-5.10457800	-0.07866500	0.00005000
H	-4.35995900	1.26890200	0.88406100
H	-4.35996600	1.26890100	-0.88396700
H	-0.64076100	-2.42848900	-0.00013000
H	-3.35858100	-2.27320400	-0.00002900
C	0.55840400	0.36955600	-0.00002000
C	1.65998300	-0.43280500	-0.00004500
C	0.60367500	1.87817700	0.00003500
C	3.07947400	-0.02885500	-0.00002300
C	4.07300900	-1.18671300	0.00013200
O	3.48697600	1.12942100	-0.00011700
H	3.92706900	-1.82284700	0.88262700
H	3.92705400	-1.82313600	-0.88215000
H	5.09097900	-0.79258800	0.00006600
H	1.50164600	-1.50947100	-0.00005600
H	1.63174800	2.23162400	-0.00003200
H	0.07633000	2.27083400	-0.87770700
H	0.07646500	2.27076300	0.87789000

prod4

E (B3LYP/BS1) = -538.698349 au

H(B3LYP/BS1) = -538.489224 au

G(B3LYP/BS1) = -538.538596 au

E(M06/BS2//B3LYP/BS1) = -538.491786 au

C	-0.63172800	0.47621200	-0.00012600
C	-1.66167000	-0.41152100	0.00009000
C	-0.81970100	1.97270500	-0.00043900
C	-3.11345700	-0.13110800	0.00000000
C	-4.00236500	-1.37066900	0.00024700
O	-3.61969300	0.98684300	-0.00027200
H	-3.80083300	-1.99197200	-0.88191700
H	-3.80086700	-1.99159900	0.88268100
H	-5.05093000	-1.06728400	0.00016200
H	-1.41821300	-1.47235200	0.00037800
C	1.94983600	0.82817200	0.00017100
C	3.02507500	-0.00620400	0.00015000

H	1.98759400	1.90804300	0.00033700
C	0.76125500	0.00627400	-0.00004600
H	-1.87421300	2.23838200	-0.00057800
H	-0.33422500	2.41324400	0.88043300
H	-0.33405100	2.41290600	-0.88138300
O	2.58593200	-1.30793700	-0.00008100
C	1.23122700	-1.28471800	-0.00020200
C	4.50481800	0.19477700	0.00043400
H	4.83688900	0.75250500	-0.88309000
H	4.83700900	0.74959700	0.88575400
H	5.01029600	-0.77478500	-0.00117600
H	0.75190400	-2.25145900	-0.00045800

prod5

E (B3LYP/BS1) = -500.609825 au

H(B3LYP/BS1) = -500.404694 au

G(B3LYP/BS1) = -500.456483 au

E(M06/BS2//B3LYP/BS1) = -500.425192 au

C	-1.89808700	-1.56929800	0.21285600
C	-2.79944300	-0.45172700	0.23806900
C	-0.66364300	-1.07032300	-0.07776600
C	-2.05603600	0.65788700	-0.03192000
C	-2.37067000	2.10833000	-0.15197800
O	-0.74690100	0.29259100	-0.22607500
H	-3.43804900	2.27158500	0.02171900
H	-1.81112800	2.70726300	0.57819000
H	-2.12285900	2.49394000	-1.14891300
H	-2.14068000	-2.60916500	0.38517800
H	-3.86282800	-0.47328900	0.43444500
C	0.68364800	-1.68866500	-0.25653300
C	1.78555700	-1.00152100	0.57457400
C	2.30776500	0.28094800	-0.08187700
C	2.64608400	1.43259200	0.84364500
O	2.46253200	0.35102200	-1.28577100
H	1.71834700	1.81598100	1.28827500
H	3.28423500	1.09880200	1.67145000
H	3.14067100	2.23200500	0.28803500
H	1.44507200	-0.80635400	1.59754500
H	0.99326700	-1.64961900	-1.30915200
H	2.65214200	-1.67452200	0.65222400
H	0.60571600	-2.74486500	0.02135200

prod6

E (B3LYP/BS1) = -539.922761 au

H(B3LYP/BS1) = -539.688027 au

G(B3LYP/BS1) = -539.742460 au

E(M06/BS2//B3LYP/BS1) = -539.718285 au

C	1.76762800	1.52699800	0.14050500
C	2.78666500	0.51584400	0.17991200
C	0.58744500	0.88704300	-0.10003600
C	2.16528200	-0.67716200	-0.03402700

C	2.63523500	-2.08764400	-0.11680600
O	0.81995100	-0.46389100	-0.20443000
H	3.71950400	-2.12579800	0.02128000
H	2.17193100	-2.71726200	0.65400800
H	2.39782100	-2.53500100	-1.09008600
H	1.90534000	2.59082100	0.27177900
H	3.84522200	0.66197700	0.34704600
C	-0.83391200	1.33769000	-0.27133100
C	-1.80011500	0.46190500	0.56134800
C	-2.08927600	-0.89674100	-0.08533400
C	-2.14854200	-2.09709800	0.83768000
O	-2.28884700	-0.98909900	-1.28145800
H	-1.14806200	-2.27748300	1.25121900
H	-2.81785000	-1.90722800	1.68630800
H	-2.48233100	-2.98027400	0.28898900
H	-1.43381100	0.34159800	1.58740300
H	-1.12658700	1.19116400	-1.32079600
C	-0.97890000	2.82688900	0.07087700
H	-0.73576400	3.02027600	1.12230900
H	-0.31543000	3.44052000	-0.54798200
H	-2.00664400	3.15972700	-0.10873900
H	-2.77124000	0.97454800	0.62764300

prod7

E (B3LYP/BS1) = -808.061146 au

H(B3LYP/BS1) = -807.742896 au

G(B3LYP/BS1) = -807.810172 au

E(M06/BS2//B3LYP/BS1) = -807.759037 au

C	-1.32700600	-1.81476500	-0.65952500
C	-2.74563200	-1.95645500	-0.82606800
C	-1.13596900	-0.71832500	0.12697400
C	-3.32864800	-0.94480300	-0.12494400
C	-4.73750200	-0.51772900	0.09779200
O	-2.35282200	-0.18594500	0.47162900
H	-5.41760600	-1.20588500	-0.41226400
H	-4.99653700	-0.51072800	1.16445700
H	-4.92078800	0.49227300	-0.29088200
H	-0.55377000	-2.44181700	-1.07791900
H	-3.26222400	-2.71174800	-1.40281800
C	0.06708300	-0.08277800	0.78420200
C	-0.13467900	1.45128700	0.95991200
C	-0.37344400	2.27406500	-0.30251200
C	-0.24017200	3.78048100	-0.13172500
O	-0.66039400	1.78249200	-1.37619400
H	-0.61914900	4.28804400	-1.02126800
H	-0.77636300	4.13223800	0.75788800
H	0.81722500	4.04254200	0.00611400
H	-0.99750100	1.62849400	1.61747700
H	0.73407400	1.86313400	1.49000900
C	1.31365300	-0.35256300	-0.02920000
C	1.58572500	-0.44891600	-1.36247800

