Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Nazarov cyclizations initiated by DDQ-oxidised pentadienyl ether: A mechanistic investigation from the DFT perspective

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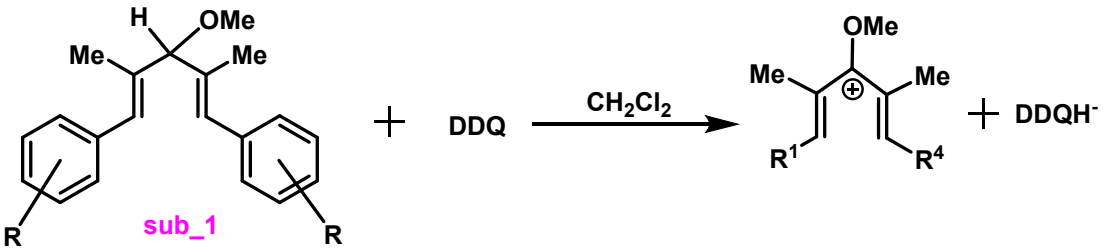
Table S1 Relative Gibbs free energy (kcal/mol) of transition structures **TS_A**, **TS_B**, and **TS_D** and intermediates **2_D** and **2_A** calculated at the M06-2X-D3 (Table S1a) and B3LYP-D3 (Table S1b) levels for cases where the pentadienyl ether is substituted by a variety of R groups.



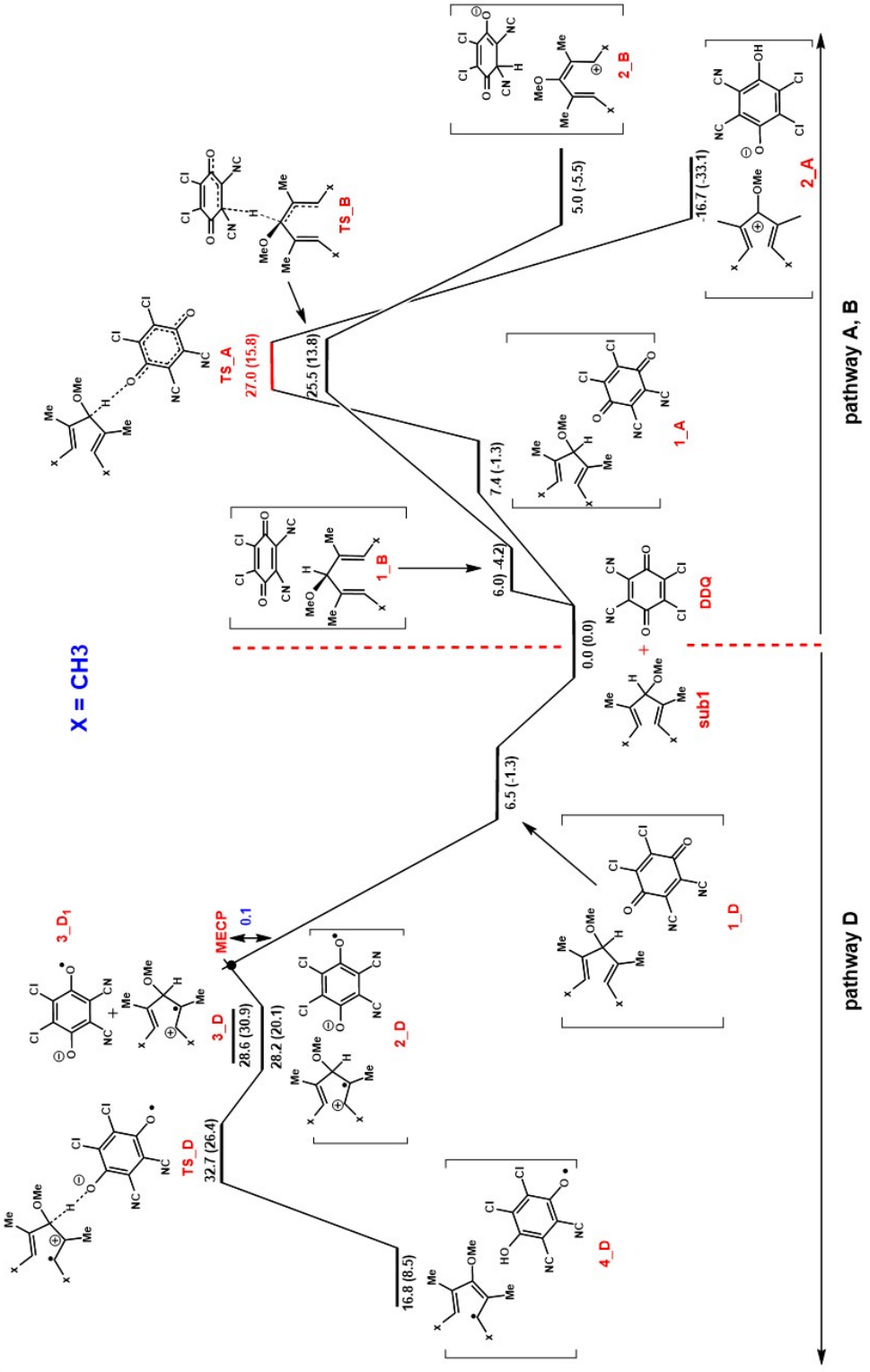
(S1a)

Entry	R-Ph	ΔG (kcal/mol) M06-2X-D3				
		(TS_A)	**(TS_B)**	**(TS_D)**	**(2_D)**	**(2_A)**
1	para-CN-Ph	24.2	29.5	35.1	33.8	-16.1
2	para-Cl-Ph	21.6	27.4	32.7	27.9	-16.9
3	Ph	19.7	26.3	32.0	25.7	-16.2
4	para-Me-Ph	19.0	25.5	30.0	24.1	-17.1
5	para-OMe-Ph	17.0	23.9	28.4	18.2	-17.5
6	para-NH_2-Ph	14.0	22.1	25.9	9.6	-18.0
7	para-NMe_2-Ph	11.4	20.4	22.4	7.8	-19.3
8	meta-CN-Ph	27.0	37.9	38.2	39.9	-15.4
9	meta-OMe-Ph	20.1	26.9	32.0	25.1	-16.5
10	meta-Me-Ph	18.5	24.9	30.1	25.3	-17.8

(S1b)

Entry	R-Ph	ΔG (kcal/mol) B3LYP-D3				
		(TS_A)	**(TS_B)**	**(TS_D)**	**(2_D)**	**(2_A)**
1	para-CN-Ph	14.3	23.0	25.7	22.2	-7.6
2	para-Cl-Ph	11.1	20.5	23.4	16.0	-8.6
3	Ph	9.6	19.4	23.0	14.4	-8.9
4	para-Me-Ph	8.5	18.3	21.0	12.2	-9.0
5	para-OMe-Ph	5.8	16.2	19.3	6.7	-9.7
6	para-NH_2-Ph	2.0	13.5	16.7	-1.0	-10.1
7	para-NMe_2-Ph	-1.4	11.6	12.9	-5.1	-11.5
8	meta-CN-Ph	16.9	24.7	28.7	27.2	-7.0
9	meta-OMe-Ph	9.0	19.7	22.6	13.1	-8.4
10	meta-Me-Ph	7.7	17.7	21.8	13.2	-9.6

Scheme ESI1 Energy profile for the reaction between pentadienyl ether (**sub_1** when X=Me) and DDQ through pathways A, B, and D. The relative Gibbs and potential energies (in parentheses) obtained from M06-2X/6-311+G(2d,p)//B3LYP/6-31G(d) calculations are given in kcal/mol.



Cartesian coordinates and total energies for all of the calculated structures in CH_2Cl_2

Fig. 1
sub_1
E(B3LYP/BS1) = -850.566216 au
H(B3LYP/BS1) = -850.178419 au
G(B3LYP/BS1) = -850.250818 au
E(M06-2X/BS2//B3LYP/BS1) = -850.436541 au

C	0.00031100	1.91110300	-0.19352400
C	1.43547800	1.37216800	-0.12392500
C	-1.07740400	0.95889700	0.31702400
C	1.65346100	0.04373000	-0.06456900
H	0.78068100	-0.59763200	0.04495100
C	-1.94163600	0.42985300	-0.57330200
H	-1.83641800	0.75965600	-1.60801500
C	2.93016700	-0.69846300	-0.10393300
C	4.01679100	-0.34402500	-0.92551700
C	3.05361900	-1.86184000	0.68092700
C	5.18938900	-1.10138700	-0.93220100
H	3.93392200	0.51237700	-1.58665400

C	4.22581000	-2.61578100	0.67950900
H	2.21734300	-2.16832400	1.30517400
C	5.30363400	-2.23525700	-0.12497900
H	6.01218000	-0.80858800	-1.57927800
H	4.29687300	-3.50328900	1.30292500
H	6.21718100	-2.82351000	-0.13193000
C	-3.05308000	-0.51583100	-0.36838100
C	-3.08247800	-1.49032800	0.64819500
C	-4.13858800	-0.47171300	-1.26645300
C	-4.16683200	-2.35914800	0.77707100
H	-2.24107500	-1.59205200	1.32423100
C	-5.22392200	-1.33537900	-1.13489500
H	-4.12663200	0.25863400	-2.07226400
C	-5.24536600	-2.28227300	-0.10696000
H	-4.16298500	-3.10571500	1.56695900
H	-6.05111400	-1.27304800	-1.83705900
H	-6.08796100	-2.96047500	-0.00381300
C	2.51497800	2.42238500	-0.20381400
H	3.49957800	2.01370200	0.03038000
H	2.56279100	2.86814500	-1.20803800
H	2.29570200	3.23890200	0.48882000
C	-1.10260600	0.74295900	1.81127000
H	-0.74736800	1.64736900	2.31434100
H	-2.10859000	0.51391700	2.17337000
H	-0.44133800	-0.07666900	2.12099400
O	-0.03497600	3.15105400	0.52499100
H	-0.20649400	2.13257900	-1.25619800
C	-1.15658900	3.96140300	0.21012500
H	-1.04058300	4.89153800	0.77219200
H	-1.19191400	4.19225700	-0.86543400
H	-2.10479000	3.48534700	0.49441200

DDQ

E(B3LYP/BS1) = -1485.107254 au

H(B3LYP/BS1) = -1485.031251 au

G(B3LYP/BS1) = -1485.084679 au

E(M06-2X/BS2//B3LYP/BS1) = -1485.08086 au

O	-0.14245300	2.67207600	-0.00005800
C	-0.11925600	1.45737100	-0.00002900
C	-1.40399400	0.67819700	-0.00003900
C	1.15361100	0.67729700	-0.00002400
C	-1.40402000	-0.67817700	-0.00009800
C	1.15359200	-0.67731900	-0.00003200
C	-0.11930400	-1.45734900	-0.00009000
O	-0.14253600	-2.67205100	-0.00012100
Cl	2.59322100	1.61598400	0.00003800
Cl	2.59316200	-1.61604000	0.00006000
C	-2.60629000	1.44836800	0.00005000
C	-2.60632400	-1.44832400	0.00004800
N	-3.58402900	2.07636200	0.00002200
N	-3.58406800	-2.07631000	0.00013000

1_A

E(B3LYP/BS1) = -2335.675559 au
H(B3LYP/BS1) = -2335.209679 au
G(B3LYP/BS1) = -2335.321691 au
E(M06-2X/BS2//B3LYP/BS1) = -2335.520358 au

C	1.88532000	-0.13574300	1.58345200
C	2.01545100	1.36522800	1.29428800
C	2.95791400	-1.01659500	0.94985600
C	2.67829100	1.78202600	0.19762300
H	3.20523500	1.02509900	-0.38138100
C	2.59311900	-1.87288500	-0.02643900
H	1.53066100	-1.90679800	-0.27239500
C	2.81723400	3.14878600	-0.34655700
C	1.76823400	4.08740400	-0.37169100
C	4.04482700	3.52005600	-0.92929500
C	1.95379400	5.35546300	-0.92524900
H	0.79104200	3.81505700	0.01448800
C	4.23257000	4.78785000	-1.47727300
H	4.86154600	2.80178800	-0.94196400
C	3.18693300	5.71536500	-1.47327100
H	1.12651300	6.06044700	-0.93688200
H	5.19363200	5.05077000	-1.91164700
H	3.32837400	6.70292300	-1.90394000
C	3.40852100	-2.82148000	-0.80596800
C	4.76510100	-2.61742700	-1.12486100
C	2.78786700	-3.98827900	-1.29576100
C	5.47510300	-3.55798700	-1.87228100
H	5.26232200	-1.70549800	-0.81365700
C	3.49769300	-4.93036000	-2.03732000
H	1.73506600	-4.15566600	-1.07998400
C	4.84936700	-4.72145300	-2.32551200
H	6.51997400	-3.37473500	-2.10885100
H	2.99544300	-5.82560700	-2.39433300
H	5.40519100	-5.45179800	-2.90707400
C	1.28903800	2.26590200	2.26091200
H	1.52869300	3.31793600	2.09670700
H	0.20082900	2.14449100	2.16973200
H	1.54811000	1.99910400	3.28897600
C	4.34178500	-0.88450000	1.53856000
H	4.26060900	-0.63802700	2.60163200
H	4.91847900	-1.80769400	1.43651300
H	4.91550100	-0.07730300	1.06518100
O	1.86551300	-0.31047200	3.00641900
H	0.90029900	-0.44711000	1.19363400
C	1.30957900	-1.54977300	3.41834800
H	1.30438200	-1.54473000	4.51137200
H	0.27802600	-1.66250200	3.05265400
H	1.90030700	-2.40634200	3.06587700
O	-1.82561900	0.03706600	1.42743900
C	-2.81741100	-0.03257800	0.72771300
C	-3.38336100	1.20712600	0.09521900
C	-3.52267900	-1.32013000	0.46000100

C	-4.49750300	1.15698500	-0.67706400
C	-4.63320000	-1.37111200	-0.31458100
C	-5.20900300	-0.14101000	-0.93464200
O	-6.20923800	-0.16229300	-1.62365300
Cl	-2.82989300	-2.70898800	1.19818600
Cl	-5.47727500	-2.82948400	-0.65056900
C	-2.68209500	2.42353000	0.35361500
C	-5.06325700	2.31666100	-1.28817400
N	-2.10768400	3.41173300	0.56360900
N	-5.52503300	3.25960600	-1.78613400

TS_A

E(B3LYP/BS1) = -2335.651003 au

H(B3LYP/BS1) = -2335.191202 au

G(B3LYP/BS1) = -2335.292982 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.502807 au

C	1.27543000	-2.04497800	-0.41603400
C	2.55201700	-1.41259100	0.06244000
C	0.36538200	-1.36746000	-1.34819000
C	3.16929600	-0.47429900	-0.70135100
H	2.73163800	-0.26506700	-1.67515400
C	0.08979000	-0.02856800	-1.10903800
H	0.71945700	0.45072900	-0.36759400
C	4.40031500	0.27199000	-0.42519500
C	4.79641000	0.67052900	0.86795400
C	5.20348300	0.66200000	-1.51747600
C	5.96691400	1.40335800	1.05812100
H	4.16532000	0.44502800	1.72037300
C	6.37839100	1.38288000	-1.32381300
H	4.89963100	0.38420800	-2.52372400
C	6.76714000	1.75337600	-0.03261200
H	6.24973700	1.71033700	2.06118000
H	6.98747500	1.66313400	-2.17865500
H	7.67978600	2.32246400	0.12041000
C	-0.84474400	0.88156900	-1.74011400
C	-1.98757800	0.49300500	-2.48154200
C	-0.63507100	2.26797500	-1.52705600
C	-2.85577200	1.44842800	-2.99804700
H	-2.21808200	-0.55419400	-2.62484400
C	-1.49990300	3.21885300	-2.05605600
H	0.23060300	2.58833000	-0.95404200
C	-2.61610100	2.81181000	-2.79247100
H	-3.73198500	1.12921300	-3.55418700
H	-1.31160900	4.27446700	-1.88601200
H	-3.30050000	3.55106200	-3.19795900
C	3.09765000	-1.97571800	1.35270900
H	4.18219700	-1.86237300	1.41500400
H	2.65367800	-1.47913500	2.22431400
H	2.85826300	-3.04064600	1.42365200
C	-0.25733100	-2.17317700	-2.45769100
H	0.39588000	-3.00932600	-2.71797800
H	-1.23663400	-2.58755100	-2.18731300

H	-0.39964000	-1.54913300	-3.34380700
O	1.47342200	-3.41415300	-0.58185400
H	0.49964300	-1.91231800	0.67146000
C	0.44101300	-4.33631800	-0.20023300
H	0.85399600	-5.32809400	-0.39092600
H	0.20796700	-4.23080600	0.86319600
H	-0.47134700	-4.20517700	-0.78751400
O	-0.26642900	-1.72268100	1.67925100
C	-1.13686400	-0.79386200	1.46189400
C	-0.85718200	0.57077200	1.84244900
C	-2.45693300	-1.07540900	0.92490900
C	-1.77219900	1.58800400	1.63472200
C	-3.37465800	-0.08222700	0.71239600
C	-3.08761700	1.33331300	1.01786200
O	-3.89156900	2.24128300	0.80435300
Cl	-2.82663300	-2.73860700	0.59064200
Cl	-4.96144200	-0.40498000	0.09707000
C	0.40641600	0.83374600	2.46126000
C	-1.49975700	2.93053600	2.02726100
N	1.43044600	1.05323700	2.96701000
N	-1.27890500	4.02747800	2.34765600

2_A

E(B3LYP/BS1) = -2335.694636 au

H(B3LYP/BS1) = -2335.228269 au

G(B3LYP/BS1) = -2335.329554 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.568667 au

C	-0.84977900	0.28126700	1.83825200
C	-2.18893600	-0.23959900	1.28886300
C	-0.27480100	1.53015100	1.16519900
C	-2.83217300	0.41191000	0.29769000
H	-2.37727200	1.31967100	-0.08527500
C	0.10990300	1.46413300	-0.12872600
H	-0.04685300	0.52253100	-0.64990900
C	-4.12758900	0.10098800	-0.33227100
C	-4.64491500	-1.19932400	-0.48945800
C	-4.87691100	1.17439100	-0.85571700
C	-5.87329800	-1.40987900	-1.11715200
H	-4.07293300	-2.05474500	-0.14937400
C	-6.10828800	0.96541200	-1.47238800
H	-4.48493300	2.18478100	-0.76587900
C	-6.61474000	-0.33082000	-1.60302200
H	-6.24783800	-2.42350700	-1.23259000
H	-6.66970700	1.81256400	-1.85713200
H	-7.57190100	-0.49858800	-2.08900600
C	0.67114800	2.51493400	-0.99449700
C	1.48893200	3.56280200	-0.52989500
C	0.41103100	2.44127600	-2.37776600
C	1.99789800	4.51525700	-1.41320300
H	1.75966900	3.61478700	0.51851200
C	0.91019600	3.39920600	-3.25716500
H	-0.19841000	1.62544200	-2.75916400

C	1.70427700	4.44444700	-2.77677300
H	2.63362600	5.31056100	-1.03372100
H	0.68591000	3.32671900	-4.31786400
H	2.10092600	5.18924700	-3.46107000
C	-2.76221900	-1.42523000	2.03439800
H	-3.85462600	-1.37636400	2.05794300
H	-2.48154700	-2.37742100	1.57415200
H	-2.39564100	-1.43777300	3.06175300
C	-0.31348700	2.81107900	1.96677100
H	-1.14661800	2.79023700	2.67356300
H	0.60283200	2.97316800	2.54721600
H	-0.43739400	3.67247100	1.30526800
O	-1.08442200	0.43630300	3.19970000
H	4.09699400	-2.81357500	-2.29101900
C	-0.01002200	0.47905300	4.14641200
H	0.58050000	-0.43869800	4.10329200
H	0.64384900	1.34056800	4.00036300
H	-0.49943100	0.55529500	5.11932000
O	4.32531900	-2.10052000	-1.66670600
C	3.28159600	-1.83090100	-0.86555800
C	3.44096000	-0.82665100	0.09920600
C	2.04770900	-2.50287100	-0.93380100
C	2.37731600	-0.49358400	0.97518000
C	0.99510400	-2.16743400	-0.07744400
C	1.12735600	-1.14288000	0.89525100
O	0.12996100	-0.91883500	1.77103300
Cl	1.88986100	-3.76540400	-2.12490800
Cl	-0.49920100	-3.03530700	-0.19051700
C	4.69681400	-0.15257500	0.18493500
C	2.62449500	0.51540600	1.95561200
N	5.71998000	0.39629200	0.25453000
N	2.89820000	1.33504400	2.73447300

1_B

E(B3LYP/BS1) = -2335.674351 au

H(B3LYP/BS1) = -2335.208896 au

G(B3LYP/BS1) = -2335.318809 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.524777 au

C	-0.72095500	-0.91007600	1.95604300
C	0.50605200	-1.69864200	1.46282700
C	-2.01835400	-1.30766500	1.25673200
C	0.72417500	-1.74756400	0.12530800
H	-0.04368000	-1.29541500	-0.50269500
C	-2.65295400	-0.39515800	0.49321500
H	-2.16316800	0.57288100	0.37895700
C	1.79505600	-2.40235100	-0.63841200
C	3.11614900	-2.58095100	-0.17592700
C	1.48884100	-2.85679100	-1.93971000
C	4.06971200	-3.22495300	-0.96472700
H	3.41117800	-2.18637300	0.78906400
C	2.43964800	-3.50385900	-2.72334900
H	0.48319800	-2.70919500	-2.32597300

C	3.73632100	-3.69747100	-2.23543000
H	5.08105800	-3.34700100	-0.58658300
H	2.17206900	-3.85509400	-3.71621700
H	4.48161800	-4.19940100	-2.84608900
C	-3.90980600	-0.51422000	-0.27016200
C	-5.01306600	-1.27941200	0.15335200
C	-4.03553800	0.21401500	-1.46979300
C	-6.17901100	-1.33951400	-0.61151300
H	-4.97407800	-1.80454600	1.10151100
C	-5.19708300	0.14942900	-2.23671000
H	-3.20376100	0.83038400	-1.80325300
C	-6.27462100	-0.63343000	-1.81253300
H	-7.01914200	-1.93298400	-0.26058900
H	-5.26380400	0.71387600	-3.16301200
H	-7.18364100	-0.68187300	-2.40569600
C	1.35786600	-2.37267900	2.50438500
H	1.95610400	-3.17714700	2.07199800
H	2.04436500	-1.66215500	2.98655000
H	0.72999000	-2.78161900	3.29902400
C	-2.47290700	-2.72373500	1.50914600
H	-1.61092700	-3.39889800	1.54742400
H	-2.98880900	-2.81351300	2.47376300
H	-3.15243900	-3.08104300	0.73175000
O	-0.83056300	-1.09206700	3.36669100
H	-0.53996300	0.16091200	1.75858100
C	-1.67366500	-0.14350200	4.00431600
H	-2.70844500	-0.20036500	3.64180000
H	-1.65312200	-0.37620800	5.07166200
H	-1.30482000	0.88166300	3.85219700
O	-0.45928900	3.91416500	0.58484400
C	0.39017700	3.11193400	0.24289100
C	1.31203300	2.50543600	1.25561400
C	0.56337300	2.68236000	-1.17458100
C	2.27633400	1.61618900	0.89141500
C	1.53116200	1.80607000	-1.53872400
C	2.48686700	1.23956800	-0.54270600
O	3.41499300	0.51938600	-0.86196400
Cl	-0.54028300	3.37964800	-2.29664000
Cl	1.76963500	1.29401000	-3.16341800
C	1.12059400	2.91905700	2.60860500
C	3.16826000	1.02568100	1.83615300
N	0.96191200	3.25616000	3.70978500
N	3.88696600	0.53419200	2.60677100