O	2.48752700	-0.46031000	0.68160400
C	3.00252500	-0.63556600	-1.48139200
H	0.86111300	-0.36999200	-2.15836500
C	3.50833400	-0.63471400	-0.21544800
H	3.57008600	-0.75630200	-2.39427700
C	0.21790200	-0.69412600	2.20653300
H	0.39634800	-1.77114000	2.14010400
H	1.05260200	-0.23893800	2.74792600
H	-0.70293300	-0.53147900	2.77546900
C	4.87745200	-0.78947100	0.35021800
H	4.94804900	-1.66525300	1.00797800
H	5.60095700	-0.91404400	-0.46045200
H	5.17420100	0.08697600	0.94047300

prod8

E (B3LYP/BS1) = -652.005961 au

H(B3LYP/BS1) = -651.782230 au

G(B3LYP/BS1) = -651.838430 au

E(M06/BS2//B3LYP/BS1) = -651.788548 au

C	0.06514500	-1.23337800	-0.03262500
C	-2.29677500	-1.13106800	-1.13642300
C	-3.06784900	0.55531700	0.12534800
C	-3.43037700	-0.29297800	-0.88081400
H	-2.22037700	-1.92783700	-1.86364800
H	-4.39094000	-0.32061700	-1.37672300
C	-1.31983900	-0.73610800	-0.27243500
O	-1.77899700	0.29628700	0.50338800
C	-3.77186900	1.64674100	0.85412700
H	-4.78828100	1.75721600	0.46603400
H	-3.83544800	1.43493200	1.92863100
H	-3.25499300	2.60793400	0.74024400
O	0.12256700	-1.84382700	1.26573200
C	1.12126300	1.16450300	-0.47393600
C	3.23135300	0.48162800	-0.09895600
C	2.49494000	1.57920100	-0.43152900
H	0.25787800	1.77550800	-0.69131400
H	2.88252700	2.57091200	-0.62124100
H	0.25534200	-2.00106200	-0.80192500
H	1.06440700	-1.96458900	1.47084700
C	1.10831400	-0.16118400	-0.16755900
O	2.39490000	-0.59490900	0.06042700
C	4.68475600	0.23904100	0.11485300
H	5.24198600	1.16646900	-0.04389600
H	4.89067400	-0.11217400	1.13399600
H	5.07509600	-0.51739300	-0.57767500

prod9

E (B3LYP/BS1) = -844.944509 au

H(B3LYP/BS1) = -844.642052 au

G(B3LYP/BS1) = -844.709501 au

E(M06/BS2//B3LYP/BS1) = -844.618496 au

C	1.93165500	1.26106700	0.76498000
C	3.35655800	1.11218800	0.85210300
C	1.50645800	0.35686700	-0.16124500
C	3.70422300	0.12778800	-0.02507400
C	4.99870600	-0.49494200	-0.41784200
O	2.57941500	-0.34293400	-0.65130400
H	5.81575400	-0.04132100	0.15029400
H	5.00339800	-1.57457700	-0.22186900
H	5.20678100	-0.35557600	-1.48629800
H	1.30435800	1.94666100	1.31511200
H	4.03371700	1.67067900	1.48403500
C	0.16196100	-0.03850500	-0.71311500
C	-1.43256000	1.78214500	-1.73488400
C	-2.11359000	2.61906600	0.23448600
C	-2.27261700	2.76462400	-1.11155800
H	-1.30775500	1.60308500	-2.79402200
H	-2.91443000	3.48317400	-1.60293800
C	-0.81590400	1.10509300	-0.72718500
O	-1.22437700	1.60399700	0.48254900
C	-2.68998100	3.30767600	1.42226300
H	-3.38837500	4.08416200	1.09754700
H	-3.23266300	2.60767300	2.06987800
H	-1.91183400	3.78267800	2.03328300
C	-0.13269300	-1.84346700	1.19757500
C	-1.76206400	-2.97903200	0.14555500
C	-1.02574600	-2.96324600	1.29292600
H	0.59978100	-1.52048500	1.92318800
H	-1.10579800	-3.66691500	2.11046900
H	0.31167300	-0.31385500	-1.76592500
C	-0.38577600	-1.25329600	-0.00280800
O	-1.37811900	-1.93565900	-0.65749200
C	-2.83884600	-3.86500000	-0.37724600
H	-3.05351700	-4.65456600	0.34849800
H	-3.76640200	-3.30833300	-0.56171000
H	-2.54872900	-4.33987200	-1.32315300

sub2

E (B3LYP/BS1) = -270.5523331 au
 H(B3LYP/BS1) = -270.425856 au
 G(B3LYP/BS1) = -270.465292 au
 E(M06/BS2//B3LYP/BS1) = -270.447079 au

C	-1.38131900	0.28550400	0.00015600
C	-0.27229200	-0.46805500	-0.00027400
C	1.08411900	0.14813400	-0.00005200
C	2.26029600	-0.81442900	0.00019300
O	1.25068500	1.35925900	-0.00010800
H	3.19762200	-0.25498000	0.00051500
H	2.22132400	-1.46771900	0.88161100
H	2.22183200	-1.46723600	-0.88163500
H	-0.33632700	-1.55562800	-0.00063300
H	-1.24225000	1.36673100	0.00056500

C	-2.78636100	-0.22698400	0.00004500
H	-3.33367400	0.13994900	0.87902700
H	-3.33375700	0.14072900	-0.87856000
H	-2.82691000	-1.32093800	-0.00043500

sub3

E (B3LYP/BS1) = -231.230767 au
H(B3LYP/BS1) = -231.134151 au
G(B3LYP/BS1) = -231.169869 au
E(M06/BS2//B3LYP/BS1) = -231.1478191 au

C	2.01532800	-0.10448200	0.00011900
C	0.80326300	-0.66776400	-0.00013800
C	-0.44110000	0.16362000	-0.00002000
C	-1.75663200	-0.59448600	0.00011800
O	-0.40129000	1.38345300	-0.00007000
H	-1.82346000	-1.24510900	-0.88171000
H	-1.82312100	-1.24590500	0.88134100
H	-2.59156500	0.10855400	0.00049500
H	0.68623700	-1.75012200	-0.00037800
H	2.10993000	0.97822500	0.00030100
H	2.92714300	-0.69459200	0.00004300

sub4

E (B3LYP/BS1) = -382.664087 au
H(B3LYP/BS1) = -382.548264 au
G(B3LYP/BS1) = -382.588289 au
E(M06/BS2//B3LYP/BS1) = -382.544276 au

C	-2.18497000	0.07110000	0.00020700
C	-0.08650800	1.56051700	0.00012100
C	1.38255200	-0.12760100	-0.00024500
C	1.29890000	1.24337300	-0.00023600
H	-0.53691500	2.54408200	0.00030200
H	2.13235200	1.93193500	-0.00046300
C	-0.76204000	0.36300800	0.00021100
O	0.13931600	-0.67073200	-0.00035900
C	2.52970200	-1.07591400	0.00029000
H	3.47321400	-0.52411100	-0.00589100
H	2.50941800	-1.72048100	0.88727200
H	2.50263400	-1.72921800	-0.88001500
O	-2.68121600	-1.04168800	-0.00012900
H	-2.81132300	0.99025700	0.00061400

TS1'+5

E (B3LYP/BS1) = -3570.323870 au
H(B3LYP/BS1) = -3570.104460 au
G(B3LYP/BS1) = -3570.199618 au
E(M06/BS2//B3LYP/BS1) = -3570.765278 au

C	-0.66875100	0.97238300	1.04777000
C	-0.25149700	2.30426400	1.24150600
C	-1.80685700	0.98596400	0.22872300
C	-1.15269900	3.09066100	0.56455500
C	-1.25360200	4.55902500	0.34609600

O	-2.10221500	2.32112600	-0.01787700
H	-1.10418200	4.81527100	-0.71047200
H	-2.24432500	4.92920900	0.63524300
H	-0.49509600	5.07939700	0.93695600
H	-0.19493300	0.08815100	1.44086000
H	0.62439700	2.63590700	1.78122500
Au	-3.39969700	-0.32376400	0.16657200
Cl	-2.14576700	-1.90634400	1.43743000
Cl	-5.24589700	-1.87537200	0.11965800
Cl	-4.69513700	1.20572000	-1.11870100
C	-0.86906400	0.23218400	-1.65392300
C	-0.27691700	-1.00334700	-1.46923300
C	-1.20030300	1.16887500	-2.51209800
C	1.00650000	-1.15453000	-0.93174300
C	1.61720400	-2.51661000	-0.75973100
O	1.64875800	-0.09611900	-0.55768700
H	1.88571900	-2.66321500	0.29390500
H	0.92663500	-3.30625900	-1.06334300
H	2.53592700	-2.58631500	-1.35407700
H	-0.86907300	-1.89785300	-1.63955300
H	-0.83792900	1.07034800	-3.53523500
H	-1.82522200	2.01868100	-2.27175300
Au	3.62909900	-0.09311500	0.01561800
Cl	2.91217100	0.06572100	2.27531600
Cl	4.26286900	-0.32503600	-2.26182000
Cl	5.86698600	0.07747700	0.67083500

[**sub1**H- (H₂O)₃]⁺

E (B3LYP/BS1) = -498.954407 au

H(B3LYP/BS1) = -498.758766 au

G(B3LYP/BS1) = -498.820388 au

E(M06/BS2//B3LYP/BS1) = -498.928127 au

C	-3.58249900	-0.28231600	0.23912700
C	-2.51083800	-1.02903700	-0.01828500
C	-4.63433600	0.43063900	0.48517000
C	-1.21303500	-0.44914900	-0.26083400
C	-0.03720900	-1.32158400	-0.56809300
O	-1.08186600	0.81624300	-0.21142200
H	0.76458500	-1.13610500	0.15944200
H	-0.30144800	-2.37947800	-0.56229700
H	0.36476800	-1.05345300	-1.55355600
H	-2.59656800	-2.11189300	-0.05830400
H	-5.27592300	0.78583700	-0.32012400
H	-4.91085600	0.69776500	1.50413300
H	-0.07767100	1.18496400	-0.41861800
O	1.19619000	1.61314400	-0.71073100
H	1.86186700	1.22850600	-0.05613500
O	2.70260200	0.30302600	0.96505800
H	3.57113200	-0.02611800	0.61607600
O	5.06061400	-0.61137600	-0.01410100
H	5.80207400	-0.03282300	-0.24904900
H	1.30186900	2.57786900	-0.73251200

H	2.88115400	0.63366100	1.85876500
H	5.46218900	-1.42834400	0.31923300

[**sub2**H- (H₂O)₃]⁺

E (B3LYP/BS1) = -500.210561 au

H(B3LYP/BS1) = -499.990606 au

G(B3LYP/BS1) = -500.054955 au

E(M06/BS2//B3LYP/BS1) = -500.178138 au

C	-3.39581300	-0.71722100	-0.10950300
C	-2.75548300	0.45651200	-0.33134100
C	-1.38592700	0.67671300	0.06027100
C	-0.74483400	1.99962600	-0.22328800
O	-0.74248500	-0.25957000	0.63589200
H	0.27055500	2.05923800	0.17097400
H	-0.72624900	2.16406900	-1.30888900
H	-1.35755000	2.80389700	0.20255200
H	-3.26401000	1.28321000	-0.81957000
H	0.29846700	-0.03728800	0.91756700
O	1.57686800	0.23567200	1.26334900
H	2.27379000	-0.29840200	0.73973600
O	3.26508900	-1.14285500	-0.11855300
H	4.13023300	-0.71550200	-0.34495400
O	5.61282700	0.05322700	-0.78449800
H	6.44123300	-0.06125600	-0.29391900
H	1.75909700	0.11338800	2.20911100
H	3.47283700	-2.04395500	0.17012300
H	5.86177600	0.03306500	-1.72146200
H	-2.84244500	-1.51509300	0.38466000
C	-4.80245600	-1.00665000	-0.48758200
H	-5.29254800	-0.16192300	-0.97763700
H	-4.83794800	-1.87992900	-1.15370300
H	-5.37854000	-1.28918800	0.40455100