TS_B

E(B3LYP/BS1) = -2335.639038 au

H(B3LYP/BS1) = -2335.178289 au

G(B3LYP/BS1) = -2335.280737 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.49227 au

C	0.09830200	-1.32048200	1.69634500
C	1.42872700	-1.58915500	1.13760100
C	-1.12560000	-1.81877300	0.94700800

C	1.56437900	-1.40702300	-0.22151100
H	0.63989800	-1.20111300	-0.75630200
C	-1.93579900	-1.01686100	0.23316800
H	-1.66256300	0.03040000	0.14878600
C	2.71532200	-1.52064900	-1.10075500
C	4.06842900	-1.55079100	-0.68856400
C	2.44355800	-1.58247600	-2.48918000
C	5.08990700	-1.66731800	-1.62668500
H	4.32861900	-1.44774500	0.35510700
C	3.46679700	-1.71019500	-3.42056300
H	1.41130300	-1.54008200	-2.82614900
C	4.79650400	-1.75688000	-2.99071700
H	6.12278300	-1.68213200	-1.29153100
H	3.23141500	-1.76616400	-4.47916700
H	5.60031900	-1.85174900	-3.71508500
C	-3.15407900	-1.37435100	-0.51988500
C	-4.10720600	-2.29494200	-0.04790100
C	-3.40183500	-0.72735800	-1.74543900
C	-5.25222900	-2.57995400	-0.79280100
H	-3.97116400	-2.76563700	0.92016900
C	-4.54092500	-1.01947600	-2.49290300
H	-2.68665000	0.00187500	-2.11721800
C	-5.46986600	-1.95066900	-2.02022800
H	-5.97941800	-3.28909500	-0.40711100
H	-4.70654400	-0.51619800	-3.44141200
H	-6.36188800	-2.17451300	-2.59849700
C	2.54142500	-1.97179400	2.08040300
H	3.18488300	-2.72409100	1.61578400
H	3.17194300	-1.11436500	2.34543800
H	2.13589700	-2.38357400	3.00493500
C	-1.28316700	-3.32326800	1.07715800
H	-0.30902800	-3.81478800	0.98506500
H	-1.69977500	-3.61665600	2.04839800
H	-1.94110600	-3.71305500	0.29784500
O	0.05662100	-1.48306800	3.05073300
H	0.13241400	0.12559000	1.55762500
C	-1.16935100	-1.18309800	3.74430800
H	-1.97115500	-1.86331800	3.44825700
H	-0.93769700	-1.31589600	4.80060600
H	-1.47245300	-0.14904000	3.55818800
O	-1.61970200	2.30619400	2.22267300
C	-0.80162700	2.14587700	1.33741000
C	0.52301500	1.44191500	1.61479500
C	-1.04830200	2.56497000	-0.06750000
C	1.58858400	1.62100600	0.66690600
C	-0.07955400	2.48286600	-1.01092400
C	1.33478400	2.05089700	-0.69424000
O	2.20628400	2.12249400	-1.55755800
Cl	-2.63663400	3.17540000	-0.38882200
Cl	-0.35554800	2.94075600	-2.64843000
C	0.89004500	1.51231900	3.01932500

C	2.94036900	1.43030900	1.03870600
N	1.19377900	1.55957700	4.13889800
N	4.05447800	1.28669000	1.35720600

2_B

E(B3LYP/BS1) = -2335.682057 au

H(B3LYP/BS1) = -2335.21514 au

G(B3LYP/BS1) = -2335.326858 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.524065 au

C	-3.25323400	-0.01397900	1.86169700
C	-3.03760100	-1.28296300	1.22601200
C	-3.36198300	1.25803200	1.15427100
C	-3.24875700	-1.34930100	-0.13841500
H	-3.70487000	-0.48004000	-0.60147700
C	-2.37380100	1.55460100	0.25242500
H	-1.54945300	0.84722400	0.19377100
C	-3.01854400	-2.44585300	-1.05543800
C	-2.06930700	-3.47346200	-0.84478900
C	-3.76667900	-2.45068400	-2.25688500
C	-1.90815800	-4.47942100	-1.79213800
H	-1.41888800	-3.45142800	0.02204100
C	-3.61698500	-3.47215500	-3.18652400
H	-4.47794000	-1.65001500	-2.44113800
C	-2.68766700	-4.49171900	-2.95373900
H	-1.16462100	-5.25381600	-1.62929000
H	-4.21108300	-3.47070000	-4.09526900
H	-2.55912600	-5.28509900	-3.68443200
C	-2.17757700	2.73212800	-0.58604000
C	-3.16666800	3.69336400	-0.89475500
C	-0.88961800	2.89136400	-1.14925000
C	-2.87030600	4.77119700	-1.72427200
H	-4.17390400	3.59458700	-0.51439700
C	-0.59879600	3.97751200	-1.96913700
H	-0.12054300	2.15867000	-0.91710800
C	-1.58727000	4.92172100	-2.25937300
H	-3.64545300	5.49538200	-1.95760300
H	0.39842900	4.08570800	-2.38594700
H	-1.36276100	5.76741100	-2.90333000
C	-2.69388300	-2.47402000	2.09089600
H	-3.05670900	-3.39856400	1.63659600
H	-1.60991200	-2.56586100	2.22418800
H	-3.14906800	-2.37176400	3.07749400
C	-4.55019700	2.13812600	1.49122000
H	-5.11688500	1.74794000	2.33807300
H	-4.25464200	3.16780500	1.71629300
H	-5.24440600	2.16220300	0.64334300
O	-3.36997600	-0.07296500	3.17385400
H	4.16847800	-1.87308000	1.91178800
C	-3.19961100	1.08072400	4.03261100
H	-4.17849200	1.46244500	4.32510400
H	-2.66934700	0.70625100	4.90800100
H	-2.61551600	1.85146500	3.52788400

O	6.21385300	-1.11313800	0.34402300
C	5.05669800	-0.73514100	0.39638600
C	3.94438600	-1.70930300	0.84325900
C	4.64843400	0.64556900	0.09008400
C	2.51414800	-1.23117600	0.67810500
C	3.34118300	1.00817200	0.03109700
C	2.16973400	0.07769300	0.29584600
O	1.00744500	0.52644900	0.17549300
Cl	5.95839300	1.74583900	-0.24817000
Cl	2.89895900	2.63263100	-0.37129600
C	4.17088000	-3.00115400	0.17218800
C	1.48625800	-2.12655800	1.01617100
N	4.31511100	-4.02466000	-0.35581500
N	0.65641700	-2.90153800	1.30728500

1_D

E(B3LYP/BS1) = -2335.675341 au

H(B3LYP/BS1) = -2335.209622 au

G(B3LYP/BS1) = -2335.324388 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.52029 au

C	2.94211500	0.13742200	1.81915900
C	3.40574900	1.30381100	0.93846800
C	3.04195800	-1.24750600	1.19296400
C	3.53940800	1.13806200	-0.39213700
H	3.41046700	0.12908200	-0.78036200
C	1.90520700	-1.88272800	0.84068000
H	0.97662900	-1.32683100	0.97797600
C	3.86533000	2.13495500	-1.43163400
C	3.38995900	3.45996800	-1.42248900
C	4.65078600	1.72764300	-2.52817200
C	3.71781100	4.34784000	-2.44849300
H	2.73406300	3.79067200	-0.62400600
C	4.98334100	2.61465800	-3.55038000
H	5.00922400	0.70158400	-2.56805800
C	4.52157600	3.93344200	-3.51272000
H	3.33406500	5.36438900	-2.41976400
H	5.59927400	2.27566100	-4.37925500
H	4.77525300	4.62623200	-4.31042700
C	1.70582600	-3.21018900	0.23222500
C	2.57096200	-4.30686900	0.41565700
C	0.55174300	-3.40932900	-0.55293200
C	2.30741900	-5.53628800	-0.19029600
H	3.43753300	-4.21293100	1.05995900
C	0.29185900	-4.63495500	-1.16220500
H	-0.14503200	-2.58557700	-0.68384400
C	1.17366800	-5.70546200	-0.98825000
H	2.98816100	-6.36816700	-0.02888900
H	-0.60332600	-4.75289500	-1.76704500
H	0.97258300	-6.66425800	-1.45842300
C	3.61572700	2.60380300	1.67485400
H	4.15406400	3.33537400	1.06910900
H	2.65640200	3.05203400	1.97223800

H	4.17648100	2.42419000	2.59553700
C	4.44466800	-1.78776800	1.04428100
H	5.15556400	-0.96812600	0.90514500
H	4.76359700	-2.33512700	1.94113700
H	4.53101800	-2.46995100	0.19377700
O	3.70384500	0.18217500	3.03533700
H	1.88476800	0.33343000	2.07303100
C	3.10509600	-0.52707600	4.10832700
H	3.75547400	-0.39327800	4.97658400
H	2.10600500	-0.12903600	4.34252500
H	3.00880600	-1.60038200	3.89416200
O	-1.59678300	-0.47052900	0.10091800
C	-2.73428600	-0.04571600	0.04370200
C	-3.75634500	-0.73546000	-0.81475800
C	-3.17901600	1.15774500	0.80566400
C	-5.03245700	-0.28156900	-0.88952000
C	-4.45345100	1.61134200	0.73063900
C	-5.47531100	0.92898900	-0.11746100
O	-6.62361600	1.31692900	-0.19767900
Cl	-1.97034200	1.90947200	1.76890100
Cl	-5.01082300	2.99143900	1.58896600
C	-3.30683700	-1.88353900	-1.53468200
C	-6.02835200	-0.91387800	-1.69364200
N	-2.93930500	-2.81780700	-2.12001000
N	-6.83980300	-1.42765600	-2.34778200

2_D

E(B3LYP/BS1) = -2335.656198 au

H(B3LYP/BS1) = -2335.191604 au

G(B3LYP/BS1) = -2335.304158 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.488257 au

C	2.20945900	-0.66349900	2.04252400
C	2.42163700	0.73698500	1.48051800
C	2.56454900	-1.73394800	1.02150300
C	3.38379200	0.93901400	0.52761000
H	4.03066600	0.09447900	0.29969000
C	1.60550400	-1.95557400	0.04625800
H	0.70869800	-1.34266100	0.13580000
C	3.72779500	2.15180900	-0.19344500
C	2.80387900	3.18270400	-0.48993700
C	5.05479500	2.28114400	-0.67239000
C	3.20784900	4.30530300	-1.20336100
H	1.76248000	3.08558000	-0.20620600
C	5.45616800	3.41222900	-1.37074400
H	5.76756400	1.48561100	-0.47240300
C	4.53364200	4.43181800	-1.63562200
H	2.48429600	5.08140500	-1.43399700
H	6.48163900	3.50095200	-1.71656600
H	4.84254800	5.31381200	-2.18905500
C	1.58695800	-2.83789300	-1.08923600
C	2.53215400	-3.86299100	-1.36608300
C	0.50685400	-2.66035700	-2.00039800

C	2.40415100	-4.64798100	-2.50168800
H	3.34743500	-4.05992500	-0.68415700
C	0.39214100	-3.44255300	-3.13852200
H	-0.22588300	-1.88709300	-1.79008800
C	1.34239700	-4.43958900	-3.39467100
H	3.12904700	-5.43191600	-2.69743200
H	-0.43324000	-3.28573600	-3.82570800
H	1.25374100	-5.05859200	-4.28246400
C	1.52937400	1.78249900	2.07780000
H	1.95761800	2.78450200	2.01056000
H	0.55452900	1.78540100	1.57260900
H	1.35056800	1.54601200	3.13269400
C	3.89440500	-2.40896600	1.14728400
H	4.50496500	-1.90591100	1.89939900
H	3.77038700	-3.45127900	1.47362000
H	4.43393700	-2.43295500	0.19479400
O	2.90415100	-0.76811600	3.27073800
H	1.12463300	-0.74379100	2.22832300
C	2.37402000	-1.75732300	4.15480200
H	2.96611800	-1.70205400	5.07028100
H	1.32084500	-1.55246100	4.38811800
H	2.45653100	-2.76831700	3.73475900
O	-0.89819700	0.16555300	0.25754600
C	-2.12379400	0.39402700	0.15155700
C	-2.63508200	1.70472200	-0.20605400
C	-3.14395700	-0.64066800	0.37993100
C	-4.00375500	1.96310500	-0.33503000
C	-4.48110400	-0.39140900	0.25627900
C	-5.01010000	0.93471600	-0.11618400
O	-6.22825500	1.15717800	-0.23276400
Cl	-2.53762300	-2.21127300	0.82530000
Cl	-5.67740600	-1.62282500	0.53004700
C	-1.66573800	2.72557200	-0.42115600
C	-4.47906600	3.25715800	-0.69090900
N	-0.86624100	3.55656000	-0.59064100
N	-4.86073000	4.31877500	-0.98242200

MECP

E(B3LYP/BS1) = -

H(B3LYP/BS1) = -

G(B3LYP/BS1) = -

E(M06-2X/BS2//B3LYP/BS1) = -3590.594393 au

6	2.2101472	-0.6637476	2.0433706
6	2.4202736	0.7363769	1.4800614
6	2.5658628	-1.7324828	1.0215936
6	3.3837801	0.9385859	0.5261198
1	4.0320433	0.0946776	0.3003323
6	1.6046552	-1.9545514	0.0441896
1	0.7079115	-1.3415923	0.1348436
6	3.7274681	2.1511694	-0.1937162
6	2.8033662	3.1826581	-0.4898855
6	5.0550182	2.2807431	-0.6724961

6	3.2075425	4.3050882	-1.2031364
1	1.7619577	3.0858112	-0.2065708
6	5.4563676	3.4119043	-1.3704506
1	5.7679000	1.4854010	-0.4725326
6	4.5334900	4.4313841	-1.6353389
1	2.4841683	5.0812658	-1.4339146
1	6.4817158	3.5008995	-1.7164391
1	4.8423685	5.3133806	-2.1887984
6	1.5870133	-2.8373973	-1.0889669
6	2.5329658	-3.8629318	-1.3658872
6	0.5058825	-2.6600385	-2.0001882
6	2.4046024	-4.6478650	-2.5010808
1	3.3479060	-4.0597497	-0.6836733
6	0.3915443	-3.4420444	-3.1382205
1	-0.2265369	-1.8866051	-1.7900391
6	1.3422823	-4.4389380	-3.3939012
1	3.1291322	-5.4319523	-2.6972263
1	-0.4334316	-3.2855790	-3.8257876
1	1.2538053	-5.0580435	-4.2817364
6	1.5287828	1.7821726	2.0774962
1	1.9578306	2.7838212	2.0104813
1	0.5541534	1.7851530	1.5722463
1	1.3504035	1.5457032	3.1325517
6	3.8945438	-2.4083867	1.1472600
1	4.5051598	-1.9056749	1.8996756
1	3.7692945	-3.4506559	1.4736067
1	4.4335980	-2.4332150	0.1946465
8	2.9044294	-0.7684315	3.2705652
1	1.1251151	-0.7444876	2.2277312
6	2.3739597	-1.7575770	4.1552181
1	2.9663393	-1.7019150	5.0703491
1	1.3208841	-1.5522465	4.3882153
1	2.4566315	-2.7684464	3.7350889
8	-0.8948268	0.1636015	0.2580688
6	-2.1223886	0.3945435	0.1514325
6	-2.6337832	1.7025770	-0.2053228
6	-3.1429585	-0.6382914	0.3791446
6	-4.0052728	1.9615767	-0.3346126
6	-4.4809120	-0.3888541	0.2556412
6	-5.0108264	0.9358449	-0.1164506
8	-6.2310747	1.1571120	-0.2328708
17	-2.5374185	-2.2108735	0.8246739
17	-5.6770880	-1.6223970	0.5300004
6	-1.6656760	2.7242840	-0.4208879
6	-4.4794103	3.2560108	-0.6906274
7	-0.8668669	3.5561544	-0.5905752
7	-4.8600770	4.3180396	-0.9822591

3_D

E(B3LYP/BS1) = -850.3554464 au

H(B3LYP/BS1) = -849.967738 au

G(B3LYP/BS1) = -850.041271 au

E(M06-2X/BS2//B3LYP/BS1) = -850.1994928 au

C	-0.02226600	2.10766500	-0.35392500
C	1.24998900	1.30820700	-0.61318600
C	-1.09620700	1.25191300	0.30474000
C	1.58403900	0.29022200	0.23964400
H	0.95380400	0.16686400	1.11734600
C	-1.77771900	0.39678300	-0.54414900
H	-1.46553900	0.44408000	-1.58681700
C	2.70721500	-0.62769000	0.20071400
C	3.38743100	-1.00706100	-0.98188400
C	3.11336900	-1.21619900	1.42465300
C	4.44350600	-1.90831200	-0.93004800
H	3.06275300	-0.62723300	-1.94272800
C	4.17876400	-2.10479300	1.47316000
H	2.58617200	-0.95157300	2.33716000
C	4.85079900	-2.45204700	0.29495400
H	4.94857900	-2.19770000	-1.84654500
H	4.48431800	-2.53436500	2.42224100
H	5.67964700	-3.15288600	0.32850200
C	-2.81952300	-0.56465500	-0.30555600
C	-3.51401200	-0.74718900	0.92234900
C	-3.18739000	-1.38807100	-1.40822000
C	-4.50480900	-1.71003500	1.03304700
H	-3.29401200	-0.12476900	1.77769300
C	-4.17301700	-2.35349700	-1.28725000
H	-2.67326700	-1.25463800	-2.35555400
C	-4.83570500	-2.51994500	-0.06371400
H	-5.03023300	-1.83387700	1.97462400
H	-4.43276200	-2.97562600	-2.13767000
H	-5.61205400	-3.27258600	0.03487600
C	2.04915400	1.78199800	-1.79226500
H	3.11467100	1.56939400	-1.68282200
H	1.70584200	1.31448800	-2.72580800
H	1.92043500	2.86344500	-1.90862200
C	-1.29656600	1.39470300	1.78096600
H	-0.51769000	2.02831400	2.20861900
H	-2.26241900	1.87270900	1.99626500
H	-1.29721100	0.42514900	2.29008300
O	0.32339400	3.27374800	0.36524400
H	-0.40652900	2.39655500	-1.34767000
C	-0.59951300	4.35446900	0.20628800
H	-0.19140200	5.19266700	0.77375700
H	-0.69220700	4.63875400	-0.85004800
H	-1.59328000	4.10405600	0.59924500

3_D_1

E(B3LYP/BS1) = -1485.284423 au

H(B3LYP/BS1) = -1485.209595 au

G(B3LYP/BS1) = -1485.262837 au

E(M06-2X/BS2//B3LYP/BS1) = -1485.270249 au

O	0.13018200	2.72289000	-0.00048800
C	0.13488000	1.47800800	0.00031800

C	1.36384500	0.70009000	0.00013400
C	-1.10810700	0.68239800	0.00037000
C	1.36375200	-0.69996400	0.00010100
C	-1.10811400	-0.68231000	0.00023300
C	0.13474000	-1.47762900	0.00020800
O	0.12986600	-2.72262000	-0.00022600
Cl	-2.58552700	1.60501000	-0.00015600
Cl	-2.58552300	-1.60501200	0.00006500
C	2.58222700	1.43646100	-0.00013200
C	2.58195600	-1.43675000	-0.00014100
N	3.58283200	2.03421100	0.00040200
N	3.58236600	-2.03477200	-0.00029800

TS_D

E(B3LYP/BS1) = -2335.634589 au

H(B3LYP/BS1) = -2335.176494 au

G(B3LYP/BS1) = -2335.283183 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.477062 au

C	-1.32106500	0.98452200	1.94911800
C	-2.38661800	0.09213500	1.46282800
C	-0.91253200	2.20746100	1.19106400
C	-2.94523300	0.29060300	0.21460100
H	-2.71734600	1.23596000	-0.26990600
C	-0.35515200	2.04761500	-0.04254300
H	-0.23098800	1.01959100	-0.37945900
C	-3.86121500	-0.55029100	-0.53518300
C	-3.93872300	-1.95816800	-0.41498400
C	-4.69302300	0.08006800	-1.49234600
C	-4.83151600	-2.68788500	-1.19399800
H	-3.26845000	-2.48540500	0.25356900
C	-5.59360800	-0.65149200	-2.25732000
H	-4.62957300	1.15808000	-1.61594600
C	-5.66987700	-2.04066000	-2.10808600
H	-4.86751100	-3.76902000	-1.09560800
H	-6.23117000	-0.14392200	-2.97539500
H	-6.36701200	-2.61634700	-2.71012000
C	0.07745700	3.02614200	-1.04030300
C	0.36141800	4.38475800	-0.78066900
C	0.24865700	2.56082900	-2.36388100
C	0.77368600	5.23490300	-1.80502800
H	0.29355900	4.77770200	0.22497400
C	0.65013100	3.41424600	-3.38655300
H	0.05227900	1.51450200	-2.58390000
C	0.91217000	4.75963200	-3.11158900
H	0.99409100	6.27436900	-1.57860900
H	0.76443400	3.03015000	-4.39624400
H	1.23122300	5.42850100	-3.90581800
C	-2.80551600	-1.02529400	2.38808400
H	-3.81798000	-1.36368100	2.16086800
H	-2.13008800	-1.88456700	2.30203000
H	-2.77069300	-0.68444900	3.42399000
C	-1.20572100	3.53801800	1.84657400

H	-1.90683200	3.40880200	2.67387600
H	-0.30643500	4.01991100	2.24963500
H	-1.64500600	4.22945700	1.11996000
O	-1.35464000	1.11815700	3.33580000
H	-0.30611400	0.06852100	1.74060000
C	-0.12426000	1.39431900	4.01611300
H	-0.39405900	1.55728500	5.06075200
H	0.55430400	0.53953500	3.93733400
H	0.37040700	2.28860000	3.62562900
O	0.39683700	-0.99542200	1.77780400
C	1.34249000	-1.32545100	0.96024400
C	1.25503400	-2.59489900	0.29419200
C	2.51675000	-0.51971800	0.71303100
C	2.24334400	-3.02815900	-0.58815600
C	3.49911300	-0.93461000	-0.15455400
C	3.42213900	-2.21600600	-0.87358600
O	4.30129500	-2.59125500	-1.66605900
Cl	2.65882400	0.96781300	1.59600600
Cl	4.91334700	0.01135800	-0.45251900
C	0.09732900	-3.39032300	0.55442900
C	2.14169400	-4.27824800	-1.26205700
N	-0.84614200	-4.03966500	0.76016000
N	2.05614200	-5.30113400	-1.81137200

4_D

E(B3LYP/BS1) = -2335.662503au

H(B3LYP/BS1) = -2335.199484 au

G(B3LYP/BS1) = -2335.306852 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.508779 au

C	-2.00449300	-0.03616700	2.12216900
C	-2.84220700	-0.93112700	1.37604600
C	-1.59538300	1.30369200	1.76115400
C	-3.72028100	-0.44502900	0.41923800
H	-3.83494800	0.63522200	0.37924300
C	-1.48039700	1.66930500	0.42982700
H	-1.68740300	0.87771700	-0.28633100
C	-4.57926300	-1.15529000	-0.51619400
C	-4.34496100	-2.46559900	-0.99605300
C	-5.70694800	-0.46888000	-1.02866900
C	-5.21218600	-3.06116800	-1.90954100
H	-3.46178600	-3.00819000	-0.68034200
C	-6.57472400	-1.06893000	-1.93499200
H	-5.89848600	0.54771000	-0.69323700
C	-6.33569100	-2.37405400	-2.37858900
H	-5.00294000	-4.06655500	-2.26553500
H	-7.43716100	-0.51787600	-2.30066400
H	-7.00918300	-2.84422900	-3.08961400
C	-1.17406300	2.93984500	-0.22018900
C	-0.78145900	4.14329700	0.41449100
C	-1.27178500	2.96369300	-1.63463100
C	-0.51567600	5.29331600	-0.32733000
H	-0.67134600	4.19043200	1.48845900

C	-1.00941200	4.11363000	-2.37036800
H	-1.56682500	2.05469900	-2.15337100
C	-0.62909800	5.29169500	-1.71978100
H	-0.21514600	6.19986200	0.19140400
H	-1.10079400	4.09183800	-3.45300900
H	-0.42100200	6.19283800	-2.28953800
C	-2.79473500	-2.39870500	1.75865500
H	-3.74017400	-2.90054800	1.54145000
H	-1.99973600	-2.92953000	1.21753300
H	-2.58248300	-2.50114000	2.82419800
C	-1.30914300	2.25747700	2.90627100
H	-1.52812600	1.78593100	3.86483500
H	-0.26658800	2.59580300	2.92224700
H	-1.94036100	3.14915200	2.81953100
O	-1.61957900	-0.49478600	3.36794200
H	0.55440200	0.39886300	0.36322800
C	-0.21686700	-0.69855200	3.58385700
H	-0.11397400	-1.02190500	4.62169300
H	0.16586200	-1.47796400	2.91581900
H	0.35841300	0.22164400	3.43406900
O	0.80946500	-0.54365400	0.24373700
C	2.09260300	-0.71569400	-0.03447100
C	2.52497100	-2.05993300	-0.20390600
C	3.02484700	0.35631200	-0.16340200
C	3.85626400	-2.33668000	-0.50484300
C	4.34624800	0.10297500	-0.46000500
C	4.84571900	-1.26787500	-0.65166300
O	6.03121300	-1.51078200	-0.91977400
Cl	2.41939800	1.96715300	0.06535100
Cl	5.49609500	1.36822000	-0.62497500
C	1.56056600	-3.10454100	-0.05318900
C	4.31467000	-3.67242700	-0.68237400
N	0.77693700	-3.95396500	0.07298800
N	4.68948000	-4.76444300	-0.82767600

Fig. 2 (a)

5

E(B3LYP/BS1) = -849.7965245 au

H(B3LYP/BS1) = -849.41832 au

G(B3LYP/BS1) = -849.488803 au

E(M06-2X/BS2//B3LYP/BS1) = -849.6468837 au

C	-0.06159300	2.10163300	0.02370800
C	1.25843800	1.56275300	-0.16872400
C	-1.23975700	1.31933400	0.38506000
C	1.51748500	0.31428400	0.36234600
H	0.74783100	-0.10436000	1.00322400
C	-1.45163900	0.16448200	-0.32127000
H	-0.71423800	-0.05871200	-1.08718400
C	2.69502800	-0.52073200	0.25406500
C	3.65848000	-0.42385900	-0.77769500
C	2.85495500	-1.53493600	1.22881800

C	4.74490800	-1.29064100	-0.80960300
H	3.53763900	0.29887700	-1.57451700
C	3.95355500	-2.38501100	1.20374600
H	2.10972000	-1.63694500	2.01295500
C	4.90292300	-2.26320700	0.18393900
H	5.46957400	-1.21349900	-1.61431000
H	4.06703400	-3.14754900	1.96800200
H	5.75752600	-2.93276200	0.15528800
C	-2.52250200	-0.82105900	-0.26680100
C	-3.71527400	-0.70595300	0.48251000
C	-2.33968400	-1.98574100	-1.04850400
C	-4.66729900	-1.72082300	0.45583900
H	-3.91776900	0.17828300	1.07020100
C	-3.28811200	-3.00192200	-1.06348100
H	-1.43493800	-2.08720900	-1.64179200
C	-4.45725800	-2.87236200	-0.30873400
H	-5.58019600	-1.61158300	1.03362200
H	-3.12045000	-3.88968100	-1.66572700
H	-5.20420400	-3.66071000	-0.32103800
C	2.29391900	2.43299800	-0.84552900
H	3.29707600	2.20260200	-0.48227100
H	2.28235500	2.29441700	-1.93375900
H	2.09242400	3.48729800	-0.65091200
C	-2.10903600	1.84649100	1.51054000
H	-1.60567700	2.64783600	2.05628200
H	-3.07740500	2.22625100	1.16699000
H	-2.30032500	1.04204700	2.22764600
O	-0.14372200	3.40563100	-0.13781100
C	-1.39679900	4.09816300	-0.36783700
H	-1.13229800	4.95349800	-0.98817900
H	-2.09931000	3.44585000	-0.88887300
H	-1.80901800	4.43765000	0.58249400

TS $_{5\text{-}6}$

E(B3LYP/BS1) = -849.7756265 au

H(B3LYP/BS1) = -849.400241 au

G(B3LYP/BS1) = -849.469144 au

E(M06-2X/BS2//B3LYP/BS1) = -849.6318092 au

C	-2.43634300	-0.58256500	-0.15853000
C	-1.41867400	-1.53215900	-0.38242700
C	-1.96227300	0.72306400	0.09434200
C	-0.12937800	-0.95302800	-0.61794400
H	-0.08082500	-0.26201800	-1.45459800
C	-0.57948400	0.74255700	0.48316300
H	-0.34175200	0.13437800	1.35118400
C	1.14818100	-1.60712600	-0.32151300
C	1.30876200	-2.48027500	0.77290600
C	2.26362300	-1.32017600	-1.13154700
C	2.54354000	-3.06824800	1.02929600
H	0.46989900	-2.68636800	1.43136800
C	3.49739400	-1.91305900	-0.87491700

H	2.15445700	-0.63695500	-1.96957400
C	3.63868800	-2.78930000	0.20419400
H	2.65627300	-3.73872700	1.87587700
H	4.34747400	-1.69010500	-1.51250600
H	4.60158100	-3.24838400	0.40835400
C	0.34055100	1.87246500	0.29468300
C	0.32672900	2.67248200	-0.86512000
C	1.30704900	2.12997200	1.28464200
C	1.23505800	3.71677200	-1.01200100
H	-0.38305600	2.46518400	-1.66127300
C	2.21045400	3.18060200	1.13875800
H	1.33946300	1.50786700	2.17509700
C	2.17450700	3.97688700	-0.00831000
H	1.21686600	4.32428800	-1.91175900
H	2.94386200	3.37414600	1.91565300
H	2.88240900	4.79201500	-0.12653900
C	-1.71522300	-2.99908700	-0.36042600
H	-0.84969600	-3.59864300	-0.64218900
H	-2.07328800	-3.31938400	0.62586200
H	-2.53288800	-3.19859200	-1.06368500
C	-2.79963500	1.95558500	-0.08843500
H	-3.39049600	1.90961800	-1.00886500
H	-3.50231100	2.05664800	0.74815300
H	-2.18496900	2.85507900	-0.09893800
O	-3.71091800	-0.99020800	-0.25353700
C	-4.72421800	-0.42481300	0.60393600
H	-5.49994600	-1.18737500	0.67696000
H	-4.31630200	-0.21629000	1.59667600
H	-5.14526400	0.48198900	0.16454000

6

E(B3LYP/BS1) = -849.7961841 au

H(B3LYP/BS1) = -849.419816 au

G(B3LYP/BS1) = -849.4909 au

E(M06-2X/BS2//B3LYP/BS1) = -849.6576538 au

C	0.53860400	2.29007200	0.23509600
C	1.24497600	1.24004500	0.82881100
C	-0.57817200	1.79804200	-0.44774100
C	0.55773600	-0.06616500	0.57803200
H	0.07350000	-0.33473300	1.52888200
C	-0.58392300	0.29880900	-0.43373800
H	-0.24437500	-0.00622000	-1.43516200
C	1.47055800	-1.21638600	0.18364100
C	2.29690600	-1.12253900	-0.94663200
C	1.48807700	-2.39068900	0.94503700
C	3.12429400	-2.18619900	-1.30566400
H	2.29708200	-0.21866300	-1.55223900
C	2.31494100	-3.45657200	0.58373400
H	0.85126400	-2.47446000	1.82191400
C	3.13515200	-3.35613100	-0.54090800
H	3.75929400	-2.10133900	-2.18277800

H	2.31653000	-4.36273800	1.18253100
H	3.77908400	-4.18432500	-0.82224400
C	-1.92980300	-0.35959400	-0.18000000
C	-2.66566300	-0.06508200	0.97799800
C	-2.44244200	-1.28523800	-1.09613500
C	-3.89176300	-0.68734800	1.21203100
H	-2.28381500	0.65186800	1.70189300
C	-3.66839400	-1.91096900	-0.85962600
H	-1.88047600	-1.52119700	-1.99622400
C	-4.39544300	-1.61280300	0.29383400
H	-4.45224400	-0.45011300	2.11166900
H	-4.05271000	-2.62960400	-1.57768500
H	-5.34939500	-2.09837200	0.47809600
C	2.47939900	1.39467300	1.62161800
H	3.32574500	0.99218800	1.04603200
H	2.67702400	2.44191500	1.85557000
H	2.42823200	0.79763600	2.53973300
C	-1.59926600	2.63129600	-1.11103400
H	-1.52139000	3.67958100	-0.81708000
H	-1.46422400	2.55892800	-2.20133200
H	-2.60352800	2.24817100	-0.90293200
O	0.84634200	3.59869500	0.39940300
C	1.52184500	4.23129100	-0.71266900
H	1.67352300	5.26776100	-0.41243300
H	2.48692100	3.74975400	-0.89799200
H	0.90751400	4.19332600	-1.61756000

DDQH$^-$

E(B3LYP/BS1) = -1485.89077 au

H(B3LYP/BS1) = -1485.80373 au

G(B3LYP/BS1) = -1485.856894 au

E(M06-2X/BS2//B3LYP/BS1) = -1485.887946 au

H	0.74392200	3.09753700	0.00014200
O	-0.16609200	2.75330800	0.00026800
C	-0.12729400	1.39052600	0.00058800
C	-1.33138000	0.68710700	0.00043700
C	1.07542400	0.64543600	0.00069600
C	-1.35296700	-0.73709800	0.00034100
C	1.07549100	-0.73887600	0.00059100
C	-0.14887900	-1.53968300	0.00041100
O	-0.14507400	-2.79197100	0.00024200
Cl	2.57584800	1.56776500	-0.00013200
Cl	2.57443600	-1.63332200	-0.00063100
C	-2.55181300	1.42797700	-0.00034200
C	-2.58895300	-1.43293900	0.00007000
N	-3.55271600	2.02380100	-0.00102700
N	-3.60545700	-2.00786800	-0.00011800

7

E(B3LYP/BS1) = -2335.71063 au

H(B3LYP/BS1) = -2335.244529 au

G(B3LYP/BS1) = -2335.348995 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.573339 au

H	6.45253400	1.01897500	-0.32278000
O	6.08751500	0.15043300	-0.07661800
C	4.73873900	0.17026700	-0.20670500
C	4.02749200	-0.99459200	0.09222500
C	4.01258600	1.30528300	-0.63388800
C	2.61108400	-1.03103800	-0.01890500
C	2.62937600	1.28214900	-0.74451700
C	1.83910600	0.10743100	-0.43217600
O	0.57138800	0.08898200	-0.53345000
Cl	4.94155000	2.74167600	-1.01994000
Cl	1.76217400	2.68365000	-1.30830100
C	4.75186500	-2.15094200	0.51239400
C	1.90945700	-2.23403800	0.26621200
N	5.33283800	-3.09917000	0.85681200
N	1.34257200	-3.22927800	0.48807200
C	-0.96760800	-0.74899500	1.82899100
C	-1.90573800	-1.61279200	1.28418900
C	-1.08160200	0.53052800	1.24060400
C	-2.79901600	-0.87428300	0.31442100
H	-3.78817500	-0.79649600	0.78774700
C	-2.18097500	0.55798100	0.22823600
H	-1.68150000	0.66953800	-0.74088100
C	-2.99180800	-1.58507800	-1.01936500
C	-1.89685700	-1.85022900	-1.85677100
C	-4.27033800	-1.98744800	-1.42370800
C	-2.08549000	-2.50392300	-3.07455200
H	-0.90188800	-1.53173000	-1.55439700
C	-4.45829900	-2.64122500	-2.64437900
H	-5.12574700	-1.78573900	-0.78317300
C	-3.36551700	-2.90212900	-3.47209200
H	-1.23063000	-2.70315500	-3.71529800
H	-5.45744400	-2.94446500	-2.94511800
H	-3.50874000	-3.41094800	-4.42140900
C	-3.16150200	1.71075100	0.39484900
C	-3.90420500	1.86285800	1.57572000
C	-3.34026200	2.63700000	-0.63947700
C	-4.80621800	2.91730600	1.71628100
H	-3.77896800	1.15401500	2.39147100
C	-4.24480800	3.69274600	-0.50116600
H	-2.77162100	2.53001300	-1.55971700
C	-4.97914700	3.83594700	0.67696800
H	-5.37353900	3.02157900	2.63698600
H	-4.37350400	4.40113500	-1.31480100
H	-5.68243200	4.65673700	0.78615800
C	-2.08422300	-3.07503200	1.51819000
H	-2.97516100	-3.44305200	1.00535300
H	-1.21222600	-3.61776600	1.12869600
H	-2.16691000	-3.31798000	2.58120600
C	-0.36380200	1.72551200	1.73416800
H	0.65194500	1.47177600	2.04515600
H	-0.35007100	2.52426800	0.99185800

H	-0.89041800	2.09715600	2.62692000
O	0.00533900	-0.91354300	2.74924600
C	0.03093200	-2.06431800	3.60511400
H	0.84680400	-1.87928100	4.30472700
H	-0.90693000	-2.15778200	4.16125700
H	0.24018700	-2.97335200	3.03735500

8

E(B3LYP/BS1) = -2335.707918 au
H(B3LYP/BS1) = -2335.242777 au
G(B3LYP/BS1) = -2335.352179 au
E(M06-2X/BS2//B3LYP/BS1) = -2335.568306 au

H	6.56461800	1.09674600	0.17084800
O	6.29530500	0.16235300	0.12982800
C	4.93840800	0.08260300	0.15561500
C	4.34451800	-1.17915500	0.10232900
C	4.09141400	1.21127900	0.23574200
C	2.92931600	-1.32284000	0.12643200
C	2.70973100	1.08610900	0.25797700
C	2.03474000	-0.19871600	0.20407500
O	0.77475000	-0.32197000	0.22401100
Cl	4.87182500	2.78338600	0.30661800
Cl	1.69160000	2.49904700	0.35898800
C	5.18587400	-2.32982700	0.02360400
C	2.33837400	-2.61337500	0.07734400
N	5.86303600	-3.27498800	-0.04031500
N	1.84573700	-3.67061600	0.04077900
C	-2.25615500	-2.37980100	-0.14919700
C	-1.93837800	-1.51812000	0.90950900
C	-2.79513300	-1.66073800	-1.21194400
C	-2.23336600	-0.10326700	0.54008200
H	-1.22984900	0.31771400	0.35399200
C	-2.97771100	-0.21891400	-0.83221900
H	-4.05407000	-0.09721400	-0.63834800
C	-2.91738500	0.73293600	1.60783900
C	-4.16008200	0.35032400	2.13538000
C	-2.31524400	1.90850300	2.07198100
C	-4.78813400	1.13104200	3.10578700
H	-4.64104200	-0.56190600	1.78825100
C	-2.94491500	2.69191900	3.04186100
H	-1.35036800	2.21068000	1.67311900
C	-4.18186300	2.30531600	3.56064000
H	-5.74987900	0.82246000	3.50592000
H	-2.46689100	3.60286700	3.39095800
H	-4.67174200	2.91419300	4.31526400
C	-2.58513000	0.78523300	-1.90498500
C	-1.24777700	0.91205300	-2.31159400
C	-3.56262600	1.58276700	-2.51182000
C	-0.90214100	1.82359400	-3.30985100
H	-0.47533300	0.31505600	-1.83194500
C	-3.21394300	2.49614800	-3.50935100
H	-4.60094100	1.49295300	-2.20176200

C	-1.88296100	2.61675700	-3.91188900
H	0.13643000	1.91637100	-3.61505300
H	-3.98246300	3.11175300	-3.96836600
H	-1.60966600	3.32684200	-4.68738500
C	-1.29265000	-1.92490600	2.16789300
H	-1.75436000	-1.43192300	3.02930700
H	-1.27868900	-3.00803100	2.29648000
H	-0.25675900	-1.55630900	2.10293600
C	-3.14209900	-2.22362400	-2.53359900
H	-2.81073000	-3.25838900	-2.63412600
H	-4.23069100	-2.17512500	-2.68051700
H	-2.70065000	-1.61127600	-3.32826900
O	-1.97124900	-3.70701300	-0.15723400
C	-3.08662900	-4.58222600	0.11577000
H	-2.69114500	-5.59568600	0.04785500
H	-3.48047100	-4.40208000	1.12143200
H	-3.88371400	-4.44521500	-0.62242900

Fig. 2 (b)

TS $_{7\text{-}9}$

E(B3LYP/BS1) = -2335.701661 au

H(B3LYP/BS1) = -2335.241159 au

G(B3LYP/BS1) = -2335.348813 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.56179 au

H	6.45837000	1.38445700	0.99819200
O	6.31954700	0.47135200	0.68903000
C	5.04354000	0.31953700	0.26777200
C	4.65446900	-0.93226000	-0.21919100
C	4.08561900	1.35616200	0.29135700
C	3.32908600	-1.14745200	-0.68257800
C	2.78229300	1.14668300	-0.14758700
C	2.34607100	-0.11900800	-0.66134000
O	1.13326200	-0.29145800	-1.08847400
Cl	4.60483800	2.90969200	0.90635300
Cl	1.60915400	2.42906000	-0.09662800
C	5.61412300	-1.98859600	-0.24874700
C	2.95263200	-2.41880300	-1.20345400
N	6.38960800	-2.85609700	-0.27569100
N	2.64050400	-3.45641300	-1.63204300
C	-2.43242000	-1.75964000	-1.35666600
C	-1.62074900	-1.51330600	-0.20663000
C	-3.45089300	-0.84920800	-1.45421400
C	-2.18614900	-0.33583500	0.55269100
H	-1.42076600	0.44907000	0.53357300
C	-3.41988100	0.12709100	-0.30142100
H	-4.33906500	-0.00546400	0.28314000
C	-2.49697100	-0.64655600	2.01077000
C	-3.39621100	-1.66786200	2.35325000
C	-1.88902600	0.09043500	3.03384500
C	-3.68248700	-1.94142800	3.69059300
H	-3.87469700	-2.25473500	1.57244600

C	-2.17583400	-0.18218600	4.37391200
H	-1.19049500	0.88440400	2.78200300
C	-3.07277000	-1.19852600	4.70565800
H	-4.38008100	-2.73622400	3.93991600
H	-1.69742400	0.40130000	5.15565100
H	-3.29603200	-1.41197400	5.74722000
C	-3.36241500	1.58429500	-0.74825300
C	-2.27887700	2.06136800	-1.50247700
C	-4.39570900	2.46770000	-0.41558400
C	-2.23198800	3.39497200	-1.90908800
H	-1.46261200	1.39287300	-1.76720200
C	-4.34940400	3.80375700	-0.82227600
H	-5.24027000	2.11083100	0.16890100
C	-3.26796200	4.27042700	-1.57070800
H	-1.38597000	3.74991300	-2.49106500
H	-5.15836700	4.47696800	-0.55213400
H	-3.23022800	5.30885100	-1.88783900
C	-0.38763600	-2.12086300	0.07835400
H	-0.04068100	-2.05414300	1.11091100
H	-0.17618900	-3.06984800	-0.41302300
H	0.38453600	-1.29056700	-0.50910600
C	-4.46177700	-0.79046500	-2.54097500
H	-4.28481000	-1.56123400	-3.29387800
H	-5.47136500	-0.91453700	-2.12695700
H	-4.44311800	0.19453500	-3.02331000
O	-2.15485100	-2.72870100	-2.27592300
C	-2.67798100	-4.03305900	-1.95878600
H	-2.34390400	-4.69416500	-2.75936900
H	-2.29037600	-4.39203500	-0.99920400
H	-3.77293200	-4.01327400	-1.92647900

TS **8-10**

E(B3LYP/BS1) = -2335.710569 au

H(B3LYP/BS1) = -2335.245291 au

G(B3LYP/BS1) = -2335.346464 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.573526 au

H	6.40650600	0.98583200	-0.32392200
O	6.03553600	0.12547600	-0.05803900
C	4.68998500	0.14448000	-0.20021400
C	3.97652000	-1.01614600	0.11542400
C	3.96900200	1.26938100	-0.65804400
C	2.56214500	-1.05294900	-0.00399100
C	2.58497500	1.24301100	-0.77728800
C	1.79837300	0.07805500	-0.44021500
O	0.52397300	0.05555500	-0.55292700
Cl	4.89991400	2.69477200	-1.07212600
Cl	1.72659100	2.62538700	-1.39613700
C	4.69846900	-2.16515700	0.55955200
C	1.86273900	-2.25842300	0.28445200
N	5.27835500	-3.10661400	0.92328300
N	1.30650400	-3.25905000	0.50554000
C	-0.91366900	-0.73041500	1.77050000