[**sub3**H- (H₂O)₃]⁺

E (B3LYP/BS1) = -460.882597 au

H(B3LYP/BS1) = -460.692619 au

G(B3LYP/BS1) = -460.751799 au

E(M06/BS2//B3LYP/BS1) = -460.875504 au

C	-4.03710600	0.01795100	0.38806600
C	-3.01839600	-0.81196600	0.09303700
C	-1.67274200	-0.32169100	-0.15650300
C	-0.56812000	-1.26692200	-0.51080500
O	-1.45056600	0.92394000	-0.07643800
H	0.29191700	-1.11138600	0.15355900
H	-0.88916100	-2.30793100	-0.46108500
H	-0.22363000	-1.04875900	-1.53081200
H	-3.16925500	-1.88439400	0.02513100
H	-0.40028700	1.26026800	-0.29517600
O	0.82405400	1.63911600	-0.58359000
H	1.50161400	1.19008400	0.02611100
O	2.33957200	0.20548500	0.94150300

H	3.18083500	-0.13560600	0.53750400
O	4.60600800	-0.73184300	-0.19423200
H	5.37183300	-0.17374300	-0.39893700
H	0.95596100	2.60101400	-0.55409900
H	2.56429200	0.48030200	1.84381700
H	4.97029900	-1.59610000	0.05140800
H	-3.89129900	1.09227600	0.45432300
H	-5.03748100	-0.36384300	0.56753700

[**sub4**H-(H₂O)₃]⁺

E (B3LYP/BS1) = -612.329060 au

H(B3LYP/BS1) = -612.119171 au

G(B3LYP/BS1) = -612.178408 au

E(M06/BS2//B3LYP/BS1) = -612.275973 au

C	0.06083200	-1.55040800	0.04374500
O	3.78019600	-1.27914400	0.04038800
H	4.05550900	0.08746500	-0.05985100
O	4.10818700	1.16848400	-0.11160700
H	3.10145000	1.53430000	-0.03330200
O	1.69835800	1.77221600	-0.03253500
H	1.24365700	0.88946800	-0.01140000
H	4.12119300	-1.80707900	-0.70078800
H	4.66563500	1.51524400	0.60843200
H	1.32989500	2.30395300	0.69077400
C	-2.48878600	-1.63542300	0.00328800
C	-2.75717100	0.58647400	-0.01818400
C	-3.45153500	-0.60882200	-0.02623700
H	-2.66589300	-2.70291500	0.00447900
H	-4.52652200	-0.71591900	-0.05199300
C	-1.24887600	-1.01520200	0.02694300
O	-1.42379500	0.35216700	0.01572400
C	-3.19906900	2.00391300	-0.03987800
H	-4.28816000	2.05781300	-0.09775400
H	-2.87313100	2.53019900	0.86534100
H	-2.77547700	2.53124200	-0.90260000
O	1.11347000	-0.87502400	0.04457600
H	2.78962400	-1.36801600	0.04263000
H	0.11851900	-2.64853100	0.05559400

[**prod3**H-(H₂O)₃]⁺

E (B3LYP/BS1) = -768.383147 au

H(B3LYP/BS1) = -768.076775 au

G(B3LYP/BS1) = -768.153668 au

E(M06/BS2//B3LYP/BS1) = -768.241921 au

C	-1.37314500	0.33269800	-0.09432300
C	-0.25253000	-0.46906100	-0.34248800
C	1.08021600	-0.05098400	-0.44708500
C	2.17689900	-1.03672600	-0.72742500
O	1.40156400	1.20363900	-0.30161000
H	2.91431000	-1.02098700	0.08578200
H	1.79209600	-2.05066200	-0.84506300

H	2.71079700	-0.74641200	-1.64056500
H	-0.40772200	-1.53299600	-0.47827200
H	2.41577400	1.38399500	-0.42213500
O	3.89068300	1.62093700	-0.63100300
H	4.42561500	1.10557800	0.03833500
O	5.06300800	0.00043700	1.11071700
H	5.87832100	-0.46268800	0.79751200
O	7.31831700	-1.27944700	0.23833900
H	8.15462700	-0.82350100	0.05983700
H	4.17197600	2.54736500	-0.58108400
H	5.24969500	0.27795900	2.02007200
H	7.56468700	-2.15723400	0.56696700
C	-1.28928600	1.82060300	0.11157900
H	-0.62917300	2.04927500	0.95453600
H	-0.83449000	2.29760000	-0.76282600
H	-2.27009000	2.25766200	0.29162100
C	-2.64969400	-0.28395800	-0.03609400
C	-3.09736400	-1.59663700	-0.18115700
O	-3.75092400	0.51565200	0.21112600
C	-4.49123800	-1.58274600	-0.01784600
H	-2.48391700	-2.46335000	-0.38325400
C	-4.84817600	-0.26634500	0.22073700
H	-5.16782500	-2.42405000	-0.06642500
C	-6.15411900	0.39396000	0.47038200
H	-6.95978100	-0.34305800	0.45288200
H	-6.15758600	0.89534700	1.44555900
H	-6.35787600	1.15558200	-0.29169700