C	-1.90194600	-1.56866700	1.29503100
C	-0.97574200	0.53387300	1.12595400
C	-2.78844600	-0.83411800	0.31301400
H	-3.77049100	-0.71279600	0.79119600
C	-2.13122900	0.57806100	0.16993700
H	-1.69577800	0.67216900	-0.82966600
C	-3.01759900	-1.58147200	-0.99522700
C	-1.94274400	-1.90705400	-1.83727500
C	-4.31225900	-1.95910800	-1.37166400
C	-2.16587000	-2.59434500	-3.03052600
H	-0.93543300	-1.60885900	-1.55728700
C	-4.53550900	-2.64695300	-2.56749400
H	-5.15316000	-1.71105800	-0.72810000
C	-3.46194500	-2.96741800	-3.39944400
H	-1.32544000	-2.83985100	-3.67439300
H	-5.54703800	-2.93021400	-2.84567800
H	-3.63232100	-3.50289100	-4.32945800
C	-3.07254100	1.75574600	0.38896800
C	-3.76372200	1.91689700	1.59975000
C	-3.26678000	2.69780300	-0.62828500
C	-4.62990500	2.99414900	1.78579800
H	-3.62626000	1.19710800	2.40388800
C	-4.13545800	3.77662400	-0.44463000
H	-2.73879300	2.58468800	-1.57178200
C	-4.81864900	3.92793100	0.76283100
H	-5.15717800	3.10430500	2.72938500
H	-4.27663100	4.49628300	-1.24628300
H	-5.49426200	4.76633700	0.90737300
C	-2.14679000	-3.01032500	1.60293600
H	-3.06489700	-3.35624000	1.12303300
H	-1.31318800	-3.61707600	1.22526700
H	-2.22527100	-3.20065700	2.67694800
C	-0.25078800	1.72833300	1.61850500
H	0.76823100	1.47496100	1.91894400
H	-0.24361800	2.53090800	0.88080200
H	-0.76964300	2.09349200	2.51781600
O	0.07782400	-0.89795800	2.67376600
C	0.04896200	-1.98961300	3.60201800
H	0.88629600	-1.81200900	4.27804000
H	-0.88390500	-1.98958200	4.17459100
H	0.19151600	-2.94556400	3.09337200

9

E(B3LYP/BS1) = -849.3647303 au
H(B3LYP/BS1) = -849.000235 au
G(B3LYP/BS1) = -849.070471 au
E(M06-2X/BS2//B3LYP/BS1) = -849.2453483 au

C	0.50407100	2.29616100	0.22882200
C	1.25563700	1.24996500	0.92576700
C	-0.50101300	1.80991100	-0.52881500
C	0.55143100	-0.07282200	0.62230000
H	0.00624900	-0.36730700	1.52686200

C	-0.52790000	0.29166000	-0.47458800
H	-0.18768200	-0.09339000	-1.44685700
C	1.45492400	-1.22715700	0.23439200
C	2.39083500	-1.10066800	-0.80498900
C	1.35393100	-2.46027600	0.89111500
C	3.19694900	-2.17616400	-1.17681100
H	2.49394000	-0.14917200	-1.32111700
C	2.16072400	-3.54070900	0.52252100
H	0.63574900	-2.57668700	1.69953800
C	3.08472100	-3.40244000	-0.51381400
H	3.91592700	-2.05710500	-1.98329400
H	2.06579300	-4.48780700	1.04727200
H	3.71429200	-4.23984400	-0.80232000
C	-1.89339300	-0.31943000	-0.20236400
C	-2.67121700	0.10593600	0.88634700
C	-2.39785300	-1.33541100	-1.02382200
C	-3.91416100	-0.47130900	1.14711800
H	-2.29951300	0.89934200	1.53122200
C	-3.64164900	-1.91808000	-0.76547900
H	-1.81049300	-1.67514000	-1.87393100
C	-4.40416000	-1.48778600	0.32147500
H	-4.50196400	-0.12644100	1.99389300
H	-4.01316900	-2.70634900	-1.41508500
H	-5.37253200	-1.93746600	0.52364200
C	2.32277300	1.43285700	1.71484300
H	2.82815300	0.59974100	2.19453400
H	2.71425800	2.42814500	1.90426100
C	-1.43717700	2.60343800	-1.38180400
H	-1.26601900	3.67653100	-1.25931300
H	-1.31319800	2.35060700	-2.44423500
H	-2.48259400	2.38686700	-1.12864300
O	0.81293800	3.62849200	0.37783600
C	1.80946600	4.10739500	-0.53592700
H	1.99450000	5.15102900	-0.27254100
H	2.74059400	3.53676800	-0.44292800
H	1.45257700	4.04931500	-1.57137100

10

E(B3LYP/BS1) = -2335.725188 au
H(B3LYP/BS1) = -2335.257182 au
G(B3LYP/BS1) = -2335.357279 au
E(M06-2X/BS2//B3LYP/BS1) = -2335.603068 au

H	-6.20710700	1.00238800	0.45988000
O	-5.85653100	0.15997000	0.11642800
C	-4.51663200	0.14150800	0.20538500
C	-3.85143700	-1.02005900	-0.21698000
C	-3.75394500	1.20489400	0.72414000
C	-2.43805800	-1.09103400	-0.16875100
C	-2.35914800	1.12994300	0.77705400
C	-1.66856200	-0.00026200	0.27687700
O	-0.32511600	-0.08838900	0.37215100
Cl	-4.61721300	2.60063900	1.31007300

Cl	-1.45142100	2.40379700	1.52646400
C	-4.62484300	-2.12598600	-0.68296800
C	-1.80181300	-2.33169200	-0.48668600
N	-5.25210900	-3.02803200	-1.06482900
N	-1.33853200	-3.37804900	-0.69436400
C	0.92134100	-0.83168300	-1.61647900
C	2.08721400	-1.44152800	-1.31896200
C	0.62044800	0.35858500	-0.73644600
C	2.80135400	-0.70136700	-0.19693100
H	3.80026900	-0.41277800	-0.54885900
C	1.95835700	0.60581900	0.02807200
H	1.70138500	0.70467600	1.08449000
C	3.01642000	-1.52711900	1.06862700
C	1.97300900	-2.25550400	1.66063600
C	4.27853800	-1.55857700	1.67710900
C	2.18693800	-2.98698100	2.82981900
H	0.98927900	-2.24613000	1.20101400
C	4.49609900	-2.28791300	2.84887400
H	5.10082000	-1.00515200	1.22853200
C	3.44926300	-3.00558300	3.42994600
H	1.36614900	-3.54583700	3.27229400
H	5.48356500	-2.29742800	3.30315700
H	3.61491000	-3.57681500	4.33949200
C	2.70443600	1.86639200	-0.38035400
C	3.36893000	1.97199800	-1.61339500
C	2.74958800	2.96227400	0.49185400
C	4.05205700	3.13729800	-1.96213700
H	3.34972500	1.13650100	-2.30904800
C	3.43453900	4.13082400	0.14756700
H	2.24762000	2.89834200	1.45446300
C	4.08802900	4.22268000	-1.08195700
H	4.55838700	3.19705700	-2.92195100
H	3.45895400	4.96551600	0.84315700
H	4.62315900	5.12888000	-1.35226200
C	2.77120200	-2.65682100	-1.88110000
H	3.75397500	-2.38455000	-2.29056500
H	2.95985600	-3.38090500	-1.07824400
H	2.21283300	-3.16826200	-2.66293200
C	0.02690700	1.53475300	-1.49954500
H	-0.94826100	1.27379500	-1.91776900
H	-0.07004300	2.41823800	-0.86701300
H	0.68396700	1.78643600	-2.33540600
O	-0.05440600	-1.05185800	-2.53764600
C	0.07331000	-2.08825000	-3.50956800
H	-0.79079300	-1.98131600	-4.16789500
H	0.99197700	-1.96790400	-4.09326700
H	0.04781800	-3.07502300	-3.03774200

Table 1
para-CN-Ph (TS_A)
E(B3LYP/BS1) = -2520.140977 au

H(B3LYP/BS1) = -2519.680333 au
G(B3LYP/BS1) = -2519.790971 au
E(M06-2X/BS2//B3LYP/BS1) = -2519.987686 au

C	0.98818200	-2.18337800	-1.02428200
C	2.30947700	-1.71032100	-0.48455500
C	0.03087300	-1.27409900	-1.67156000
C	2.88529700	-0.59122500	-0.99346500
H	2.38934300	-0.10834900	-1.83216600
C	-0.20347500	-0.05876300	-1.05192100
H	0.47505400	0.19730900	-0.24609600
C	4.15049600	0.03758800	-0.60090800
C	4.61263300	0.07798700	0.73033400
C	4.91444100	0.68288800	-1.59576600
C	5.80945100	0.70749600	1.05024200
H	4.01189800	-0.34661500	1.52627400
C	6.11689900	1.30406700	-1.29020600
H	4.56013900	0.68298000	-2.62253400
C	6.57490400	1.31474700	0.03988300
H	6.15054500	0.74027200	2.07954500
H	6.70099000	1.78445500	-2.06795500
C	-1.15135800	0.99845100	-1.36134600
C	-2.33830300	0.83078800	-2.11324700
C	-0.89450400	2.27520900	-0.80461400
C	-3.20422700	1.89389100	-2.32495500
H	-2.60783300	-0.13822300	-2.51032800
C	-1.74967300	3.34590700	-1.01888700
H	0.00297400	2.42557500	-0.21239800
C	-2.91248700	3.16009000	-1.78610200
H	-4.11294900	1.74801400	-2.89856900
H	-1.52835500	4.31854600	-0.59353800
C	2.93954700	-2.61736600	0.54420700
H	4.02511900	-2.50417900	0.57263500
H	2.54834100	-2.41081100	1.54771900
H	2.70807000	-3.65981100	0.30890600
C	-0.66776800	-1.73947500	-2.92205700
H	-0.05164200	-2.48057000	-3.43614500
H	-1.64368700	-2.19793000	-2.72156500
H	-0.83455500	-0.89531500	-3.59647200
O	1.13682200	-3.45686100	-1.55481100
H	0.28718000	-2.33585800	0.12939400
C	0.10152300	-4.43750000	-1.37358800
H	0.46017000	-5.33285800	-1.88286800
H	-0.03862300	-4.64766900	-0.30956200
H	-0.84823000	-4.12504100	-1.81349800
O	-0.36891000	-2.41648400	1.19848400
C	-1.22639900	-1.46186500	1.34382700
C	-0.86731500	-0.27238000	2.08278700
C	-2.59982100	-1.57481100	0.88319300
C	-1.77376100	0.74734500	2.30298300
C	-3.51042800	-0.57430900	1.08908000
C	-3.15799300	0.67653400	1.79183000

O	-3.95823100	1.59388000	1.96629100
Cl	-3.03681900	-3.05342500	0.08891600
Cl	-5.15613300	-0.69948100	0.57062000
C	0.46482600	-0.20067600	2.60205400
C	-1.42688600	1.90991800	3.05063600
N	1.54652700	-0.13991300	3.02444100
N	-1.14419800	2.86049800	3.65945700
C	7.81218600	1.95800600	0.36699100
N	8.81842000	2.47985800	0.63179600
C	-3.80612800	4.25660000	-2.01309900
N	-4.53110200	5.14714800	-2.20105900

para-CN-Ph (TS_B)

E(B3LYP/BS1) = -2520.129803 au

H(B3LYP/BS1) = -2519.668282 au

G(B3LYP/BS1) = -2519.779326 au

E(M06-2X/BS2//B3LYP/BS1) = -2519.979612 au

C	0.01917500	-1.08680700	-2.05123300
C	1.36025500	-0.48643300	-2.03847400
C	-1.19414500	-0.17357400	-2.01335400
C	1.55212400	0.54625500	-1.15049900
H	0.65988900	0.89927800	-0.63891500
C	-1.95339800	0.00744900	-0.91822500
H	-1.65083700	-0.48253700	0.00133100
C	2.73847100	1.32621700	-0.82601500
C	4.06926900	0.96436600	-1.13639400
C	2.52581300	2.53112800	-0.11523700
C	5.13046100	1.78591200	-0.78023500
H	4.28910400	0.02671500	-1.62474900
C	3.57790700	3.36248600	0.23535700
H	1.51313800	2.81748100	0.15210300
C	4.89203900	2.99349200	-0.10198700
H	6.14688900	1.49329100	-1.02000400
H	3.39319800	4.28779300	0.76990300
C	-3.15484300	0.85066100	-0.76853000
C	-4.14916900	0.95159900	-1.75890600
C	-3.34183600	1.54482100	0.44254200
C	-5.27474200	1.74431800	-1.56348500
H	-4.06125400	0.38243700	-2.67725600
C	-4.45706900	2.34643900	0.64704500
H	-2.59610000	1.46262600	1.22765700
C	-5.43097500	2.45382300	-0.36131800
H	-6.03671000	1.80905300	-2.33290400
H	-4.58165500	2.88547600	1.58015800
C	2.41991000	-1.08622200	-2.92768600
H	3.06386100	-0.29978300	-3.33022000
H	3.05744200	-1.79659800	-2.38759100
H	1.96243400	-1.62066300	-3.76058700
C	-1.40225000	0.52258800	-3.34626700
H	-0.44125800	0.85157700	-3.75441400
H	-1.85755000	-0.14015400	-4.09198200
H	-2.04470000	1.39804900	-3.23451300

O	-0.07308200	-2.14440700	-2.90011000
H	0.12102500	-1.74580100	-0.73369900
C	-1.30873700	-2.88552000	-2.95897100
H	-2.12785200	-2.26395400	-3.32696800
H	-1.11593100	-3.70158400	-3.65407400
H	-1.55775000	-3.28672400	-1.97289900
O	-1.56024700	-3.47376300	0.81581800
C	-0.73441600	-2.63578100	1.11933800
C	0.55717200	-2.48564300	0.31362900
C	-0.93819800	-1.67330900	2.23352900
C	1.64799100	-1.78034100	0.93042700
C	0.04365900	-0.82503800	2.62374300
C	1.43456900	-0.85831700	2.03102400
O	2.32444100	-0.16331300	2.51358300
Cl	-2.49331600	-1.73645200	2.99059400
Cl	-0.18264400	0.31606800	3.89244400
C	0.89838100	-3.71215300	-0.39023500
C	2.98527600	-1.99474700	0.52090000
N	1.17933500	-4.68311100	-0.96095000
N	4.08724800	-2.18657400	0.18637100
C	5.98951600	3.84229300	0.25574200
C	-6.58787500	3.27434700	-0.15809900
N	-7.52690800	3.94204100	0.00628800
N	6.88047300	4.53286300	0.54470400

para-CN-Ph (TS_D)

E(B3LYP/BS1) = -2520.12572 au

H(B3LYP/BS1) = -2519.66698 au

G(B3LYP/BS1) = -2519.783696 au

E(M06-2X/BS2//B3LYP/BS1) = -2519.962837 au

C	-0.45990500	0.65861500	2.54276100
C	-1.84359100	0.53057400	2.04528200
C	0.46517500	1.71149100	2.01016600
C	-2.26173900	1.27437000	0.95910600
H	-1.61722700	2.09215000	0.65004200
C	0.85473800	1.62105200	0.70774000
H	0.47282300	0.76799800	0.15008200
C	-3.49447700	1.17050300	0.19790700
C	-4.21437000	-0.03326400	0.01271800
C	-3.96811100	2.33809700	-0.44731100
C	-5.37267500	-0.05844500	-0.75036600
H	-3.84286800	-0.96286700	0.42678000
C	-5.13251000	2.32574200	-1.19814600
H	-3.41410300	3.26565500	-0.33809000
C	-5.84717100	1.12280700	-1.35017700
H	-5.90964300	-0.98974400	-0.89478600
H	-5.49125700	3.23273700	-1.67248400
C	1.67964300	2.51026200	-0.10897500
C	2.58230400	3.47188200	0.39528600
C	1.58080900	2.36882200	-1.51202100
C	3.32787100	4.27111700	-0.46157600
H	2.73281900	3.58235000	1.46015700

C	2.31304400	3.16765000	-2.37692100
H	0.90814900	1.62174900	-1.92307000
C	3.19240500	4.13225700	-1.85359900
H	4.02169200	5.00035000	-0.05717300
H	2.21424300	3.04926000	-3.45059800
C	-2.72982900	-0.44633000	2.77641500
H	-3.78488000	-0.23918100	2.59255900
H	-2.51885700	-1.47566200	2.46357300
H	-2.53953400	-0.38675200	3.84940700
C	0.84404600	2.81836200	2.96580900
H	0.17120700	2.82520300	3.82584800
H	1.86622500	2.71313400	3.34946500
H	0.78242800	3.79019900	2.46546700
O	-0.38721900	0.42856900	3.91112800
H	-0.03704600	-0.49448500	2.00425000
C	0.84463100	-0.07017400	4.45131100
H	0.70481800	-0.08891200	5.53284100
H	1.03362500	-1.08234900	4.08204100
H	1.69313100	0.57452600	4.20472800
O	0.05064200	-1.77519000	1.68920300
C	0.69398800	-2.29412800	0.69816800
C	-0.02211100	-3.14820500	-0.20893600
C	2.10933500	-2.11094300	0.46553500
C	0.60684000	-3.75501000	-1.29496500
C	2.74270100	-2.70468700	-0.59992700
C	2.02897700	-3.56121500	-1.56038900
O	2.59423500	-4.09106200	-2.53064300
Cl	2.98318200	-1.14795100	1.61631600
Cl	4.43475000	-2.50425200	-0.88392200
C	-1.41883900	-3.32519200	0.03210200
C	-0.11377300	-4.58064700	-2.20387600
N	-2.55827800	-3.46285900	0.22452800
N	-0.70646500	-5.25506900	-2.94497800
C	-7.04791400	1.09762900	-2.12967900
C	3.95665300	4.96264800	-2.73514800
N	-8.02477000	1.07899500	-2.76235000
N	4.57683700	5.63889100	-3.45134400

para-CN-Ph (2_D)

E(B3LYP/BS1) = -2520.143046 au

H(B3LYP/BS1) = -2519.677612 au

G(B3LYP/BS1) = -2519.796647 au

E(M06-2X/BS2//B3LYP/BS1) = -2519.97013 au

C	2.29443900	1.54846200	-2.41907300
C	2.54576200	0.22481000	-1.70626600
C	2.08625800	2.49646700	-1.23208300
C	3.76365600	0.07193600	-1.07875900
H	4.48815300	0.86424200	-1.24564700
C	0.83617300	2.46607500	-0.63357000
H	0.12312100	1.76559900	-1.06386000
C	4.27011700	-1.03829500	-0.29905400
C	3.45495300	-1.94663000	0.42039200

C	5.67811400	-1.18353600	-0.21238600
C	4.02284000	-2.97172500	1.16042200
H	2.37847900	-1.83388400	0.44745500
C	6.25146300	-2.21533900	0.51051900
H	6.31694800	-0.48030600	-0.73790800
C	5.42228500	-3.12132600	1.19992100
H	3.38840400	-3.65309500	1.71652500
H	7.32927900	-2.32529200	0.55476500
C	0.29045500	3.21592600	0.47054400
C	0.94971700	4.25371100	1.18318500
C	-1.03740500	2.87864000	0.85661700
C	0.31781900	4.90917500	2.22484900
H	1.95218200	4.55877700	0.92405900
C	-1.67126700	3.52874100	1.90055800
H	-1.54748900	2.07919800	0.32761700
C	-0.99551700	4.55154500	2.59244900
H	0.82984400	5.70095400	2.76032300
H	-2.68093600	3.25573700	2.18670400
C	1.45697000	-0.79887000	-1.79624100
H	1.83173200	-1.80720500	-1.61401400
H	0.63689200	-0.61315100	-1.08909300
H	1.01556600	-0.76693100	-2.79902600
C	3.24728700	3.34283200	-0.80476900
H	4.12533300	3.13165600	-1.41550700
H	3.00055900	4.40322200	-0.94716700
H	3.49948500	3.20135200	0.25070000
O	3.37910200	1.88401500	-3.24693600
H	1.36927300	1.47433600	-3.00476300
C	3.08705600	2.92925000	-4.17803200
H	3.98506300	3.05892900	-4.78423900
H	2.24524100	2.65060500	-4.82492400
H	2.85336600	3.87464500	-3.67200200
O	-1.51982100	-0.04268500	-0.48696200
C	-2.45801300	-0.86077600	-0.35175300
C	-2.27575000	-2.15161800	0.28533000
C	-3.82088600	-0.57548200	-0.82486000
C	-3.32440700	-3.06614000	0.43174200
C	-4.84704500	-1.46561800	-0.68369200
C	-4.67111900	-2.78299500	-0.04225600
O	-5.60627500	-3.59280200	0.08417000
Cl	-4.04352600	0.97413100	-1.58706500
Cl	-6.45279300	-1.11871900	-1.25078600
C	-0.96714100	-2.44855200	0.76158100
C	-3.11946900	-4.32721000	1.05986100
N	0.10601300	-2.68635100	1.14877000
N	-2.94338300	-5.35743500	1.57488000
C	6.00640700	-4.18634600	1.95796500
N	6.48340200	-5.05178800	2.57266700
C	-1.64174200	5.23421500	3.67183000
N	-2.16591600	5.79020600	4.54960600

para-CN-Ph (2_A)

E(B3LYP/BS1) = -2520.189284 au
H(B3LYP/BS1) = -2519.722099 au
G(B3LYP/BS1) = -2519.832321 au
E(M06-2X/BS2//B3LYP/BS1) = -2520.059354 au

C	-0.49949500	-0.64812200	2.02292800
C	-1.92484000	-0.76262200	1.44469200
C	0.21617200	0.68930400	1.79318100
C	-2.50314200	0.28270000	0.81809000
H	-1.94141600	1.20824400	0.74882400
C	0.54650400	1.05174200	0.53413500
H	0.24868100	0.39256000	-0.27733700
C	-3.85420700	0.37906000	0.24180600
C	-4.54732800	-0.70120500	-0.33919300
C	-4.47292300	1.64662400	0.22646700
C	-5.81572500	-0.53163600	-0.88246900
H	-4.08277100	-1.67772000	-0.39679600
C	-5.74260300	1.82856400	-0.30327600
H	-3.94685900	2.49838300	0.64824200
C	-6.42691400	0.73336500	-0.86029400
H	-6.33271100	-1.37314200	-1.33174200
H	-6.20644200	2.80931700	-0.29423800
C	1.21426300	2.27654200	0.06586900
C	2.19137200	2.96810900	0.80813100
C	0.89034400	2.75734600	-1.21945400
C	2.79543600	4.11377100	0.30301500
H	2.50998600	2.59124100	1.77253100
C	1.47836400	3.90561500	-1.73115300
H	0.15754300	2.22364500	-1.81801700
C	2.43550000	4.59630400	-0.96658200
H	3.55158600	4.63173900	0.88350900
H	1.20766600	4.26897800	-2.71690300
C	-2.62993900	-2.06258700	1.76115000
H	-3.70509100	-1.90441500	1.88147900
H	-2.48583700	-2.80885600	0.97419500
H	-2.23899700	-2.48502200	2.68763800
C	0.37272400	1.58542000	2.99920600
H	-0.44286000	1.41216800	3.70523700
H	1.31135100	1.40322700	3.53614100
H	0.36169900	2.63735000	2.70347100
O	-0.66570800	-0.96483400	3.36646600
H	3.82877400	-2.63617100	-3.30653500
C	0.43068000	-1.41281600	4.17418100
H	0.87980800	-2.31424900	3.75196500
H	1.19757900	-0.64663100	4.30039900
H	-0.01547600	-1.64391600	5.14313100
O	4.17345100	-2.23066000	-2.48963600
C	3.20071700	-2.13293900	-1.57004100
C	3.53206600	-1.57768000	-0.32605000
C	1.87724400	-2.56068900	-1.78101100
C	2.55047200	-1.44518800	0.68753500
C	0.90632400	-2.42055400	-0.78485800

C	1.21614700	-1.84830100	0.47481900
O	0.28369100	-1.83551100	1.45093000
Cl	1.50333900	-3.27161300	-3.32661600
Cl	-0.70512300	-2.97648100	-1.08798400
C	4.87743500	-1.15592800	-0.10003800
C	2.96597900	-0.89431800	1.93821700
N	5.97314200	-0.81215300	0.08435200
N	3.36938300	-0.44255400	2.93133000
C	3.05186000	5.77973600	-1.48718100
C	-7.73523700	0.90955100	-1.41527600
N	-8.79913700	1.05297000	-1.86580700
N	3.55077600	6.74229600	-1.91106800

para-Cl-Ph (TS_A)

E(B3LYP/BS1) = -3254.842071 au

H(B3LYP/BS1) = -3254.399068 au

G(B3LYP/BS1) = -3254.507295 au

E(M06-2X/BS2//B3LYP/BS1) = -3254.70702 au

C	0.92200900	-2.22220900	-1.08021800
C	2.25014900	-1.76981100	-0.54198100
C	-0.04209000	-1.28934200	-1.68092100
C	2.82095700	-0.63180500	-1.01524300
H	2.31115200	-0.12055800	-1.82877700
C	-0.26731300	-0.09319900	-1.01760000
H	0.42363800	0.13338200	-0.21350300
C	4.08821500	-0.01184000	-0.61939100
C	4.59515100	-0.04507900	0.69512600
C	4.81543900	0.70558100	-1.59112100
C	5.79521300	0.58334000	1.01934900
H	4.02936600	-0.52670600	1.48437300
C	6.02129900	1.32729000	-1.28474400
H	4.43247400	0.76650600	-2.60617700
C	6.50364600	1.25448200	0.02299100
H	6.16999700	0.56017600	2.03683900
H	6.57600500	1.86532600	-2.04567200
C	-1.21996000	0.97049400	-1.26855600
C	-2.41369700	0.84002200	-2.01833400
C	-0.96626100	2.22120700	-0.65300400
C	-3.28778900	1.90919600	-2.16822900
H	-2.68546700	-0.10761600	-2.46327600
C	-1.82802900	3.29981000	-0.80479500
H	-0.06374600	2.34923800	-0.06277800
C	-2.98597500	3.13426900	-1.56662800
H	-4.20235500	1.79238000	-2.73871700
H	-1.60964700	4.25219100	-0.33499600
C	2.89286200	-2.71333900	0.44574900
H	3.98096500	-2.61876000	0.44387200
H	2.53677300	-2.52584600	1.46612100
H	2.63706500	-3.74593100	0.19241400
C	-0.76222900	-1.71069700	-2.93490300
H	-0.15809300	-2.43835500	-3.48138500
H	-1.73773300	-2.17074900	-2.73477900

H	-0.93458300	-0.84472200	-3.57976400
O	1.06619800	-3.47321000	-1.67284800
H	0.24442600	-2.42896500	0.06227700
C	0.04389900	-4.46694300	-1.49905200
H	0.39331900	-5.34104700	-2.05049400
H	-0.06772800	-4.71794900	-0.44032300
H	-0.92035700	-4.14635800	-1.90095600
O	-0.41375600	-2.56088200	1.14565900
C	-1.26379500	-1.60616200	1.32692200
C	-0.89515500	-0.44174400	2.09762600
C	-2.63762100	-1.68945700	0.86213800
C	-1.78837900	0.58838300	2.33301000
C	-3.53501600	-0.68038200	1.08537200
C	-3.16775000	0.55257400	1.80982400
O	-3.95431200	1.48184900	1.99199700
Cl	-3.09345700	-3.14452300	0.03326800
Cl	-5.18229200	-0.77399300	0.55997200
C	0.43357700	-0.40101700	2.62848500
C	-1.42842800	1.72801200	3.10908000
N	1.51158700	-0.36469100	3.06336000
N	-1.13499400	2.65991100	3.74157200
Cl	8.02512100	2.04227100	0.42649100
Cl	-4.08667900	4.48306800	-1.76696700

para-Cl-Ph (TS_B)

E(B3LYP/BS1) = -3254.83045 au

H(B3LYP/BS1) = -3254.386642 au

G(B3LYP/BS1) = -3254.495313 au

E(M06-2X/BS2//B3LYP/BS1) = -3254.698039 au

C	0.02477800	-1.17251300	-2.04602500
C	1.36684100	-0.57945700	-2.03562600
C	-1.18349800	-0.25247900	-2.00578100
C	1.56443900	0.45959000	-1.15269600
H	0.67164800	0.81539200	-0.64374300
C	-1.94057700	-0.06617400	-0.90981300
H	-1.63644500	-0.55877900	0.00816800
C	2.74868400	1.23511400	-0.82753900
C	4.07951300	0.89145300	-1.16048100
C	2.54227000	2.42543100	-0.09021100
C	5.14237400	1.71246300	-0.80074300
H	4.30205600	-0.03285800	-1.67298700
C	3.59472300	3.25789000	0.26549700
H	1.53220200	2.70337600	0.19651500
C	4.89204200	2.89337800	-0.09959600
H	6.15862900	1.43460700	-1.05724900
H	3.41537400	4.17144700	0.82120500
C	-3.13923300	0.78026500	-0.75558700
C	-4.13080700	0.90078100	-1.74509600
C	-3.33136400	1.46192500	0.46050000
C	-5.25748700	1.69732400	-1.54470200
H	-4.04601000	0.34396600	-2.67171300
C	-4.44621200	2.26849200	0.67262600

H	-2.59100300	1.36972800	1.25018700
C	-5.39970800	2.38156900	-0.33909000
H	-6.01840500	1.77585700	-2.31359000
H	-4.57482300	2.79736400	1.61073900
C	2.42807700	-1.18616100	-2.91841000
H	3.05172900	-0.39860600	-3.35098600
H	3.08700100	-1.86592000	-2.36471500
H	1.97328600	-1.75322100	-3.73070400
C	-1.39378300	0.44342700	-3.33873400
H	-0.43176400	0.75174400	-3.76055200
H	-1.87354400	-0.20986100	-4.07768000
H	-2.01709900	1.33206000	-3.21981400
O	-0.07664800	-2.22638600	-2.90501900
H	0.11667400	-1.83582400	-0.74699500
C	-1.31530700	-2.96020200	-2.95506100
H	-2.13471200	-2.33479200	-3.31649300
H	-1.13299800	-3.77731900	-3.65214500
H	-1.56115000	-3.36174900	-1.96807200
O	-1.56878300	-3.56230300	0.81443500
C	-0.73641700	-2.72829500	1.11379200
C	0.55336000	-2.58709500	0.30918700
C	-0.93301500	-1.76215300	2.22649600
C	1.64874700	-1.88357900	0.91945700
C	0.05357300	-0.91767200	2.61258900
C	1.44240700	-0.95654100	2.01560400
O	2.33528100	-0.26044700	2.49274900
Cl	-2.48686700	-1.81677800	2.98815000
Cl	-0.16503300	0.22691600	3.88070600
C	0.88654700	-3.81250800	-0.39834600
C	2.98371100	-2.10063000	0.50401500
N	1.16195700	-4.78367800	-0.97170900
N	4.08430100	-2.29488200	0.16598700
Cl	6.23493100	3.93246600	0.34288900
Cl	-6.81840300	3.39354400	-0.08080400

para-Cl-Ph (TS_D)

E(B3LYP/BS1) = -3254.826306 au

H(B3LYP/BS1) = -3254.385196 au

G(B3LYP/BS1) = -3254.498903 au

E(M06-2X/BS2//B3LYP/BS1) = -3254.682472 au

C	-0.42778100	0.42889900	2.64495500
C	-1.80917200	0.33690600	2.13907100
C	0.51863800	1.47986400	2.15836600
C	-2.22992700	1.15576700	1.10955800
H	-1.58089400	1.98995700	0.85837100
C	0.87761400	1.46294400	0.84274800
H	0.45049800	0.66186100	0.24203500
C	-3.46250000	1.11403400	0.34413400
C	-4.21199800	-0.05973800	0.09683200
C	-3.91392000	2.31960300	-0.24387900
C	-5.37148300	-0.02310900	-0.66909400
H	-3.86571400	-1.01859500	0.46328100

C	-5.07848500	2.37141700	-0.99812400
H	-3.34272300	3.23082700	-0.09025800
C	-5.80344900	1.19439100	-1.20051000
H	-5.93018100	-0.93236300	-0.86201500
H	-5.41854500	3.30649700	-1.42936900
C	1.71850400	2.36786300	0.06190600
C	2.65180900	3.28291500	0.59506600
C	1.60471400	2.29795700	-1.34472400
C	3.41371600	4.10187900	-0.23375900
H	2.81772200	3.34518200	1.66183100
C	2.35162500	3.11630500	-2.18371000
H	0.90777700	1.59079600	-1.78593400
C	3.25192400	4.01913000	-1.61667400
H	4.13215200	4.79371100	0.19229600
H	2.24134200	3.05212500	-3.26066100
C	-2.69906900	-0.68984600	2.79729200
H	-3.75310300	-0.43573500	2.67213600
H	-2.53282600	-1.68654200	2.37197200
H	-2.47426300	-0.74780200	3.86340500
C	0.96771700	2.50883200	3.16974000
H	0.32905600	2.47650000	4.05483000
H	2.00101300	2.35204500	3.50306900
H	0.91482500	3.51367700	2.73769700
O	-0.35987600	0.13772900	4.00510800
H	-0.00908700	-0.72963200	2.04010800
C	0.85146200	-0.43343500	4.51569900
H	0.71511400	-0.49635600	5.59637500
H	1.00304900	-1.43471000	4.10169600
H	1.72477100	0.18810800	4.29626000
O	0.07602600	-1.95478100	1.66016400
C	0.72130300	-2.39654500	0.63094700
C	0.00271500	-3.16240300	-0.34880100
C	2.14019400	-2.21194600	0.42630900
C	0.63349600	-3.68420000	-1.47716300
C	2.77565300	-2.72202200	-0.68080400
C	2.05985000	-3.48538700	-1.71526500
O	2.62679800	-3.93844100	-2.72273800
Cl	3.01538200	-1.36166400	1.66113500
Cl	4.47211500	-2.51922700	-0.93447400
C	-1.39725600	-3.34683400	-0.13299500
C	-0.08875500	-4.42331500	-2.45651500
N	-2.53890300	-3.49407500	0.03759100
N	-0.68235200	-5.02728800	-3.25540400
Cl	4.20915100	5.05912800	-2.66300400
Cl	-7.27356800	1.24260800	-2.15932500

para-Cl-Ph (2_D)

E(B3LYP/BS1) = -3254.848811 au

H(B3LYP/BS1) = -3254.400778 au

G(B3LYP/BS1) = -3254.518035 au

E(M06-2X/BS2//B3LYP/BS1) = -3254.694232 au

C	-2.16072500	1.66815400	2.50161700

C	-2.49847400	0.36891700	1.78228500
C	-1.87512900	2.60632900	1.32327000
C	-3.73540500	0.27940400	1.18403700
H	-4.42001200	1.09900900	1.38551000
C	-0.61628200	2.51808100	0.75599700
H	0.05516100	1.79221600	1.21069500
C	-4.30690300	-0.78838100	0.39329800
C	-3.55262900	-1.72491200	-0.35687600
C	-5.72132200	-0.86560400	0.32276000
C	-4.18155700	-2.70672100	-1.10914800
H	-2.47201400	-1.66697300	-0.40110300
C	-6.35825300	-1.85360300	-0.41131500
H	-6.31940300	-0.14326100	0.87065900
C	-5.57901100	-2.77408500	-1.12136700
H	-3.59429800	-3.40848200	-1.69075700
H	-7.44040700	-1.91167900	-0.44349900
C	-0.01268800	3.22772100	-0.34242000
C	-0.60999300	4.27853500	-1.09010900
C	1.31091000	2.83719700	-0.69235000
C	0.07298500	4.89609100	-2.12451400
H	-1.60761700	4.62510000	-0.86504900
C	1.99803000	3.44778900	-1.72783200
H	1.77810000	2.02461800	-0.14360700
C	1.37325200	4.47813000	-2.43933700
H	-0.39124700	5.69809200	-2.68725800
H	3.00325000	3.13494700	-1.98698900
C	-1.45565400	-0.70763400	1.82784300
H	-1.88726800	-1.69464200	1.65343700
H	-0.65167100	-0.55895500	1.09550700
H	-0.97977900	-0.70802400	2.81529500
C	-2.98786900	3.50116700	0.86113400
H	-3.88467300	3.34340600	1.46088200
H	-2.69514600	4.55193200	0.98390000
H	-3.23304100	3.34792700	-0.19468000
O	-3.22591300	2.07829200	3.32452000
H	-1.24892100	1.52794800	3.09649100
C	-2.87443400	3.12251700	4.23353500
H	-3.76185100	3.31526700	4.83897200
H	-2.04759500	2.81131100	4.88556600
H	-2.58870300	4.04377900	3.70948700
O	1.63171200	-0.14360800	0.59809700
C	2.49359500	-1.03164800	0.41442200
C	2.20405500	-2.25848200	-0.30540800
C	3.87239000	-0.90143100	0.91155700
C	3.16947600	-3.25118600	-0.50712600
C	4.81655300	-1.86849900	0.71656900
C	4.53126100	-3.12018600	-0.01110500
O	5.39302400	-3.99927000	-0.18769500
Cl	4.22489800	0.56980600	1.77376600
Cl	6.44150200	-1.70479700	1.31224100
C	0.87904200	-2.40847400	-0.80444900

C	2.86013400	-4.44654100	-1.21590500
N	-0.20659700	-2.52850600	-1.21095600
N	2.59891400	-5.42221000	-1.79691900
Cl	-6.36922100	-4.01936100	-2.06132300
Cl	2.22742000	5.26095800	-3.74421900

para-Cl-Ph (2_A)

E(B3LYP/BS1) = -3254.88726 au

H(B3LYP/BS1) = -3254.43784 au

G(B3LYP/BS1) = -3254.546215 au

E(M06-2X/BS2//B3LYP/BS1) = -3254.775035 au

C	-0.44614700	-0.79059400	2.04381200
C	-1.87318500	-0.85761700	1.46993000
C	0.30049300	0.53386900	1.85586700
C	-2.43460800	0.21885200	0.88179700
H	-1.85139500	1.13281300	0.83952400
C	0.62607500	0.93523600	0.60735000
H	0.30365600	0.31024200	-0.22192400
C	-3.78568200	0.36559100	0.31408500
C	-4.51899900	-0.67881300	-0.27992800
C	-4.36658400	1.64946900	0.32126200
C	-5.78754500	-0.46038900	-0.81604000
H	-4.09061400	-1.67066100	-0.35756200
C	-5.63597000	1.88313000	-0.19980100
H	-3.81453000	2.48018600	0.75286700
C	-6.33884800	0.81817200	-0.76266000
H	-6.33594400	-1.27502200	-1.27686000
H	-6.07026600	2.87677700	-0.17443700
C	1.31986500	2.15778500	0.17063200
C	2.30864900	2.81513700	0.92630200
C	1.00990700	2.67800100	-1.10133300
C	2.93903400	3.96292900	0.44809200
H	2.62150200	2.41340200	1.88282800
C	1.62220000	3.82909700	-1.58840600
H	0.26774000	2.17599400	-1.71639600
C	2.58223600	4.46558600	-0.80182800
H	3.70531000	4.45397400	1.03816200
H	1.36258400	4.22266500	-2.56523400
C	-2.60522800	-2.15306900	1.74424800
H	-3.67134200	-1.96984200	1.90666800
H	-2.51044800	-2.86288100	0.91697800
H	-2.19968800	-2.63363900	2.63540700
C	0.49566700	1.38255300	3.09098400
H	-0.30566900	1.19406900	3.80940700
H	1.44469400	1.17347000	3.59938000
H	0.48963400	2.44458000	2.83212900
O	-0.60750600	-1.15675200	3.37544400
H	3.79151300	-2.66093900	-3.40197700
C	0.48936500	-1.64531000	4.15753200
H	0.92225300	-2.53849300	3.70198900
H	1.26841900	-0.89458900	4.30121100
H	0.04942900	-1.90196500	5.12306500

O	4.15273200	-2.29190000	-2.57510000
C	3.19217600	-2.21416600	-1.64003800
C	3.54570600	-1.70916000	-0.38107000
C	1.86064200	-2.61651700	-1.84953600
C	2.57798200	-1.59989000	0.64882200
C	0.90361400	-2.49913300	-0.83736700
C	1.23499500	-1.97661900	0.43905300
O	0.31465000	-1.98173100	1.42339800
Cl	1.45887800	-3.26663900	-3.41547800
Cl	-0.71882900	-3.02305800	-1.14012800
C	4.89956700	-1.31468700	-0.15660400
C	3.01769600	-1.10475500	1.91447200
N	6.00241900	-0.99348800	0.02623000
N	3.44413100	-0.70244300	2.91923200
Cl	-7.94529900	1.09856700	-1.43371700
Cl	3.37112400	5.92032400	-1.40780300

Ph (TS_A)

E(B3LYP/BS1) = -2335.651003 au

H(B3LYP/BS1) = -2335.191202 au

G(B3LYP/BS1) = -2335.292982 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.502807 au

C	1.27543000	-2.04497800	-0.41603400
C	2.55201700	-1.41259100	0.06244000
C	0.36538200	-1.36746000	-1.34819000
C	3.16929600	-0.47429900	-0.70135100
H	2.73163800	-0.26506700	-1.67515400
C	0.08979000	-0.02856800	-1.10903800
H	0.71945700	0.45072900	-0.36759400
C	4.40031500	0.27199000	-0.42519500
C	4.79641000	0.67052900	0.86795400
C	5.20348300	0.66200000	-1.51747600
C	5.96691400	1.40335800	1.05812100
H	4.16532000	0.44502800	1.72037300
C	6.37839100	1.38288000	-1.32381300
H	4.89963100	0.38420800	-2.52372400
C	6.76714000	1.75337600	-0.03261200
H	6.24973700	1.71033700	2.06118000
H	6.98747500	1.66313400	-2.17865500
H	7.67978600	2.32246400	0.12041000
C	-0.84474400	0.88156900	-1.74011400
C	-1.98757800	0.49300500	-2.48154200
C	-0.63507100	2.26797500	-1.52705600
C	-2.85577200	1.44842800	-2.99804700
H	-2.21808200	-0.55419400	-2.62484400
C	-1.49990300	3.21885300	-2.05605600
H	0.23060300	2.58833000	-0.95404200
C	-2.61610100	2.81181000	-2.79247100
H	-3.73198500	1.12921300	-3.55418700
H	-1.31160900	4.27446700	-1.88601200
H	-3.30050000	3.55106200	-3.19795900
C	3.09765000	-1.97571800	1.35270900

H	4.18219700	-1.86237300	1.41500400
H	2.65367800	-1.47913500	2.22431400
H	2.85826300	-3.04064600	1.42365200
C	-0.25733100	-2.17317700	-2.45769100
H	0.39588000	-3.00932600	-2.71797800
H	-1.23663400	-2.58755100	-2.18731300
H	-0.39964000	-1.54913300	-3.34380700
O	1.47342200	-3.41415300	-0.58185400
H	0.49964300	-1.91231800	0.67146000
C	0.44101300	-4.33631800	-0.20023300
H	0.85399600	-5.32809400	-0.39092600
H	0.20796700	-4.23080600	0.86319600
H	-0.47134700	-4.20517700	-0.78751400
O	-0.26642900	-1.72268100	1.67925100
C	-1.13686400	-0.79386200	1.46189400
C	-0.85718200	0.57077200	1.84244900
C	-2.45693300	-1.07540900	0.92490900
C	-1.77219900	1.58800400	1.63472200
C	-3.37465800	-0.08222700	0.71239600
C	-3.08761700	1.33331300	1.01786200
O	-3.89156900	2.24128300	0.80435300
Cl	-2.82663300	-2.73860700	0.59064200
Cl	-4.96144200	-0.40498000	0.09707000
C	0.40641600	0.83374600	2.46126000
C	-1.49975700	2.93053600	2.02726100
N	1.43044600	1.05323700	2.96701000
N	-1.27890500	4.02747800	2.34765600

Ph (TS_B)

E(B3LYP/BS1) = -2335.639038 au

H(B3LYP/BS1) = -2335.178289 au

G(B3LYP/BS1) = -2335.280737 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.49227 au

C	0.09830200	-1.32048200	1.69634500
C	1.42872700	-1.58915500	1.13760100
C	-1.12560000	-1.81877300	0.94700800
C	1.56437900	-1.40702300	-0.22151100
H	0.63989800	-1.20111300	-0.75630200
C	-1.93579900	-1.01686100	0.23316800
H	-1.66256300	0.03040000	0.14878600
C	2.71532200	-1.52064900	-1.10075500
C	4.06842900	-1.55079100	-0.68856400
C	2.44355800	-1.58247600	-2.48918000
C	5.08990700	-1.66731800	-1.62668500
H	4.32861900	-1.44774500	0.35510700
C	3.46679700	-1.71019500	-3.42056300
H	1.41130300	-1.54008200	-2.82614900
C	4.79650400	-1.75688000	-2.99071700
H	6.12278300	-1.68213200	-1.29153100
H	3.23141500	-1.76616400	-4.47916700
H	5.60031900	-1.85174900	-3.71508500
C	-3.15407900	-1.37435100	-0.51988500

C	-4.10720600	-2.29494200	-0.04790100
C	-3.40183500	-0.72735800	-1.74543900
C	-5.25222900	-2.57995400	-0.79280100
H	-3.97116400	-2.76563700	0.92016900
C	-4.54092500	-1.01947600	-2.49290300
H	-2.68665000	0.00187500	-2.11721800
C	-5.46986600	-1.95066900	-2.02022800
H	-5.97941800	-3.28909500	-0.40711100
H	-4.70654400	-0.51619800	-3.44141200
H	-6.36188800	-2.17451300	-2.59849700
C	2.54142500	-1.97179400	2.08040300
H	3.18488300	-2.72409100	1.61578400
H	3.17194300	-1.11436500	2.34543800
H	2.13589700	-2.38357400	3.00493500
C	-1.28316700	-3.32326800	1.07715800
H	-0.30902800	-3.81478800	0.98506500
H	-1.69977500	-3.61665600	2.04839800
H	-1.94110600	-3.71305500	0.29784500
O	0.05662100	-1.48306800	3.05073300
H	0.13241400	0.12559000	1.55762500
C	-1.16935100	-1.18309800	3.74430800
H	-1.97115500	-1.86331800	3.44825700
H	-0.93769700	-1.31589600	4.80060600
H	-1.47245300	-0.14904000	3.55818800
O	-1.61970200	2.30619400	2.22267300
C	-0.80162700	2.14587700	1.33741000
C	0.52301500	1.44191500	1.61479500
C	-1.04830200	2.56497000	-0.06750000
C	1.58858400	1.62100600	0.66690600
C	-0.07955400	2.48286600	-1.01092400
C	1.33478400	2.05089700	-0.69424000
O	2.20628400	2.12249400	-1.55755800
Cl	-2.63663400	3.17540000	-0.38882200
Cl	-0.35554800	2.94075600	-2.64843000
C	0.89004500	1.51231900	3.01932500
C	2.94036900	1.43030900	1.03870600
N	1.19377900	1.55957700	4.13889800
N	4.05447800	1.28669000	1.35720600