TS₅₊₁

E (B3LYP/BS1) = -3570.328943 au

H(B3LYP/BS1) = -3570.11045 au

G(B3LYP/BS1) = -3570.204656 au

E(M06/BS2//B3LYP/BS1) = -3570.851635 au

C	0.04089800	-0.68795200	1.71021900
C	-1.11769500	-1.51715700	1.71768400
C	0.87388400	-1.17319800	0.71645200
C	-0.93206600	-2.45795600	0.73909200
C	-1.73832500	-3.60209300	0.24413600
O	0.27876900	-2.24797000	0.12680300
H	-2.00363900	-3.45986300	-0.80948700
H	-1.18337300	-4.54443300	0.33517100
H	-2.66509300	-3.67489600	0.81889600
H	0.26157300	0.12342000	2.38468500
H	-1.98455000	-1.42554800	2.35702000
Au	2.71888800	-0.61390200	0.10541200
Cl	3.15637600	0.21047500	2.30580500
Cl	4.89572100	0.17436000	-0.61337700
Cl	2.22546500	-1.32796100	-2.10070000
C	-0.06508900	1.44786300	-0.37007200
C	0.89016200	2.14593000	0.16234400
C	-1.04791500	1.00842700	-1.22031600
C	1.59524000	3.21314400	-0.69060700

C	2.97998400	3.56091300	-0.19766500
O	1.07643200	3.70117200	-1.66974600
H	3.36176200	4.41173400	-0.76567700
H	2.96610500	3.78834200	0.87437300
H	3.64207400	2.69298600	-0.33179200
H	1.28719500	1.96398900	1.15706400
H	-1.54332600	1.85307300	-1.72051500
H	-0.78141200	0.17228000	-1.86744900
Au	-2.88354000	0.37710400	-0.18282000
Cl	-2.58203500	2.01114000	1.52544400
Cl	-3.22734700	-1.11483500	-2.00214000
Cl	-4.94264800	-0.33242000	0.83549000

TS_{4-1sol}

E (B3LYP/BS1) = -1918.164491 au

H(B3LYP/BS1) = -1917.996696 au

G(B3LYP/BS1) = -1918.068786 au

E(M06/BS2//B3LYP/BS1) = -1918.349777 au

C	1.70189000	-1.39928500	1.36345800
C	2.84387000	-1.56316800	0.53519200
C	1.54822400	-0.03752300	1.54496800
C	3.32438200	-0.30482500	0.27274300
C	4.46057400	0.20347500	-0.53915900
O	2.55127100	0.62819100	0.90043100
H	4.09843000	0.82339300	-1.36717400
H	5.13836100	0.81643900	0.06739500
H	5.02611300	-0.63354200	-0.95583200
H	0.92789300	0.54682800	2.20550500
H	1.06383900	-2.16501300	1.78182300
H	3.24836500	-2.48988200	0.15439900
Au	-0.68648000	-0.23650600	-0.10145000
Cl	0.60779300	0.08690200	-2.05562900
Cl	-1.86863600	-2.00778700	-1.11771400
Cl	-1.85377700	-0.54680100	1.93665200
C	-0.69183200	3.24222800	0.09026000
C	-0.88913500	4.66152600	-0.17628900
H	-0.20666300	5.25657500	0.43818800
H	-0.69170200	4.86894300	-1.23256200
H	-1.91988900	4.94479900	0.05751800
N	-0.52890200	2.11799400	0.30551200

1_sol

E (B3LYP/BS1) = -1648.829361 au

H(B3LYP/BS1) = -1648.766732 au

G(B3LYP/BS1) = -1648.821111 au

E(M06/BS2//B3LYP/BS1) = -1649.125740 au

C	2.95450700	-0.00264800	0.00004500
Au	-0.25623600	-0.00010800	0.00033300
Cl	-0.22297400	-2.38067200	0.00015000
Cl	-2.55552400	0.00400500	-0.00145100
Cl	-0.21478500	2.38036400	0.00015200
N	1.80226500	-0.00321000	0.00135200
C	4.40924700	-0.00160700	-0.00186400
H	4.77611800	-0.70082200	-0.75965500

H	4.77618500	1.00447700	-0.22709700
H	4.77775700	-0.31001700	0.98145400

TS_{1sol-1'}

E (B3LYP/BS1) = -1918.125505 au

H(B3LYP/BS1) = -1917.960200 au

G(B3LYP/BS1) = -1918.036671 au

E(M06/BS2//B3LYP/BS1) = -1918.311962 au

C	-0.39570100	3.27759900	-0.16022200
Au	0.82130500	-0.04737100	0.00419200
Cl	0.79056900	-0.26636300	-2.35572600
Cl	2.86239800	-1.17133000	0.10457200
Cl	0.76602700	0.09876300	2.36786800
C	-4.41233200	-0.70792400	0.05638000
C	-3.55728400	-1.71114400	0.02299800
C	-5.25929000	0.27833100	0.09097600
C	-2.08913200	-1.50784600	0.00861100
C	-1.21036700	-2.73553800	-0.02109000
O	-1.61373900	-0.36884400	0.01964200
H	-0.53629500	-2.71359600	0.84343600
H	-1.78145300	-3.66668900	-0.01234700
H	-0.58280700	-2.69973000	-0.91969800
H	-5.63906400	0.72982800	-0.82334800
H	-5.61054200	0.68867700	1.03561700
H	-3.92463300	-2.73512200	0.00716100
N	-0.19847600	2.13929800	-0.15373700
C	-0.65447900	4.71268500	-0.16758800
H	-1.72025300	4.90021000	-0.32954200
H	-0.35731000	5.14869300	0.79108600
H	-0.08292600	5.19051300	-0.96906800

TS_{1-9'}

E (B3LYP/BS1) = -2054.714467 au

H(B3LYP/BS1) = -2054.494545 au

G(B3LYP/BS1) = -2054.57014 au

E(M06/BS2//B3LYP/BS1) = -2054.852112 au

C	0.32197900	0.99350100	-0.05016500
C	0.21726300	2.30280500	0.12634100
C	1.11982900	-0.11538800	-0.30550000
C	1.38733200	3.23848100	0.09020900
C	1.05523900	4.69321600	0.34919700
O	2.52784800	2.86429900	-0.13508700
H	1.96531600	5.29368000	0.30645800
H	0.33640000	5.05623400	-0.39632700
H	0.58029500	4.80630600	1.33198700
H	1.33121900	-0.80456000	0.50683400
H	1.13000000	-0.51430200	-1.31680000
H	-0.75877400	2.74446700	0.30523600
Au	-1.46123200	-0.23965000	0.01388300
Cl	-1.68889200	0.13116800	-2.32146800
Cl	-3.57399800	-1.30502400	0.15278300
Cl	-1.03249200	-0.56715500	2.33008700
C	3.44049000	0.10077900	-0.64910300
H	3.29801100	0.88005800	-1.37880200

C	3.78667700	0.14119000	0.69079900
H	3.72809800	1.01877900	1.31730000
C	4.17838800	-1.17157100	1.04810500
C	4.08700900	-1.93645600	-0.09393500
H	4.48123400	-1.52451200	2.02370600
O	3.66461200	-1.16718100	-1.13316300
C	4.34051100	-3.37341400	-0.37785000
H	3.43027800	-3.87371200	-0.72948500
H	5.10110300	-3.48910500	-1.15912700
H	4.68769200	-3.87958100	0.52587600

9'

E (B3LYP/BS1) = -2054.755235 au

H(B3LYP/BS1) = -2054.531844 au

G(B3LYP/BS1) = -2054.604376 au

E(M06/BS2//B3LYP/BS1) = -2054.907475 au

C	0.17765200	0.99840800	-0.16939300
C	0.06743600	2.20334900	0.42577300
C	1.36997100	0.54647000	-0.98484000
C	1.04713800	3.31653600	0.35021900
C	0.52252100	4.67621900	0.76730100
O	2.21096600	3.18606900	-0.03353400
H	1.30819400	5.42659200	0.66331500
H	-0.34229400	4.95362500	0.15209300
H	0.17387500	4.64609700	1.80740200
H	1.15512900	-0.38389800	-1.51346500
H	1.63440400	1.32126700	-1.71373100
H	-0.86326300	2.44724100	0.93006500
Au	-1.35722500	-0.36253400	-0.02933600
Cl	-2.85639100	1.28084300	-0.79474400
Cl	-3.12578100	-1.99201600	0.14655600
Cl	0.23319500	-2.02596600	0.69619300
C	2.61424200	0.33117800	-0.10637200
H	2.96164200	1.34181300	0.17374400
C	2.55787800	-0.53897700	1.08705400
H	1.91855500	-0.33825000	1.93335100
C	3.58616400	-1.45207200	1.01415400
C	4.21441000	-1.25421600	-0.22515600
H	3.85249700	-2.20969400	1.73735400
O	3.68870900	-0.26235200	-0.90643200
C	5.35114400	-1.98229700	-0.84243700
H	5.00825800	-2.48944900	-1.75275300
H	6.13574700	-1.27747200	-1.13894400
H	5.76193200	-2.72360400	-0.15506100

Table S2. Cartesian coordinates and total energies for the structures optimized by inclusion of dispersion

1

E(B3LYP-D3/BS1) = -1785.388863 au
H(B3LYP-D3/BS1) = -1785.274810 au
G(B3LYP-D3/BS1) = -1785.335047 au
E(M06-D3/BS2//B3LYP-D3/BS1) = -1785.615988 au

C	-1.56247000	-0.00004600	-0.49367600
C	-2.38298500	-0.00002300	0.52200000
C	-0.93708400	-0.00004400	-1.68862000
C	-3.88361300	-0.00000800	0.26260400
C	-4.73817500	0.00004100	1.50982300
O	-4.32897200	-0.00004300	-0.86433400
H	-5.79263200	0.00003800	1.22943300
H	-4.51389600	-0.88303800	2.12152800
H	-4.51388400	0.88316300	2.12146300
H	-0.76798500	0.93914900	-2.21331900
H	-0.76794700	-0.93924000	-2.21330000
H	-2.01743300	0.00004100	1.54466300
Au	0.78353600	0.00000000	-0.11341800
Cl	0.70499700	-2.37032300	-0.13445300
Cl	2.83314500	0.00004400	1.01081300
Cl	0.70492800	2.37032100	-0.13451300

Cl
E(B3LYP-D3/BS1) = -460.248731 au
H(B3LYP-D3/BS1) = -460.246371 au
G(B3LYP-D3/BS1) = -460.263754 au
E(M06-D3/BS2//B3LYP-D3/BS1) = -460.371685 au

Cl	0.00000000	0.00000000	0.00000000
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furan

E (B3LYP-D3/BS1) = -269.343983 au
H(B3LYP-D3/BS1) = -269.239662 au
G(B3LYP-D3/BS1) = -269.274637 au
E(M06-D3/BS2//B3LYP-D3/BS1) = -269.234099 au

C	-1.54964100	0.61702100	0.00005900
C	-0.22195100	1.16456100	-0.00006800
C	-1.39735100	-0.73447100	-0.00002800
C	0.63868100	0.10624200	-0.00009500
C	2.12233300	-0.01343300	0.00004900
O	-0.07184600	-1.06488900	0.00004500
H	2.48154700	-0.55385900	0.88481300
H	2.48168000	-0.55497900	-0.88396900
H	2.57489100	0.98226600	-0.00054000
H	-2.08726900	-1.56482800	-0.00000200
H	-2.48389900	1.16122400	0.00010800
H	0.05540100	2.20976600	-0.00027100

(H₂O)₃

E(B3LYP-D3/BS1) = -229.266725 au
 H(B3LYP-D3/BS1) = -229.184878 au
 G(B3LYP-D3/BS1) = -229.220696 au
 E(M06-D3/BS2//B3LYP-D3/BS1) = -229.296742 au
 O -0.40218200 1.52350300 0.12209700
 H -0.45115900 1.99961800 -0.72099300
 H 0.46959900 1.05796700 0.09021300
 O 1.52854100 -0.40669500 -0.09906400
 H 0.69631100 -0.93687600 -0.15590700
 H 1.92702400 -0.66218700 0.74659200
 O -1.12810200 -1.10856400 -0.10517800
 H -1.47083500 -1.40303900 0.75214200
 H -1.15699000 -0.12143500 -0.05488700