Ph (TS_D)

E(B3LYP/BS1) = -2335.634589 au

H(B3LYP/BS1) = -2335.176494 au

G(B3LYP/BS1) = -2335.283183 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.477062 au

C	-1.32106500	0.98452200	1.94911800
C	-2.38661800	0.09213500	1.46282800
C	-0.91253200	2.20746100	1.19106400
C	-2.94523300	0.29060300	0.21460100
H	-2.71734600	1.23596000	-0.26990600
C	-0.35515200	2.04761500	-0.04254300
H	-0.23098800	1.01959100	-0.37945900
C	-3.86121500	-0.55029100	-0.53518300

C	-3.93872300	-1.95816800	-0.41498400
C	-4.69302300	0.08006800	-1.49234600
C	-4.83151600	-2.68788500	-1.19399800
H	-3.26845000	-2.48540500	0.25356900
C	-5.59360800	-0.65149200	-2.25732000
H	-4.62957300	1.15808000	-1.61594600
C	-5.66987700	-2.04066000	-2.10808600
H	-4.86751100	-3.76902000	-1.09560800
H	-6.23117000	-0.14392200	-2.97539500
H	-6.36701200	-2.61634700	-2.71012000
C	0.07745700	3.02614200	-1.04030300
C	0.36141800	4.38475800	-0.78066900
C	0.24865700	2.56082900	-2.36388100
C	0.77368600	5.23490300	-1.80502800
H	0.29355900	4.77770200	0.22497400
C	0.65013100	3.41424600	-3.38655300
H	0.05227900	1.51450200	-2.58390000
C	0.91217000	4.75963200	-3.11158900
H	0.99409100	6.27436900	-1.57860900
H	0.76443400	3.03015000	-4.39624400
H	1.23122300	5.42850100	-3.90581800
C	-2.80551600	-1.02529400	2.38808400
H	-3.81798000	-1.36368100	2.16086800
H	-2.13008800	-1.88456700	2.30203000
H	-2.77069300	-0.68444900	3.42399000
C	-1.20572100	3.53801800	1.84657400
H	-1.90683200	3.40880200	2.67387600
H	-0.30643500	4.01991100	2.24963500
H	-1.64500600	4.22945700	1.11996000
O	-1.35464000	1.11815700	3.33580000
H	-0.30611400	0.06852100	1.74060000
C	-0.12426000	1.39431900	4.01611300
H	-0.39405900	1.55728500	5.06075200
H	0.55430400	0.53953500	3.93733400
H	0.37040700	2.28860000	3.62562900
O	0.39683700	-0.99542200	1.77780400
C	1.34249000	-1.32545100	0.96024400
C	1.25503400	-2.59489900	0.29419200
C	2.51675000	-0.51971800	0.71303100
C	2.24334400	-3.02815900	-0.58815600
C	3.49911300	-0.93461000	-0.15455400
C	3.42213900	-2.21600600	-0.87358600
O	4.30129500	-2.59125500	-1.66605900
Cl	2.65882400	0.96781300	1.59600600
Cl	4.91334700	0.01135800	-0.45251900
C	0.09732900	-3.39032300	0.55442900
C	2.14169400	-4.27824800	-1.26205700
N	-0.84614200	-4.03966500	0.76016000
N	2.05614200	-5.30113400	-1.81137200

Ph (2_D)

E(B3LYP/BS1) = -2335.656198 au

H(B3LYP/BS1) = -2335.191604 au
G(B3LYP/BS1) = -2335.304158 au
E(M06-2X/BS2//B3LYP/BS1) = -2335.488257 au

C	2.20945900	-0.66349900	2.04252400
C	2.42163700	0.73698500	1.48051800
C	2.56454900	-1.73394800	1.02150300
C	3.38379200	0.93901400	0.52761000
H	4.03066600	0.09447900	0.29969000
C	1.60550400	-1.95557400	0.04625800
H	0.70869800	-1.34266100	0.13580000
C	3.72779500	2.15180900	-0.19344500
C	2.80387900	3.18270400	-0.48993700
C	5.05479500	2.28114400	-0.67239000
C	3.20784900	4.30530300	-1.20336100
H	1.76248000	3.08558000	-0.20620600
C	5.45616800	3.41222900	-1.37074400
H	5.76756400	1.48561100	-0.47240300
C	4.53364200	4.43181800	-1.63562200
H	2.48429600	5.08140500	-1.43399700
H	6.48163900	3.50095200	-1.71656600
H	4.84254800	5.31381200	-2.18905500
C	1.58695800	-2.83789300	-1.08923600
C	2.53215400	-3.86299100	-1.36608300
C	0.50685400	-2.66035700	-2.00039800
C	2.40415100	-4.64798100	-2.50168800
H	3.34743500	-4.05992500	-0.68415700
C	0.39214100	-3.44255300	-3.13852200
H	-0.22588300	-1.88709300	-1.79008800
C	1.34239700	-4.43958900	-3.39467100
H	3.12904700	-5.43191600	-2.69743200
H	-0.43324000	-3.28573600	-3.82570800
H	1.25374100	-5.05859200	-4.28246400
C	1.52937400	1.78249900	2.07780000
H	1.95761800	2.78450200	2.01056000
H	0.55452900	1.78540100	1.57260900
H	1.35056800	1.54601200	3.13269400
C	3.89440500	-2.40896600	1.14728400
H	4.50496500	-1.90591100	1.89939900
H	3.77038700	-3.45127900	1.47362000
H	4.43393700	-2.43295500	0.19479400
O	2.90415100	-0.76811600	3.27073800
H	1.12463300	-0.74379100	2.22832300
C	2.37402000	-1.75732300	4.15480200
H	2.96611800	-1.70205400	5.07028100
H	1.32084500	-1.55246100	4.38811800
H	2.45653100	-2.76831700	3.73475900
O	-0.89819700	0.16555300	0.25754600
C	-2.12379400	0.39402700	0.15155700
C	-2.63508200	1.70472200	-0.20605400
C	-3.14395700	-0.64066800	0.37993100
C	-4.00375500	1.96310500	-0.33503000

C	-4.48110400	-0.39140900	0.25627900
C	-5.01010000	0.93471600	-0.11618400
O	-6.22825500	1.15717800	-0.23276400
Cl	-2.53762300	-2.21127300	0.82530000
Cl	-5.67740600	-1.62282500	0.53004700
C	-1.66573800	2.72557200	-0.42115600
C	-4.47906600	3.25715800	-0.69090900
N	-0.86624100	3.55656000	-0.59064100
N	-4.86073000	4.31877500	-0.98242200

Ph (2_A)

E(B3LYP/BS1) = -2335.694636 au

H(B3LYP/BS1) = -2335.228269 au

G(B3LYP/BS1) = -2335.329554 au

E(M06-2X/BS2//B3LYP/BS1) = -2335.568667 au

C	-0.84977900	0.28126700	1.83825200
C	-2.18893600	-0.23959900	1.28886300
C	-0.27480100	1.53015100	1.16519900
C	-2.83217300	0.41191000	0.29769000
H	-2.37727200	1.31967100	-0.08527500
C	0.10990300	1.46413300	-0.12872600
H	-0.04685300	0.52253100	-0.64990900
C	-4.12758900	0.10098800	-0.33227100
C	-4.64491500	-1.19932400	-0.48945800
C	-4.87691100	1.17439100	-0.85571700
C	-5.87329800	-1.40987900	-1.11715200
H	-4.07293300	-2.05474500	-0.14937400
C	-6.10828800	0.96541200	-1.47238800
H	-4.48493300	2.18478100	-0.76587900
C	-6.61474000	-0.33082000	-1.60302200
H	-6.24783800	-2.42350700	-1.23259000
H	-6.66970700	1.81256400	-1.85713200
H	-7.57190100	-0.49858800	-2.08900600
C	0.67114800	2.51493400	-0.99449700
C	1.48893200	3.56280200	-0.52989500
C	0.41103100	2.44127600	-2.37776600
C	1.99789800	4.51525700	-1.41320300
H	1.75966900	3.61478700	0.51851200
C	0.91019600	3.39920600	-3.25716500
H	-0.19841000	1.62544200	-2.75916400
C	1.70427700	4.44444700	-2.77677300
H	2.63362600	5.31056100	-1.03372100
H	0.68591000	3.32671900	-4.31786400
H	2.10092600	5.18924700	-3.46107000
C	-2.76221900	-1.42523000	2.03439800
H	-3.85462600	-1.37636400	2.05794300
H	-2.48154700	-2.37742100	1.57415200
H	-2.39564100	-1.43777300	3.06175300
C	-0.31348700	2.81107900	1.96677100
H	-1.14661800	2.79023700	2.67356300
H	0.60283200	2.97316800	2.54721600
H	-0.43739400	3.67247100	1.30526800

O	-1.08442200	0.43630300	3.19970000
H	4.09699400	-2.81357500	-2.29101900
C	-0.01002200	0.47905300	4.14641200
H	0.58050000	-0.43869800	4.10329200
H	0.64384900	1.34056800	4.00036300
H	-0.49943100	0.55529500	5.11932000
O	4.32531900	-2.10052000	-1.66670600
C	3.28159600	-1.83090100	-0.86555800
C	3.44096000	-0.82665100	0.09920600
C	2.04770900	-2.50287100	-0.93380100
C	2.37731600	-0.49358400	0.97518000
C	0.99510400	-2.16743400	-0.07744400
C	1.12735600	-1.14288000	0.89525100
O	0.12996100	-0.91883500	1.77103300
Cl	1.88986100	-3.76540400	-2.12490800
Cl	-0.49920100	-3.03530700	-0.19051700
C	4.69681400	-0.15257500	0.18493500
C	2.62449500	0.51540600	1.95561200
N	5.71998000	0.39629200	0.25453000
N	2.89820000	1.33504400	2.73447300

para-Me-Ph (TS_A)

E(B3LYP/BS1) = -2414.289627 au

H(B3LYP/BS1) = -2413.770975 au

G(B3LYP/BS1) = -2413.881977 au

E(M06-2X/BS2//B3LYP/BS1) = -2414.120353 au

C	-1.07154400	2.13094500	-0.82308600
C	-2.38223700	1.63040800	-0.28615800
C	-0.13868000	1.26240400	-1.55160500
C	-2.98863200	0.56221600	-0.86793400
H	-2.51118600	0.14856000	-1.75397000
C	0.09405600	-0.00364600	-1.03001300
H	-0.57741200	-0.30527400	-0.23372000
C	-4.24901200	-0.09048300	-0.51097500
C	-4.74629900	-0.18149100	0.80472300
C	-4.99448400	-0.71175000	-1.53518000
C	-5.94646500	-0.83625400	1.06981100
H	-4.17423400	0.22616500	1.63056200
C	-6.19783200	-1.35240500	-1.26437800
H	-4.62454400	-0.67396300	-2.55697100
C	-6.69970300	-1.42685000	0.04491500
H	-6.30218700	-0.89651300	2.09559000
H	-6.75664700	-1.80804200	-2.07842200
C	1.02591500	-1.04045700	-1.41105400
C	2.19261700	-0.85722800	-2.19518500
C	0.79164500	-2.34008500	-0.89238300
C	3.04796100	-1.91861400	-2.45434000
H	2.45304300	0.12198200	-2.57440900
C	1.64738200	-3.39692900	-1.16823800
H	-0.08940000	-2.51258600	-0.28027900
C	2.79410500	-3.20911400	-1.95566800
H	3.94218300	-1.74461900	-3.04688400

H	1.43271000	-4.38025000	-0.75885600
C	-2.97064600	2.45685700	0.83186700
H	-4.06126000	2.39568500	0.84588800
H	-2.59977300	2.12735600	1.81035900
H	-2.68648000	3.50578400	0.70845500
C	0.55007100	1.81349100	-2.77166500
H	-0.06340300	2.59859600	-3.21935300
H	1.53365100	2.24519200	-2.54794300
H	0.70056000	1.02158200	-3.51024600
O	-1.23280600	3.43782800	-1.28490100
H	-0.35166900	2.22315800	0.29992000
C	-0.20374000	4.40896200	-1.04373200
H	-0.58269700	5.34285700	-1.46213900
H	-0.03213900	4.52759700	0.02995200
H	0.73714400	4.14828300	-1.53525100
O	0.36559200	2.24586400	1.36841600
C	1.22741300	1.28416500	1.38954800
C	0.90715100	0.03112400	2.02906100
C	2.57169300	1.43307700	0.86076700
C	1.80722300	-1.02128900	2.06442800
C	3.47481100	0.40454100	0.88842700
C	3.14601800	-0.91703000	1.45678900
O	3.93632100	-1.86246500	1.45613800
Cl	2.98937500	2.99014400	0.21484900
Cl	5.08992700	0.57502700	0.28350300
C	-0.38282400	-0.08290800	2.63842900
C	1.49273500	-2.25238700	2.70922900
N	-1.42888900	-0.17930900	3.13776000
N	1.23757000	-3.25892700	3.23534200
C	-7.98819500	-2.15386400	0.34322700
H	-7.81209000	-3.23032100	0.47192200
H	-8.45026200	-1.78703700	1.26517000
H	-8.70964800	-2.04075900	-0.47289100
C	3.71662900	-4.35655700	-2.27390000
H	3.44065400	-4.81923200	-3.23110400
H	4.75497000	-4.02194000	-2.36347300
H	3.66556200	-5.13542600	-1.50721200

para-Me-Ph (TS_B)

E(B3LYP/BS1) = -2414.277013 au

H(B3LYP/BS1) = -2413.757561 au

G(B3LYP/BS1) = -2413.869674 au

E(M06-2X/BS2//B3LYP/BS1) = -2414.109757 au

C	0.05018200	-0.91591800	-2.05976600
C	1.38659400	-0.31597900	-2.01765600
C	-1.16462000	-0.00411500	-2.01690900
C	1.56326800	0.71214700	-1.11335200
H	0.65744100	1.04706400	-0.61319800
C	-1.93698500	0.15813900	-0.92706400
H	-1.63696000	-0.35072400	-0.01598700
C	2.72956700	1.49003800	-0.74929200
C	4.06962100	1.20090200	-1.10252000

C	2.50159800	2.63734300	0.05008400
C	5.10485500	2.03270100	-0.69534300
H	4.31185800	0.31657700	-1.67378000
C	3.54202400	3.46600500	0.44360800
H	1.48464200	2.87805000	0.34807300
C	4.86743600	3.18038500	0.07866400
H	6.12417800	1.78565300	-0.98060200
H	3.32900500	4.34517100	1.04601900
C	-3.14251800	0.99243400	-0.76701100
C	-4.12197800	1.14199400	-1.76444000
C	-3.36274600	1.63387600	0.46672400
C	-5.25385300	1.92599500	-1.54384600
H	-4.02164400	0.61343800	-2.70665900
C	-4.48951500	2.42287400	0.67699200
H	-2.63544400	1.51744000	1.26630000
C	-5.45536100	2.59059200	-0.32703000
H	-5.99958800	2.01356800	-2.33046800
H	-4.62671100	2.91138000	1.63890400
C	2.47020000	-0.90019800	-2.88833300
H	3.06151600	-0.09653300	-3.33763100
H	3.15758300	-1.53789900	-2.31952600
H	2.03969000	-1.50181500	-3.68853700
C	-1.36439800	0.71563800	-3.33881900
H	-0.39930300	1.03347400	-3.74681500
H	-1.83750900	0.07678800	-4.09472200
H	-1.99138100	1.60004400	-3.20732000
O	-0.03549600	-1.94983900	-2.95020500
H	0.12272900	-1.60753600	-0.78926900
C	-1.26793000	-2.68960400	-3.02540300
H	-2.08959800	-2.06185300	-3.37811300
H	-1.07636100	-3.48970800	-3.73988900
H	-1.51998900	-3.11636200	-2.05024700
O	-1.57700300	-3.38515900	0.70991900
C	-0.75303700	-2.55368000	1.04077900
C	0.54850200	-2.38883900	0.26565200
C	-0.97400100	-1.61267700	2.17058500
C	1.62899900	-1.68918500	0.90615800
C	0.00063400	-0.77089800	2.59125300
C	1.39888000	-0.78593200	2.01589800
O	2.27811900	-0.09141600	2.52158900
Cl	-2.54023200	-1.69325900	2.90530200
Cl	-0.24711400	0.34391300	3.88152500
C	0.90115700	-3.59323900	-0.46620600
C	2.97176700	-1.88595100	0.50612700
N	1.19295200	-4.54837900	-1.05839700
N	4.07939000	-2.06466200	0.18256900
C	-6.66584600	3.46516100	-0.10369900
H	-7.49183000	3.18185500	-0.76377000
H	-7.01757300	3.40523400	0.93180200
H	-6.43307300	4.51938300	-0.30503600
C	6.00515100	4.05833000	0.53281400

H	5.68158100	5.09509100	0.66853400
H	6.40090700	3.71139500	1.49686900
H	6.83348400	4.04225700	-0.18248900

para-Me-Ph (TS_D)

E(B3LYP/BS1) = -2414.272744 au

H(B3LYP/BS1) = -2413.756051 au

G(B3LYP/BS1) = -2413.873462 au

E(M06-2X/BS2//B3LYP/BS1) = -2414.095142 au

C	-0.73835500	0.85794300	2.39215000
C	-2.05903100	0.46729800	1.86993800
C	0.07186400	1.94189900	1.76319500
C	-2.56370400	1.06178600	0.72981300
H	-2.04288000	1.94953500	0.38102800
C	0.46627000	1.78173300	0.46509200
H	0.16226500	0.84957900	-0.00839800
C	-3.74116800	0.72659900	-0.04729500
C	-4.31553500	-0.56405100	-0.13058800
C	-4.32954800	1.75077000	-0.82806000
C	-5.43238000	-0.79606600	-0.92382900
H	-3.85786600	-1.39893700	0.38655900
C	-5.45392600	1.51222100	-1.60593700
H	-3.89279900	2.74605000	-0.80679300
C	-6.03501700	0.23447000	-1.66484200
H	-5.84196000	-1.80158900	-0.98057400
H	-5.88681700	2.32383900	-2.18538500
C	1.20207700	2.65685900	-0.44180100
C	1.95719900	3.79058000	-0.06840100
C	1.17993200	2.32342900	-1.81573000
C	2.62749700	4.54933000	-1.02341900
H	2.05455700	4.06999600	0.97203400
C	1.84425000	3.09136500	-2.76333500
H	0.62441100	1.44543200	-2.13598200
C	2.57888900	4.22681300	-2.38776500
H	3.20911500	5.40936600	-0.70019800
H	1.79958500	2.80402100	-3.81103400
C	-2.79905000	-0.60028400	2.64138500
H	-3.87756000	-0.51299400	2.49506700
H	-2.49206500	-1.60352300	2.32301900
H	-2.57865600	-0.51180100	3.70621700
C	0.36477600	3.15765400	2.61162000
H	-0.26521300	3.16116800	3.50333500
H	1.40974300	3.20135400	2.94305900
H	0.16747900	4.07232700	2.04240300
O	-0.70076700	0.80346800	3.78609600
H	-0.10412800	-0.31943400	1.98615100
C	0.54460200	0.48213600	4.41586900
H	0.36836100	0.58121500	5.48836700
H	0.83773300	-0.54611700	4.18290800
H	1.34608700	1.16485200	4.11717900
O	0.19389700	-1.52797700	1.79052300
C	0.95727000	-1.96848500	0.84267300

C	0.42644900	-2.94563900	-0.06530500
C	2.33716400	-1.57502700	0.67151200
C	1.19268800	-3.47051800	-1.10506300
C	3.10494800	-2.08524400	-0.34833300
C	2.57770900	-3.06035300	-1.31576600
O	3.26250200	-3.51457400	-2.24662400
Cl	2.99769100	-0.47009000	1.83570500
Cl	4.75811600	-1.63240400	-0.56146200
C	-0.93200500	-3.34489700	0.12431200
C	0.65422700	-4.42126600	-2.01782800
N	-2.03858400	-3.67268600	0.27273100
N	0.21089200	-5.19866000	-2.76247500
C	3.28047800	5.07730400	-3.41746200
H	2.60668100	5.84874600	-3.81417600
H	4.14687100	5.59175600	-2.98960600
H	3.62042600	4.47712700	-4.26782800
C	-7.27016000	-0.02215100	-2.49038100
H	-7.33607400	0.66696900	-3.33834300
H	-7.28967400	-1.04736200	-2.87399000
H	-8.17801900	0.11568800	-1.88741700

para-Me-Ph (2_D)

E(B3LYP/BS1) = -2414.298894 au

H(B3LYP/BS1) = -2413.775313 au

G(B3LYP/BS1) = -2413.89553 au

E(M06-2X/BS2//B3LYP/BS1) = -2414.109437 au

C	-2.69596600	1.50781400	2.11597700
C	-2.79124300	0.10601500	1.53151900
C	-2.47140900	2.35160000	0.85626400
C	-3.97055500	-0.24650600	0.91382600
H	-4.78409500	0.46774700	1.01184300
C	-1.17322500	2.42549700	0.38671600
H	-0.43223600	1.88563300	0.97388000
C	-4.33245300	-1.46200000	0.22276400
C	-3.41319300	-2.35515500	-0.38528400
C	-5.71533600	-1.75504000	0.09395900
C	-3.86336600	-3.48649900	-1.04869200
H	-2.35093500	-2.14266600	-0.38910400
C	-6.15179400	-2.89729800	-0.55584600
H	-6.44044200	-1.07127600	0.52703800
C	-5.23420500	-3.79340600	-1.13555500
H	-3.13950400	-4.14444000	-1.52196500
H	-7.21663700	-3.10162600	-0.62791200
C	-0.60335600	3.10521600	-0.74673800
C	-1.30439600	3.91178700	-1.68540300
C	0.80017000	2.95610300	-0.93407500
C	-0.63609100	4.51975800	-2.73329200
H	-2.37040700	4.06286400	-1.59781900
C	1.45540700	3.56888300	-1.98805800
H	1.35289600	2.32640600	-0.24325500
C	0.75492700	4.36807100	-2.90941300
H	-1.19613200	5.12805800	-3.43839800