$[(\text{H}_2\text{O})_2(\text{H}_3\text{O})\text{Cl}]^+$
 E(B3LYP-D3/BS1) = -690.081082 au
 H(B3LYP-D3/BS1) = -689.988915 au
 G(B3LYP-D3/BS1) = -690.031972 au
 E(M06-D3/BS2//B3LYP-D3/BS1) = -690.106214 au
 O 0.89215400 1.94258200 -0.06016400
 H 1.81830900 0.50402700 0.06323600
 H 0.83837200 2.39128100 0.79810000
 H -0.01714800 1.60589100 -0.20799800
 O 2.22537900 -0.40482200 0.07517000
 H 2.76213200 -0.44649100 -0.73117700
 H 0.94647400 -1.40870400 -0.03596200
 O 0.07341000 -1.91679400 -0.06828600
 H 0.00942300 -2.38175300 0.78214600
 H -0.92483300 -0.88750900 -0.05695400
 Cl -1.82119300 0.21503100 -0.01089100

sub1

E(B3LYP-D3/BS1) = -269.303670 au
 H(B3LYP-D3/BS1) = -269.202014 au
 G(B3LYP-D3/BS1) = -269.240538 au
 E(M06-D3/BS2//B3LYP-D3/BS1) = -269.199529 au
 C -1.49219400 -0.34845600 -0.00004100
 C -0.24453500 -0.76389200 -0.00010400
 C -2.72243600 0.07852100 0.00004200
 C 0.91562000 0.18515700 -0.00001900
 C 2.28581900 -0.47330500 0.00004800
 O 0.77786400 1.39512600 0.00001200
 H 3.06186400 0.29424800 -0.00001200
 H 2.40099400 -1.11586700 0.88254600
 H 2.40102500 -1.11606000 -0.88230300
 H -3.25607200 0.27021700 -0.92877700
 H -3.25594300 0.27023800 0.92893000
 H -0.02843000 -1.83193100 -0.00002800

TS₁₋₂

E(B3LYP-D3/BS1) = -1785.384639 au

H(B3LYP-D3/BS1) = -1785.271607 au
 G(B3LYP-D3/BS1) = -1785.329455 au
 E(M06-D3/BS2//B3LYP-D3/BS1) = -1785.609739 au

C	1.39021000	-0.00008600	0.14696700
C	2.32939700	0.00013700	-0.77966100
C	1.32152300	-0.00040300	1.51454800
C	3.71265200	-0.00002300	-0.18171400
C	4.87002800	0.00022300	-1.14936000
O	3.86203800	-0.00034600	1.03118200
H	5.81544100	0.00023200	-0.60532000
H	4.81084900	-0.88225200	-1.79843400
H	4.81069200	0.88284300	-1.79821800
H	1.23279800	0.93797600	2.05988400
H	1.23270100	-0.93902500	2.05945000
H	2.16493600	0.00042600	-1.84983500
Au	-0.74439100	0.00000100	0.03295600
Cl	-0.65912400	-2.37225500	0.07756900
Cl	-3.02913200	0.00021000	-0.52167800
Cl	-0.65878500	2.37224500	0.07792000

TS_{1'}-8

E (B3LYP-D3/BS1) = -2054.742630 au
 H(B3LYP-D3/BS1) = -2054.522578 au
 G(B3LYP-D3/BS1) = -2054.595569 au
 E(M06-D3/BS2//B3LYP-D3/BS1) = -2054.845120 au

C	-2.86437700	1.82966100	-0.06067700
C	-1.84943400	2.44486000	0.65023800
C	-3.63146600	1.89799200	-1.12567400
C	-0.54566400	1.92396300	0.64792400
C	0.57397000	2.58732000	1.39581800
O	-0.33912700	0.83876900	-0.01302100
H	1.39270400	2.80719000	0.69995400
H	0.25297100	3.51249600	1.87955100
H	0.96101900	1.89309000	2.15231200
H	-4.45480100	1.22604400	-1.33073100
H	-3.41804100	2.67680400	-1.85618700
H	-2.07120900	3.31027200	1.26868700
Au	1.48211100	-0.13896100	-0.08497200
Cl	3.46406900	-1.33977400	-0.25396100
Cl	1.00335200	-1.07645900	2.05357600
Cl	1.87912600	0.96466100	-2.13599800
C	-2.44461900	-0.74793600	0.95879500
C	-4.02132500	-1.54629900	-0.40767700
C	-2.73569800	-1.76911100	0.03744100
H	-1.52602800	-0.63135400	1.51334400
H	-2.07656700	-2.56331700	-0.28243500
O	-4.55244500	-0.46100200	0.20520400
C	-3.55846800	0.10600400	0.99174200
H	-3.93985200	0.68993000	1.81738500
C	-4.87108700	-2.23573300	-1.41216800
H	-5.85896400	-2.46215600	-0.99547400

H	-5.02126700	-1.60412300	-2.29658600
H	-4.39643700	-3.16668200	-1.73051300

TS₁₋₉

E (B3LYP-D3/BS1) = -2054.747467 au

H(B3LYP-D3/BS1) = -2054.528041 au

G(B3LYP-D3/BS1) = -2054.602858 au

E(M06-D3/BS2//B3LYP-D3/BS1) = -2054.855406 au

C	-1.10995200	0.89559000	0.34226900
C	-1.21074100	2.07938000	-0.20228500
C	-0.62905900	-0.21829500	0.96230900
C	-2.44586200	2.90568100	-0.45920300
C	-2.15824700	4.27036600	-1.04575200
O	-3.57240000	2.51615000	-0.22136200
H	-3.09437500	4.80951200	-1.19771300
H	-1.50303300	4.83939600	-0.37409600
H	-1.62714300	4.16595100	-2.00051100
H	-0.93701500	-1.18914200	0.56766000
H	-0.48245800	-0.14932300	2.04086200
H	-0.25829000	2.53078000	-0.48531100
Au	1.42037600	-0.13658200	0.07828000
Cl	1.94332700	1.56027700	1.65329400
Cl	3.63933600	-0.20085200	-0.73833300
Cl	0.71263500	-1.78187500	-1.48155700
C	-3.67605100	-0.29314100	0.50270200
H	-4.09097200	0.52854500	1.06154200
C	-3.42691000	-0.48458800	-0.83671300
H	-3.58469300	0.24580800	-1.61531500
C	-2.93336600	-1.81320600	-0.96589900
C	-2.91533100	-2.35255200	0.29561500
H	-2.59471300	-2.30422100	-1.86625500
O	-3.38291600	-1.42703100	1.19760400
C	-2.52146200	-3.67981600	0.83635400
H	-1.79826500	-3.57498400	1.65340100
H	-3.39011000	-4.22081900	1.23170900
H	-2.06429700	-4.27932900	0.04570800