H	2.52610400	3.42885600	-2.10851200
C	-1.59078400	-0.77614400	1.71440300
H	-1.86023800	-1.83249300	1.65984700
H	-0.80224700	-0.59389600	0.97384500
H	-1.14375000	-0.58457800	2.69664200
C	-3.67507900	2.98531700	0.21912000
H	-4.57624100	2.76478700	0.79236000
H	-3.55631400	4.07598200	0.20004700
H	-3.82258800	2.65287400	-0.81362100
O	-3.86250400	1.83575700	2.83437700
H	-1.81599500	1.57216200	2.76929100
C	-3.73325100	3.02410300	3.61430700
H	-4.67462600	3.14346800	4.15388600
H	-2.90891700	2.93236000	4.33430000
H	-3.56250000	3.90969800	2.98832300
O	1.49607700	0.12781500	0.62617000
C	2.51033100	-0.58051200	0.44762100
C	2.45648900	-1.85835300	-0.24018800
C	3.84455700	-0.17411900	0.91910100
C	3.59486100	-2.64768600	-0.43925600
C	4.95647900	-0.94288600	0.72701900
C	4.91185500	-2.24149100	0.02733400
O	5.92688100	-2.93814100	-0.15043400
Cl	3.91425100	1.35598600	1.74781600
Cl	6.52580900	-0.45323600	1.29425600
C	1.17953300	-2.27701400	-0.71037000
C	3.51531300	-3.89696500	-1.11739400
N	0.13358800	-2.61849700	-1.09472800
N	3.44186000	-4.91855700	-1.67311700
C	-5.70461900	-5.04750000	-1.82172600
H	-6.70158400	-4.91856300	-2.25455600
H	-5.01435100	-5.35464700	-2.61342500
H	-5.76638600	-5.87742400	-1.10431300
C	1.46593300	5.06098500	-4.03881700
H	0.85516700	5.07301300	-4.94759100
H	1.67220900	6.10787800	-3.77660700
H	2.42374000	4.58354900	-4.26437100

para-Me-Ph (2_A)

E(B3LYP/BS1) = -2414.331407 au

H(B3LYP/BS1) = -2413.806346 au

G(B3LYP/BS1) = -2413.917727 au

E(M06-2X/BS2//B3LYP/BS1) = -2414.184597 au

C	-0.61379900	-0.38697600	2.00150000
C	-2.00563000	-0.62935200	1.39676300
C	0.05335100	0.94995900	1.67329200
C	-2.62147600	0.32697700	0.66979800
H	-2.09676100	1.26729100	0.53470200
C	0.39381100	1.22003500	0.39292800
H	0.13644000	0.47725900	-0.35889600
C	-3.95937700	0.31940200	0.05616700
C	-4.64093300	-0.83126900	-0.38329900

C	-4.59265100	1.56182100	-0.15226000
C	-5.90183800	-0.73864400	-0.97157200
H	-4.17443200	-1.80562700	-0.30013400
C	-5.85543500	1.64752000	-0.72942900
H	-4.08139500	2.47254000	0.15129500
C	-6.54072200	0.49608500	-1.14563100
H	-6.39568400	-1.64693000	-1.30964300
H	-6.31502000	2.62370800	-0.86734100
C	1.02336800	2.42064100	-0.17831300
C	1.92654800	3.24949300	0.51320200
C	0.74598400	2.74140400	-1.52227300
C	2.49482600	4.36184500	-0.10572300
H	2.22151000	3.00512100	1.52731500
C	1.30730500	3.85968300	-2.13028900
H	0.07435400	2.10327600	-2.09194000
C	2.18896600	4.69815800	-1.43132500
H	3.19874300	4.97553900	0.45162900
H	1.06512900	4.08219300	-3.16700200
C	-2.65537800	-1.93477800	1.80255900
H	-3.72818300	-1.79690400	1.96939300
H	-2.53642000	-2.70994600	1.03939600
H	-2.21012100	-2.31093400	2.72430600
C	0.15580300	1.95342000	2.79917100
H	-0.64667800	1.79374800	3.52342200
H	1.10571100	1.88280200	3.34307500
H	0.07782000	2.97227900	2.41037900
O	-0.79926300	-0.60397000	3.36233600
H	3.94253400	-2.59582000	-3.04901100
C	0.29954200	-0.90880900	4.22954300
H	0.80422800	-1.82253400	3.90806200
H	1.02401300	-0.09490800	4.29100800
H	-0.15473300	-1.06577900	5.20983700
O	4.24819600	-2.09903300	-2.26773300
C	3.25157600	-1.97892000	-1.37509700
C	3.52130400	-1.29593700	-0.18131200
C	1.96171100	-2.50611500	-1.56723700
C	2.51222800	-1.13762700	0.80192700
C	0.96367000	-2.34165900	-0.60275400
C	1.20888900	-1.64205100	0.60748100
O	0.25792600	-1.59525400	1.55783800
Cl	1.66493500	-3.36852100	-3.05261600
Cl	-0.60348100	-3.02499500	-0.87879500
C	4.83303800	-0.77102600	0.02551400
C	2.87074200	-0.46323700	2.00902400
N	5.90176200	-0.34356500	0.19321500
N	3.23594400	0.08296100	2.96907800
C	2.78033900	5.92462300	-2.08395400
H	2.10199000	6.78404300	-1.99697900
H	3.72802200	6.20962500	-1.61584500
H	2.95998500	5.76286500	-3.15219500
C	-7.92174900	0.58610800	-1.74980000

H	-8.03783800	1.49446500	-2.35080800
H	-8.13690200	-0.27702100	-2.38802200
H	-8.69391400	0.61506400	-0.96920900

para-OMe-Ph (TS_A)

E(B3LYP/BS1) = -2564.705785 au

H(B3LYP/BS1) = -2564.175125 au

G(B3LYP/BS1) = -2564.287812 au

E(M06-2X/BS2//B3LYP/BS1) = -2564.543547 au

C	-0.93796200	2.19087300	-1.05205100
C	-2.26449600	1.77526200	-0.48478300
C	0.00554200	1.22860600	-1.63050600
C	-2.87014300	0.64185300	-0.93069400
H	-2.37919300	0.11314000	-1.74558900
C	0.20623800	0.03210900	-0.94774500
H	-0.49956700	-0.16631800	-0.14872300
C	-4.13686900	0.04608000	-0.51458300
C	-4.67933800	0.15616400	0.78706400
C	-4.84796000	-0.73604200	-1.44618700
C	-5.87820300	-0.45437800	1.11836200
H	-4.13535500	0.68927900	1.55817000
C	-6.05943900	-1.34427000	-1.13154800
H	-4.44406200	-0.86172900	-2.44771100
C	-6.58798200	-1.19977000	0.16046700
H	-6.28453200	-0.37761700	2.12212000
H	-6.57524300	-1.92749500	-1.88512900
C	1.14836100	-1.03619200	-1.14949500
C	2.35549900	-0.94786200	-1.88884900
C	0.89236600	-2.26643700	-0.47767700
C	3.24250800	-2.01062700	-1.96378400
H	2.62791900	-0.02468500	-2.38242200
C	1.75925000	-3.33516800	-0.55801800
H	-0.02092700	-2.36842100	0.10148400
C	2.95347400	-3.21757800	-1.29755500
H	4.16148900	-1.89330500	-2.52476100
H	1.55118400	-4.26968100	-0.04779300
C	-2.86960000	2.74784700	0.49884200
H	-3.96152700	2.70900500	0.48294600
H	-2.53762700	2.54195600	1.52416700
H	-2.56053800	3.76769100	0.25215900
C	0.74785000	1.61620100	-2.88195800
H	0.16307200	2.34578400	-3.44667900
H	1.72815900	2.06416200	-2.67556700
H	0.91489000	0.73763800	-3.51100700
O	-1.07928400	3.42107600	-1.70399100
H	-0.24829400	2.43935400	0.05734600
C	-0.07360800	4.42907800	-1.53167800
H	-0.41397400	5.28324100	-2.11981000
H	0.00933000	4.71608900	-0.47907200
H	0.90558200	4.10682700	-1.89609300
O	0.45194800	2.61503000	1.13701100
C	1.29965100	1.65435500	1.30469300

C	0.95041600	0.49824900	2.09084400
C	2.65151200	1.71035800	0.78109600
C	1.82718800	-0.56340300	2.25995900
C	3.53140200	0.67256100	0.94014500
C	3.16621500	-0.56778500	1.64914900
O	3.92936600	-1.53216800	1.75177300
Cl	3.10882100	3.16841100	-0.04759100
Cl	5.15685400	0.73843400	0.33861000
C	-0.34614600	0.48451700	2.69620500
C	1.47930800	-1.69963600	3.04587400
N	-1.39747200	0.46909500	3.19399600
N	1.19628900	-2.62859100	3.68805300
O	3.74595100	-4.30487300	-1.30765800
O	-7.75621500	-1.74646200	0.58406200
C	-8.52315600	-2.51979700	-0.33875600
H	-7.96500500	-3.39886700	-0.68128800
H	-9.40849800	-2.84260500	0.21017900
H	-8.82772200	-1.91901200	-1.20355900
C	4.99513600	-4.25251400	-2.00670500
H	5.45245200	-5.23080600	-1.85980500
H	4.83980100	-4.07506500	-3.07608500
H	5.64375600	-3.47519000	-1.58947600

para-OMe-Ph (TS_B)

E(B3LYP/BS1) = -2564.692252 au

H(B3LYP/BS1) = -2564.161079 au

G(B3LYP/BS1) = -2564.275806 au

E(M06-2X/BS2//B3LYP/BS1) = -2564.530866 au

C	0.10931400	-1.25753600	-2.00505300
C	1.44192600	-0.65480900	-1.95880700
C	-1.10514400	-0.34706300	-2.06707700
C	1.58720700	0.44796800	-1.13554700
H	0.66275000	0.82040900	-0.70010800
C	-1.89894900	-0.09272800	-1.00963300
H	-1.61269700	-0.52102700	-0.05368400
C	2.73487500	1.24985100	-0.79156300
C	4.08763600	0.94179600	-1.07558500
C	2.48265300	2.45645000	-0.08183700
C	5.12000600	1.79191900	-0.70318000
H	4.34875900	0.01745200	-1.56973900
C	3.49931400	3.31310400	0.28487700
H	1.45735700	2.71447400	0.16822600
C	4.83516400	2.99142000	-0.02687800
H	6.14109800	1.51438800	-0.93491100
H	3.29529800	4.23586300	0.81806300
C	-3.10764200	0.74499600	-0.93917600
C	-4.04958100	0.85374400	-1.98346500
C	-3.37931700	1.44212500	0.25041700
C	-5.18264000	1.64431800	-1.85161500
H	-3.91469300	0.28649600	-2.89788700
C	-4.50717700	2.24865800	0.39445100
H	-2.68538900	1.36419600	1.08347200

C	-5.41799100	2.35795100	-0.66551600
H	-5.90893900	1.71537600	-2.65545700
H	-4.66778600	2.77590400	1.32746300
C	2.55937200	-1.30184200	-2.73711400
H	3.15404900	-0.53439000	-3.24289200
H	3.23763600	-1.87173400	-2.09057400
H	2.16232800	-1.98239500	-3.48978900
C	-1.27618400	0.26119900	-3.44796000
H	-0.29942100	0.49835100	-3.88189900
H	-1.78198500	-0.41589900	-4.14748300
H	-1.86065000	1.18262200	-3.39413300
O	0.05151500	-2.34761600	-2.83395800
H	0.13240200	-1.86531800	-0.70147300
C	-1.17692100	-3.09346500	-2.89399000
H	-1.98683300	-2.49707000	-3.32091700
H	-0.96230700	-3.94518100	-3.53920000
H	-1.46380800	-3.44681600	-1.89939200
O	-1.63129900	-3.54448800	0.84681100
C	-0.81132900	-2.69987100	1.15677800
C	0.51667800	-2.58897700	0.42327700
C	-1.06444600	-1.69238100	2.22050300
C	1.57784700	-1.85031000	1.05351300
C	-0.10047200	-0.82931100	2.62260800
C	1.31487800	-0.87815000	2.09374900
O	2.17803300	-0.14927800	2.58052100
Cl	-2.65499900	-1.72427100	2.90651500
Cl	-0.38711000	0.36137400	3.83588100
C	0.89004400	-3.83527300	-0.22116900
C	2.93180400	-2.06434000	0.70523500
N	1.20085900	-4.82512800	-0.74281000
N	4.04987400	-2.25398300	0.42590800
O	5.76229500	3.88764300	0.36903800
O	-6.55307800	3.10821600	-0.63922900
C	-6.85225800	3.84457100	0.54517000
H	-7.79018600	4.36345300	0.34312100
H	-6.98179200	3.17882000	1.40669900
H	-6.06913900	4.57941800	0.76648400
C	7.14285100	3.62613300	0.09582500
H	7.32315500	3.55144300	-0.98193800
H	7.68763600	4.47927400	0.50024100
H	7.47505900	2.70822300	0.59240900

para-OMe-Ph (TS_D)

E(B3LYP/BS1) = -2564.688141 au

H(B3LYP/BS1) = -2564.159368 au

G(B3LYP/BS1) = -2564.278339 au

E(M06-2X/BS2//B3LYP/BS1) = -2564.517583 au

C	0.45131400	-0.50342900	2.63796400
C	1.82843500	-0.46265000	2.12190100
C	-0.56859500	-1.45330800	2.11235600
C	2.21707300	-1.29986700	1.09375800
H	1.52712900	-2.10243900	0.84603600

C	-0.89011900	-1.39183700	0.78432700
H	-0.36712300	-0.62872900	0.20994200
C	3.44437000	-1.32573700	0.32815800
C	4.29550700	-0.21647800	0.11589400
C	3.80279000	-2.54392200	-0.30851800
C	5.44998300	-0.31749900	-0.65222600
H	4.03291300	0.75483200	0.51677900
C	4.95373600	-2.66066500	-1.06259600
H	3.15801900	-3.41035800	-0.18659500
C	5.79710000	-1.54608900	-1.23857800
H	6.06479100	0.56238100	-0.79983700
H	5.22566400	-3.59956400	-1.53448900
C	-1.79147100	-2.18743000	-0.03771800
C	-2.77230600	-3.08716100	0.43166400
C	-1.69266600	-2.02855800	-1.44358500
C	-3.59202100	-3.79996100	-0.44035700
H	-2.92943100	-3.22525900	1.49260400
C	-2.49401500	-2.73581000	-2.32076100
H	-0.95866500	-1.33421600	-1.84451400
C	-3.45455800	-3.63637400	-1.82660200
H	-4.33614900	-4.47273900	-0.03063100
H	-2.40093600	-2.60763800	-3.39464800
C	2.76293400	0.53217000	2.77157200
H	3.79819200	0.18684800	2.72101000
H	2.70740300	1.51079600	2.28021200
H	2.49006500	0.67369900	3.81823700
C	-1.15777400	-2.44155900	3.09260800
H	-0.58383700	-2.44646600	4.02117800
H	-2.20123700	-2.21676600	3.34682300
H	-1.13825800	-3.45174600	2.66888900
O	0.41053500	-0.27092500	4.01620000
H	0.07980700	0.74380800	2.05877000
C	-0.73105900	0.40684200	4.55074500
H	-0.59386300	0.41090200	5.63374600
H	-0.77758200	1.43599900	4.18135100
H	-1.66685700	-0.10712200	4.30877300
O	0.03718200	1.92646900	1.71002200
C	-0.60713400	2.36802800	0.67536300
C	0.12715700	3.05865500	-0.34557600
C	-2.03795000	2.25554800	0.51334500
C	-0.50292100	3.57414200	-1.47761700
C	-2.67299500	2.75806200	-0.59775400
C	-1.94326000	3.44271000	-1.67640400
O	-2.50976100	3.88885100	-2.68719400
Cl	-2.92630600	1.50463600	1.80127100
Cl	-4.38381600	2.64021400	-0.80336400
C	1.53923900	3.18268800	-0.16746600
C	0.23234800	4.24130100	-2.49795100
N	2.69006000	3.28584400	-0.03004900
N	0.83641000	4.78654600	-3.33056000
O	-4.19556000	-4.28450600	-2.76045500

C	-5.19397200	-5.20631900	-2.32183100
H	-5.65147700	-5.60070000	-3.22979200
H	-4.75067000	-6.02857800	-1.74842900
H	-5.95735500	-4.70575100	-1.71512400
O	6.90022700	-1.75564500	-1.99471500
C	7.79576700	-0.66507400	-2.22299000
H	8.21008400	-0.28995500	-1.28052800
H	8.59887200	-1.06810400	-2.84054900
H	7.29668700	0.15122100	-2.75698900

para-OMe-Ph (2_D)

E(B3LYP/BS1) = -2564.718045 au

H(B3LYP/BS1) = -2564.18256 au

G(B3LYP/BS1) = -2564.306933 au

E(M06-2X/BS2//B3LYP/BS1) = -2564.535983 au

C	-1.27825000	0.82693700	2.65818600
C	-2.12742100	-0.23565600	1.97150400
C	-1.23527100	2.14472800	1.89685900
C	-3.11394500	0.13410000	1.10399400
H	-3.31832100	1.19986800	1.02352800
C	-0.31572600	2.20877000	0.87084500
H	0.27955700	1.30655300	0.73383700
C	-3.98932900	-0.69107600	0.29397700
C	-3.65028600	-1.98002500	-0.19464200
C	-5.24558500	-0.16042500	-0.08464600
C	-4.53301700	-2.69830500	-0.97691100
H	-2.67029900	-2.39985000	-0.00073400
C	-6.14687900	-0.87689100	-0.85733200
H	-5.51924500	0.83515900	0.25434200
C	-5.79635700	-2.16361200	-1.30729900
H	-4.26808700	-3.67707500	-1.36356000
H	-7.10425900	-0.43798400	-1.11080600
C	-0.00528500	3.24730600	-0.07026700
C	-0.54152500	4.56797100	-0.08218200
C	0.94183500	2.92334700	-1.08312800
C	-0.16305400	5.47874300	-1.04228700
H	-1.24571400	4.88299900	0.67474800
C	1.32547700	3.82627300	-2.05572400
H	1.37060900	1.92558500	-1.08910500
C	0.77040800	5.12276000	-2.04531300
H	-0.56598300	6.48605200	-1.04988100
H	2.04522200	3.53238700	-2.80977100
C	-1.76986200	-1.64121700	2.36196800
H	-2.60642300	-2.33298300	2.24214200
H	-0.92771100	-2.00752900	1.76094600
H	-1.45408100	-1.65597200	3.41078600
C	-2.18823600	3.22449300	2.31910200
H	-2.87240900	2.84775300	3.08160000
H	-1.64978000	4.07745500	2.75437200
H	-2.77081800	3.60957700	1.47471800
O	-1.72642200	0.95275000	4.00048300
H	-0.25217700	0.42170400	2.65847000

C	-0.73696500	1.46163400	4.89298200
H	-1.18888200	1.46855600	5.88712700
H	0.15433500	0.81947700	4.90292400
H	-0.43405000	2.48434200	4.63091600
O	1.18255400	-0.76664600	0.64597000
C	2.18145200	-1.42096300	0.27684700
C	2.06083900	-2.70710500	-0.38619500
C	3.55865100	-0.94385800	0.48164100
C	3.17691500	-3.44144200	-0.80120100
C	4.65002200	-1.65850900	0.07769000
C	4.53716000	-2.96646000	-0.59649400
O	5.53291200	-3.61570000	-0.96301500
Cl	3.70875800	0.59721000	1.27898200
Cl	6.27240600	-1.08257900	0.32510500
C	0.73811300	-3.19165200	-0.59435700
C	3.03083900	-4.69995000	-1.45067500
N	-0.34648000	-3.58542700	-0.75889600
N	2.90342700	-5.72897500	-1.98233800
O	-6.58328600	-2.95139300	-2.06750700
C	-7.87473000	-2.47479900	-2.46038400
H	-7.78977200	-1.56682700	-3.06690500
H	-8.31271100	-3.27498000	-3.05686900
H	-8.50413600	-2.28010700	-1.58551300
O	1.06221800	6.08600500	-2.92951700
C	2.00366000	5.82132100	-3.98076000
H	2.98625000	5.57340800	-3.56774300
H	1.64932700	5.00955200	-4.62344900
H	2.06543800	6.74619400	-4.55307500

para-OMe-Ph (2_A)

E(B3LYP/BS1) = -2564.744513 au

H(B3LYP/BS1) = -2564.207454 au

G(B3LYP/BS1) = -2564.321363 au

E(M06-2X/BS2//B3LYP/BS1) = -2564.604151 au

C	-0.48888000	-0.67363600	2.07044000
C	-1.91198400	-0.70054500	1.49861900
C	0.33073400	0.59230400	1.82602900
C	-2.43015200	0.38340800	0.88039500
H	-1.79039300	1.25625000	0.80049500
C	0.65987100	0.92769200	0.55713400
H	0.28236600	0.28789500	-0.23768400
C	-3.77006800	0.61215900	0.32289100
C	-4.68539700	-0.38439100	-0.06196300
C	-4.16759000	1.95432700	0.12091200
C	-5.93605600	-0.06977100	-0.59689300
H	-4.42324500	-1.43079700	0.02538900
C	-5.40868900	2.28346200	-0.39944800
H	-3.48044500	2.75344900	0.38845400
C	-6.31066300	1.26950500	-0.76185700
H	-6.60220400	-0.87465000	-0.88518000
H	-5.70139000	3.31946800	-0.54087100
C	1.42000300	2.07791100	0.05085200

C	2.42268700	2.75311700	0.76844000
C	1.16513100	2.51551300	-1.26824300
C	3.11933600	3.83081100	0.21944100
H	2.70002700	2.41774000	1.76092300
C	1.83971500	3.59127500	-1.82272100
H	0.41316600	2.00070100	-1.86136800
C	2.82363400	4.26481600	-1.07925600
H	3.89186400	4.31310000	0.80678700
H	1.62822000	3.92571500	-2.83377500
C	-2.69956600	-1.95347900	1.81674300
H	-3.70218700	-1.69874300	2.17789900
H	-2.81994500	-2.59766800	0.94020000
H	-2.19882500	-2.53854700	2.58813300
C	0.59924400	1.47536800	3.02324100
H	-0.17981200	1.34015000	3.77738400
H	1.56132800	1.25855700	3.50391500
H	0.61447500	2.52718000	2.72376300
O	-0.66177000	-0.98685700	3.41333000
H	3.57124000	-2.91725000	-3.36524100
C	0.42049200	-1.48315700	4.21057000
H	0.79805300	-2.42465500	3.80580800
H	1.24105900	-0.76877800	4.29593900
H	-0.01574000	-1.65525300	5.19654600
O	3.96365500	-2.53098300	-2.56080300
C	3.02767500	-2.39233300	-1.60676100
C	3.42401400	-1.85237300	-0.37556800
C	1.68185100	-2.76786900	-1.77008900
C	2.48321200	-1.67769800	0.67062800
C	0.75177100	-2.58500700	-0.74320000
C	1.12407000	-2.01959200	0.50438800
O	0.22666400	-1.94431400	1.50090900
Cl	1.22788300	-3.47072800	-3.29954400
Cl	-0.88969900	-3.08146400	-0.98444900
C	4.79325100	-1.48943000	-0.19587300
C	2.96574400	-1.16170700	1.91212400
N	5.90873000	-1.19378400	-0.04958500
N	3.42930600	-0.75370500	2.89813300
O	3.43438800	5.30602600	-1.70824000
O	-7.50464400	1.68706800	-1.26685000
C	-8.45584100	0.70021500	-1.65970200
H	-8.75295000	0.07212700	-0.81135800
H	-9.32350300	1.25183200	-2.02421300
H	-8.06382600	0.06502500	-2.46306800
C	4.45082500	6.01964600	-1.00689800
H	4.79053400	6.80001600	-1.68914600
H	4.05670200	6.47994700	-0.09306200
H	5.29344800	5.36611400	-0.75164400

para-NH_2-Ph (TS_A)