TS_{4-1'}

E(B3LYP-D3/BS1) = -2054.756527 au

H(B3LYP-D3/BS1) = -2054.536850 au

G(B3LYP-D3/BS1) = -2054.613185 au

E(M06-D3/BS2//B3LYP-D3/BS1) = -2054.855788 au

C	0.54445300	2.16664200	1.52315200
C	0.46623600	3.25052500	0.60626000
C	-0.65082900	1.47988400	1.41341600
C	-0.76288400	3.16672500	0.00370800
C	-1.43342600	3.95617000	-1.06041900
O	-1.45589200	2.10277400	0.50457800
H	-1.63512100	3.32354700	-1.93169800
H	-2.38873700	4.36517700	-0.70934100
H	-0.79148200	4.78347100	-1.37274500

H	-1.09080900	0.66862800	1.97038800
H	1.36320300	1.89863400	2.17592200
H	1.23233500	3.97958600	0.38618800
Au	0.87029700	-0.37198100	0.01555900
Cl	0.38984900	0.71105900	-2.02878400
Cl	3.14066400	-0.68330200	-0.57060600
Cl	1.16984900	-1.37325700	2.12779400
C	-4.18770700	-1.26195700	0.23768500
C	-3.43817800	-1.94612500	-0.60577700
C	-4.90260700	-0.57512000	1.07772900
C	-1.97235700	-1.76807500	-0.64685700
C	-1.17986100	-2.52907700	-1.67475600
O	-1.42725300	-0.99122000	0.14791300
H	-0.30788400	-2.98393200	-1.19193700
H	-1.76807500	-3.29537600	-2.18424500
H	-0.79707100	-1.80769000	-2.40767700
H	-5.29931500	0.40296900	0.81305400
H	-5.11994700	-0.95279300	2.07498100
H	-3.88857700	-2.65217400	-1.29970600

TS₅₋₆

E (B3LYP-D3/BS1) = -2284.05757 au

H(B3LYP-D3/BS1) = -2283.753138 au

G(B3LYP-D3/BS1) = -2283.837863 au

E(M06-D3/BS2//B3LYP-D3/BS1) = -2284.176755 au

C	0.07541800	-2.43553000	0.96146900
C	1.29185600	-2.67638600	1.63809500
C	0.08622900	-1.10376700	0.50677800
C	1.99154200	-1.49512000	1.61498600
C	3.28176900	-1.06725500	2.21186600
O	1.25748800	-0.53847500	0.97638200
H	3.79105900	-1.92521400	2.65704200
H	3.92926700	-0.59602400	1.46698100
H	3.09079700	-0.31279000	2.98444500
H	-0.74770700	-3.11701300	0.81661600
H	1.62546100	-3.60312500	2.08268400
Au	-1.45035100	0.18705300	0.06751100
Cl	-2.97337600	-1.63161100	0.12928600
Cl	-3.27042700	1.64365400	-0.47162400
Cl	-0.04273700	2.12364900	0.19407400
C	0.70319200	-2.04126700	-1.38643700
C	2.08243200	-1.86037100	-1.46501600
C	-0.35687800	-2.47822300	-2.02899000
C	2.60821000	-0.61381500	-1.76861400
C	4.08098800	-0.34062700	-1.82767200
O	1.77316500	0.36700800	-2.00382600
H	4.35414400	0.33951400	-1.01114100
H	4.66360600	-1.26006200	-1.73936400
H	4.33302300	0.16002300	-2.76922300
H	2.75638900	-2.68079000	-1.24269300
H	-0.23188700	-2.79663500	-3.06357200

H	-1.35599800	-2.50338600	-1.60946200
H	2.19930100	1.29587700	-2.06474800
O	2.65315200	2.77558900	-1.81612900
H	2.95701100	2.63616500	-0.88097400
O	3.19086700	1.65362300	0.56333800
H	2.97926300	1.97872600	1.46765500
O	1.78124100	1.89004000	2.90092700
H	1.58889200	2.69443800	3.40691500
H	1.78849000	3.21200300	-1.72010400
H	2.40480600	1.10502700	0.38782600
H	1.00713400	1.78116800	2.31391400

TS₇

E (B3LYP-D3/BS1) = -1593.920206 au

H(B3LYP-D3/BS1) = -1593.716153 au

G(B3LYP-D3/BS1) = -1593.785296 au

E(M06-D3/BS2//B3LYP-D3/BS1) = -1594.031161 au

C	-0.38660600	1.11116900	0.52419100
C	-0.92372500	1.48632600	1.73498900
C	-1.90399900	2.48137800	1.44952200
Cl	2.42274600	1.60592000	-0.82161300
H	-0.64271600	1.09631100	2.70288500
Cl	2.78860900	-1.84623100	-0.30649900
C	-1.17575600	-1.11813300	0.35972500
C	-0.15082900	-1.71162000	1.04897300
C	-2.24929600	-1.00258000	-0.38527400
H	0.26118400	-2.64178800	0.65756800
H	-2.39689400	-0.13997100	-1.02724000
Au	1.12504900	-0.16377400	0.07117500
C	-3.32022900	-2.06920700	-0.30520600
O	-3.20521000	-3.04638200	0.40586000
C	-4.52900800	-1.81056300	-1.18127100
H	-5.00119100	-0.85991400	-0.90280000
H	-4.22502700	-1.72666500	-2.23224600
H	-5.24343900	-2.62731200	-1.06634800
H	-0.03803500	-1.52551100	2.11654700
O	-1.00039000	1.79600700	-0.48149700
C	-1.92447600	2.63524100	0.08936400
H	-2.51657700	3.02078800	2.15838300
C	-2.67358200	3.52399200	-0.83675600
H	-3.41855500	4.09944900	-0.28101200
H	-1.99518000	4.22552000	-1.33742100
H	-3.18566400	2.94945000	-1.61767200