E(B3LYP/BS1) = -2446.379242 au

H(B3LYP/BS1) = -2445.883208 au

G(B3LYP/BS1) = -2445.989909 au

E(M06-2X/BS2//B3LYP/BS1) = -2446.233806 au

C	-1.04933200	2.12124800	-0.83055300
C	-2.36660900	1.63365700	-0.30227600
C	-0.12002900	1.24445000	-1.54758200
C	-2.97996700	0.56402100	-0.88029200
H	-2.50070100	0.15265000	-1.76733100
C	0.09232900	-0.03809000	-1.03758600
H	-0.59574400	-0.33607900	-0.25403300
C	-4.23077200	-0.09304100	-0.52651500
C	-4.77080800	-0.14214500	0.77892400
C	-4.94205200	-0.77806800	-1.53864300
C	-5.95937000	-0.80366500	1.04794500
H	-4.23230900	0.30970900	1.60408500
C	-6.13625800	-1.43147400	-1.28426100
H	-4.54539200	-0.78044300	-2.55120600
C	-6.67592000	-1.45264900	0.02013700
H	-6.34132500	-0.83560300	2.06527500
H	-6.66126000	-1.94054200	-2.08866400
C	1.02271500	-1.06451100	-1.38847900
C	2.19409300	-0.90605100	-2.18730100
C	0.80311200	-2.36196800	-0.83290400
C	3.06065100	-1.95109900	-2.41213900
H	2.44357100	0.05987000	-2.60505200
C	1.65432100	-3.41753500	-1.06159400
H	-0.07941000	-2.52244100	-0.22000000
C	2.81613400	-3.23662600	-1.85556700
H	3.95368800	-1.79598000	-3.01087600
H	1.45024300	-4.39153900	-0.62674000
C	-2.95473500	2.46716200	0.81063700
H	-4.04725400	2.43562900	0.80166800
H	-2.61361900	2.12412000	1.79555600
H	-2.64215400	3.50971800	0.70015400
C	0.60035900	1.79754100	-2.74809600
H	0.01699700	2.61008500	-3.18631400
H	1.59376400	2.19518400	-2.50301700
H	0.73633500	1.01737300	-3.50218400
O	-1.20419900	3.42659000	-1.32665700
H	-0.35136100	2.23523200	0.28178200
C	-0.20001800	4.40566300	-1.03225500
H	-0.54872400	5.33075600	-1.49570400
H	-0.10106000	4.54904700	0.04795700
H	0.77547100	4.13927600	-1.44951000
O	0.36792500	2.29246300	1.38437300
C	1.22178900	1.32065400	1.41510300
C	0.89074700	0.07025000	2.04136500
C	2.55987200	1.44370600	0.87145400
C	1.76553600	-1.01234600	2.02894200
C	3.43331300	0.38721000	0.85009600
C	3.07838000	-0.94131800	1.37659500
O	3.83314000	-1.91882600	1.30373200
Cl	3.01432200	3.00704000	0.25592700

Cl	5.04271500	0.53314000	0.21247700
C	-0.38673200	-0.02673600	2.67736900
C	1.43101600	-2.24566200	2.65724200
N	-1.42215100	-0.11133400	3.20185600
N	1.15968500	-3.25574700	3.16982200
N	-7.83556800	-2.15130500	0.29666500
H	-8.32889400	-1.89404500	1.14231300
H	-8.45821300	-2.32414100	-0.48250800
N	3.65675900	-4.26816900	-2.10544100
H	4.54980800	-4.10409800	-2.54845100
H	3.56132500	-5.13821200	-1.60055100

para-NH_2-Ph (TS_B)

E(B3LYP/BS1) = -2446.363605 au

H(B3LYP/BS1) = -2445.866991 au

G(B3LYP/BS1) = -2445.975649 au

E(M06-2X/BS2//B3LYP/BS1) = -2446.219545 au

C	0.10274100	-0.85805400	-2.07377500
C	1.43686400	-0.27609500	-1.99083900
C	-1.10489700	0.06373900	-2.03609900
C	1.60187500	0.77144200	-1.09064400
H	0.68202300	1.11607300	-0.62420200
C	-1.87826500	0.23315600	-0.94540600
H	-1.57395400	-0.27889300	-0.03679800
C	2.75016800	1.52450400	-0.69069600
C	4.10343000	1.27213900	-1.05756300
C	2.52202700	2.63230300	0.17744500
C	5.13181900	2.07338300	-0.61185500
H	4.35271800	0.42820400	-1.68375300
C	3.54039100	3.44288900	0.62427600
H	1.50398400	2.84589400	0.49152900
C	4.87935900	3.18337100	0.23554300
H	6.15474900	1.85430400	-0.90511000
H	3.32718700	4.28176700	1.28070500
C	-3.07870500	1.06486200	-0.77462900
C	-4.02830100	1.30274100	-1.78785900
C	-3.33984800	1.62921900	0.49073100
C	-5.15528300	2.08431600	-1.56086800
H	-3.90643200	0.84420400	-2.76321600
C	-4.45576000	2.42040000	0.72589400
H	-2.64054000	1.45573700	1.30494800
C	-5.38767600	2.66844100	-0.30119300
H	-5.87430900	2.23818200	-2.36192600
H	-4.61941900	2.84829300	1.71200100
C	2.54882800	-0.88007700	-2.81015100
H	3.09757600	-0.08884900	-3.33284300
H	3.26940400	-1.42500400	-2.18863100
H	2.15237000	-1.57004500	-3.55383900
C	-1.30079800	0.78479900	-3.35778900
H	-0.33190600	1.02562800	-3.80720400
H	-1.85298100	0.18270100	-4.09050700
H	-1.85271300	1.71655100	-3.21072500

O	0.01728200	-1.86274300	-3.01238500
H	0.13435800	-1.58879700	-0.84946700
C	-1.21089700	-2.60309900	-3.09382500
H	-2.03936600	-1.97208200	-3.42623900
H	-1.02517300	-3.38693900	-3.82849800
H	-1.45857700	-3.05507200	-2.12850200
O	-1.62144700	-3.41831500	0.54631700
C	-0.79961900	-2.60462000	0.93236100
C	0.52447100	-2.42312100	0.21886100
C	-1.05448000	-1.70029900	2.08459200
C	1.58241300	-1.72833200	0.90665200
C	-0.09620800	-0.86764700	2.55959400
C	1.31402900	-0.84544200	2.01855200
O	2.16797900	-0.13658100	2.55408000
Cl	-2.64088900	-1.81127000	2.77566800
Cl	-0.38948200	0.20193800	3.88211400
C	0.90640700	-3.59883000	-0.53922700
C	2.93613300	-1.89413600	0.53467700
N	1.22513500	-4.53189900	-1.15338700
N	4.05584100	-2.04468800	0.23706600
N	-6.54124800	3.40449200	-0.05585000
N	5.89313800	3.98948900	0.64237300
H	-6.48357900	4.05893000	0.71533600
H	-6.97000400	3.82629300	-0.87103900
H	6.85304200	3.71085300	0.49516500
H	5.73599100	4.67836300	1.36447600

para-NH_2-Ph (TS_D)

E(B3LYP/BS1) = -2446.358995 au

H(B3LYP/BS1) = -2445.864849 au

G(B3LYP/BS1) = -2445.977134 au

E(M06-2X/BS2//B3LYP/BS1) = -2446.207808 au

C	-0.79968200	0.92873000	2.39102500
C	-2.10899800	0.52003000	1.86653300
C	0.06180300	1.93429800	1.71569500
C	-2.60743400	1.07854800	0.70344800
H	-2.07306400	1.95004700	0.33313200
C	0.44239600	1.70426500	0.42007800
H	0.07354500	0.77621100	-0.01456600
C	-3.77235600	0.73736100	-0.07502900
C	-4.42562400	-0.52347100	-0.07821800
C	-4.29229100	1.72319700	-0.95666400
C	-5.52990600	-0.76591200	-0.87418700
H	-4.03312400	-1.33917800	0.51577200
C	-5.40171700	1.49592000	-1.74661500
H	-3.80292700	2.69300400	-1.00222300
C	-6.05397100	0.24087400	-1.71851900
H	-5.99823100	-1.74681300	-0.86405600
H	-5.77824000	2.27872900	-2.39990800
C	1.23801200	2.47400400	-0.52120100
C	1.97629900	3.64980900	-0.24074500
C	1.30019500	1.99761700	-1.85480700

C	2.70747800	4.30178700	-1.22193400
H	1.99871900	4.05959700	0.75971300
C	2.02227200	2.64357000	-2.84291500
H	0.75344000	1.09390800	-2.11341600
C	2.74503000	3.81858300	-2.54678000
H	3.26796400	5.19791500	-0.96703100
H	2.03907700	2.24432000	-3.85394600
C	-2.85650100	-0.52683600	2.66184100
H	-3.93704700	-0.38589500	2.57671600
H	-2.61990500	-1.53898500	2.31193500
H	-2.57740200	-0.46803200	3.71470600
C	0.45264700	3.15851200	2.51302200
H	-0.10625500	3.19983000	3.44950200
H	1.52205500	3.18136700	2.75811700
H	0.23150300	4.06833200	1.94332700
O	-0.79039200	0.96354700	3.79242100
H	-0.14948300	-0.33711600	2.04609600
C	0.41501200	0.58421400	4.46193700
H	0.23416100	0.75912700	5.52462700
H	0.63643500	-0.47507700	4.29670000
H	1.27221300	1.18517000	4.14046600
O	0.16713300	-1.48388900	1.90411800
C	0.92843000	-1.88624400	0.92956800
C	0.38713400	-2.78971200	-0.04196400
C	2.31827600	-1.51713400	0.80467200
C	1.15711900	-3.26949200	-1.10195200
C	3.08979900	-1.98029700	-0.23506500
C	2.55426200	-2.88046000	-1.26829700
O	3.24206100	-3.29329000	-2.21615300
Cl	2.98502900	-0.50235800	2.04448600
Cl	4.75596900	-1.55443200	-0.39725300
C	-0.98006900	-3.17656800	0.10745800
C	0.61177200	-4.15261700	-2.07607000
N	-2.09200500	-3.49977000	0.22127900
N	0.16258200	-4.87446100	-2.87156100
N	3.51805400	4.44007900	-3.50892400
N	-7.18422700	0.01685200	-2.46412100
H	-7.46286800	-0.94173700	-2.62754700
H	-7.37340200	0.63940900	-3.23865000
H	3.27498900	4.25528400	-4.47409300
H	3.75332000	5.41073000	-3.34401500

para-NH_2-Ph (2_D)

E(B3LYP/BS1) = -2446.396866 au

H(B3LYP/BS1) = -2445.89612 au

G(B3LYP/BS1) = -2446.015414 au

E(M06-2X/BS2//B3LYP/BS1) = -2446.234186 au

C	-1.75877900	0.85301600	2.25297200
C	-2.38855000	-0.41319900	1.68628100
C	-1.89491700	2.08195000	1.36555300
C	-3.27338900	-0.34380100	0.65352800
H	-3.57502200	0.65331200	0.33762900

C	-0.89346000	2.28705400	0.44962200
H	-0.10720000	1.53210300	0.45383400
C	-3.92677500	-1.40856900	-0.08289700
C	-3.39086300	-2.70938600	-0.26733100
C	-5.16585500	-1.12683700	-0.71535500
C	-4.06539200	-3.67062200	-0.99433000
H	-2.40953400	-2.95448700	0.12158800
C	-5.85706600	-2.08053800	-1.43362600
H	-5.58875300	-0.13013800	-0.61825700
C	-5.32337600	-3.38570200	-1.58315100
H	-3.62490300	-4.65427800	-1.13298900
H	-6.81120900	-1.83760000	-1.89321900
C	-0.69896400	3.30881500	-0.54397100
C	-1.48556200	4.48465900	-0.71129300
C	0.39688400	3.13939400	-1.44103800
C	-1.21076900	5.40221800	-1.70031800
H	-2.31284300	4.68726700	-0.04546500
C	0.68104600	4.04266500	-2.43756800
H	1.02292200	2.25850000	-1.33159200
C	-0.12387400	5.20357000	-2.59606400
H	-1.82347000	6.29333000	-1.80241600
H	1.51997300	3.87831900	-3.10753800
C	-1.92427200	-1.67024300	2.37007000
H	-2.65709800	-2.47742200	2.29845200
H	-0.97917700	-2.02165500	1.93639700
H	-1.74220300	-1.46163700	3.42932400
C	-3.10920600	2.94465100	1.57768800
H	-3.80176400	2.45902900	2.26781700
H	-2.83752800	3.91238800	2.02122200
H	-3.63306200	3.15574200	0.63875800
O	-2.29065900	1.05410900	3.56263200
H	-0.68296800	0.62703200	2.33903400
C	-1.44937800	1.83046000	4.40918200
H	-1.94376200	1.87999700	5.38219000
H	-0.46250100	1.36125200	4.52779800
H	-1.30971500	2.85146900	4.02803800
O	1.08638800	-0.54907300	0.87028300
C	2.18372100	-0.99376000	0.47300000
C	2.31858700	-2.31546900	-0.11478100
C	3.43150800	-0.21657900	0.56462300
C	3.54585300	-2.80941800	-0.57123100
C	4.63042700	-0.69789100	0.12278700
C	4.77449600	-2.03481200	-0.48478700
O	5.86752100	-2.46756000	-0.89208000
Cl	3.28153400	1.36463700	1.27907500
Cl	6.09616000	0.23192200	0.23890600
C	1.13100400	-3.09569500	-0.20521400
C	3.64846700	-4.10617800	-1.15008600
N	0.15978800	-3.73637300	-0.27474500
N	3.72423500	-5.16820200	-1.62369300
N	-6.00833500	-4.34701500	-2.26192600

H	-6.81207400	-4.09688200	-2.82089600
H	-5.55087100	-5.21373700	-2.50815700
N	0.13815900	6.10125700	-3.57059300
H	-0.42404900	6.93281700	-3.68482700
H	0.91381700	5.97777800	-4.20597200

para-NH_2-Ph (2_A)

E(B3LYP/BS1) = -2446.412822 au

H(B3LYP/BS1) = -2445.910273 au

G(B3LYP/BS1) = -2446.017046 au

E(M06-2X/BS2//B3LYP/BS1) = -2446.291813 au

C	-0.60771800	-0.37942200	2.05337100
C	-1.99933900	-0.56062600	1.44401400
C	0.12206700	0.93036700	1.76578500
C	-2.56941100	0.40635100	0.69202100
H	-1.96167700	1.27889700	0.47513500
C	0.48216300	1.22228700	0.49311500
H	0.19139600	0.51056900	-0.27659600
C	-3.90016200	0.47538200	0.07453600
C	-5.04886100	-0.22138900	0.50422400
C	-4.06616700	1.34797100	-1.02290100
C	-6.27294600	-0.07785800	-0.13941100
H	-5.00281000	-0.86607700	1.37316600
C	-5.27995500	1.49097100	-1.68035800
H	-3.20972700	1.91950200	-1.37391200
C	-6.41320700	0.77302600	-1.25172100
H	-7.13946800	-0.62359400	0.22685300
H	-5.36247700	2.16740400	-2.52791300
C	1.17214600	2.39487400	-0.05414200
C	2.05928400	3.22210900	0.66543100
C	0.97554000	2.70689000	-1.41652000
C	2.68507400	4.31025500	0.06927600
H	2.29481800	2.99709000	1.69891700
C	1.58478800	3.79831800	-2.01867000
H	0.31560300	2.07949200	-2.01165300
C	2.45293000	4.62884600	-1.28256800
H	3.37276600	4.91981100	0.65062600
H	1.40079800	4.01297500	-3.06867600
C	-2.68351400	-1.84816500	1.84602100
H	-3.31620800	-1.70888300	2.73158200
H	-3.31825500	-2.22337500	1.03796500
H	-1.94895300	-2.61669600	2.08935300
C	0.27273100	1.89727100	2.91860400
H	-0.50647600	1.72575200	3.66499300
H	1.24024200	1.80544100	3.42857900
H	0.19031400	2.92841500	2.56251600
O	-0.80543400	-0.63959500	3.40406700
H	3.57758800	-2.65229200	-3.25844400
C	0.29454400	-0.98305500	4.25677600
H	0.71435900	-1.95023600	3.97125400
H	1.08446000	-0.23017400	4.24940500
H	-0.13617300	-1.04914700	5.25795400

O	3.95292900	-2.19247900	-2.48506700
C	3.02067600	-2.06056800	-1.52596000
C	3.39649800	-1.43087700	-0.33104000
C	1.69933900	-2.52836700	-1.65092000
C	2.45667100	-1.25861800	0.71563800
C	0.77098200	-2.35475000	-0.62095900
C	1.12157000	-1.69653900	0.58667200
O	0.24528400	-1.61948600	1.59828000
Cl	1.27416000	-3.33490400	-3.13729400
Cl	-0.83447800	-2.97966300	-0.80047000
C	4.74240400	-0.97618900	-0.18838700
C	2.90502300	-0.64874600	1.92729800
N	5.83885800	-0.60582000	-0.07091100
N	3.33221200	-0.16437100	2.89502600
N	3.11939300	5.68442500	-1.89347600
N	-7.65091700	0.95800100	-1.86084600
H	-8.30565500	0.19275400	-1.74956700
H	-7.61604300	1.27691000	-2.82195500
H	3.43871700	6.41740400	-1.27136800
H	2.67032800	6.06405000	-2.71835800

para-NMe_2-Ph (TS_A)

E(B3LYP/BS1) = -2603.606008 au

H(B3LYP/BS1) = -2602.990086 au

G(B3LYP/BS1) = -2603.112138 au

E(M06-2X/BS2//B3LYP/BS1) = -2603.411289 au

C	0.77455600	-2.39274800	-1.16329600
C	2.12361700	-1.97893000	-0.66109500
C	-0.19151900	-1.42787400	-1.70124900
C	2.69714200	-0.82318100	-1.10402200
H	2.16500000	-0.29239600	-1.89214400
C	-0.36997700	-0.22835500	-1.01110000
H	0.35705200	-0.03971400	-0.22876400
C	3.95541600	-0.20452200	-0.72534500
C	4.58825300	-0.35769300	0.53005500
C	4.58269300	0.67032500	-1.64281200
C	5.77454300	0.28786600	0.83576300
H	4.11924600	-0.95745100	1.30152200
C	5.77400500	1.31344600	-1.36054000
H	4.11542400	0.83964800	-2.61028100
C	6.41888500	1.13371100	-0.10664900
H	6.20078600	0.14723600	1.82156700
H	6.20491800	1.96706100	-2.10907100
C	-1.31830700	0.82979200	-1.16142700
C	-2.52796800	0.78561800	-1.91368700
C	-1.08037100	2.03089900	-0.42901200
C	-3.41332600	1.83905800	-1.92890400
H	-2.79631000	-0.10616200	-2.46370400
C	-1.94847100	3.09683000	-0.44355800
H	-0.16781400	2.11100400	0.15501500
C	-3.16060300	3.03646700	-1.19154900
H	-4.32792200	1.73771400	-2.49911000

H	-1.70428700	3.97868200	0.13432000
C	2.78540500	-2.96259800	0.27363000
H	3.87463700	-2.92754400	0.18750300
H	2.52197700	-2.76532000	1.32052900
H	2.45693200	-3.97916600	0.03849600
C	-0.98331200	-1.81638900	-2.92160600
H	-0.43905400	-2.57326000	-3.49024600
H	-1.96962400	-2.23046500	-2.67476400
H	-1.14489500	-0.94545900	-3.56299500
O	0.88238600	-3.62179100	-1.83907800
H	0.15386400	-2.65315700	-0.03719600
C	-0.10246500	-4.63274600	-1.59425400
H	0.18251400	-5.47820100	-2.22391100
H	-0.09527200	-4.93774000	-0.54322600
H	-1.11093800	-4.30580100	-1.86460200
O	-0.49593600	-2.87668800	1.09873600
C	-1.33157700	-1.91718200	1.33677500
C	-0.93760800	-0.77141200	2.10675300
C	-2.70719400	-1.95262700	0.88237700
C	-1.79640800	0.30585800	2.31805200
C	-3.56575100	-0.90206700	1.08351100
C	-3.15760200	0.33152600	1.77456400
O	-3.90840500	1.30662700	1.91316700
Cl	-3.22628400	-3.40385200	0.07144300
Cl	-5.21845600	-0.94648100	0.54721100
C	0.38564700	-0.76955300	2.64914500
C	-1.39280200	1.43734700	3.08194500
N	1.45781200	-0.76315800	3.10221900
N	-1.06407600	2.36594300	3.70388600
N	-4.03940700	4.07201000	-1.20166900
N	7.60353900	1.76011500	0.18553500
C	8.20769700	1.61029000	1.50338100
H	8.42884700	0.55873300	1.72462700
H	9.14553000	2.16520500	1.53040500
H	7.55636200	1.99799100	2.29850400
C	8.21108800	2.66738000	-0.77930700
H	7.56473300	3.52922500	-0.99463400
H	9.15199700	3.04025500	-0.37449600
H	8.42794500	2.15683400	-1.72585300
C	-5.29304200	3.97774800	-1.94806500
H	-5.92957400	3.17168400	-1.56264300
H	-5.83354700	4.91853000	-1.85219800
H	-5.10606800	3.79814600	-3.01248500
C	-3.79406900	5.25369300	-0.37649500
H	-2.86189500	5.75202700	-0.66589400
H	-4.61362000	5.95811500	-0.51208700
H	-3.73524700	4.98999000	0.68642600

para-NMe_2-Ph (TS_B)

E(B3LYP/BS1) = -2603.589351 au

H(B3LYP/BS1) = -2602.972915 au

G(B3LYP/BS1) = -2603.095936 au

E(M06-2X/BS2//B3LYP/BS1) = -2603.396663 au

C	-0.07649400	1.50740900	-1.98640100
C	-1.41690000	0.93534500	-1.99499600
C	1.12189900	0.57479000	-2.01985100
C	-1.61062800	-0.20804900	-1.22524200
H	-0.70416300	-0.61375000	-0.78229600
C	1.85367800	0.26505700	-0.93034300
H	1.51839700	0.66731400	0.02185900
C	-2.77289200	-0.98644500	-0.93644600
C	-4.11592000	-0.68937600	-1.30528400
C	-2.57915100	-2.18236900	-0.18574000
C	-5.16152400	-1.52149200	-0.97205400
H	-4.34707100	0.21541600	-1.84824200
C	-3.61173700	-3.02613400	0.15056400
H	-1.57151300	-2.44097400	0.12871000
C	-4.95066800	-2.72558900	-0.23653600
H	-6.16209000	-1.24038700	-1.27509500
H	-3.39449500	-3.92078500	0.71994700
C	3.03741600	-0.59600900	-0.81594000
C	4.01173400	-0.75380200	-1.82068100
C	3.26842700	-1.28054500	0.39392200
C	5.12273100	-1.56951600	-1.64726100
H	3.92887000	-0.19683800	-2.74784600
C	4.36543500	-2.10846400	0.58156500
H	2.55972700	-1.16751100	1.21100800
C	5.32436400	-2.29400000	-0.44627000
H	5.84671100	-1.63079100	-2.45074700
H	4.48089100	-2.60805400	1.53577000
C	-2.50761300	1.64125000	-2.75955500
H	-3.04166800	0.92387100	-3.39273700
H	-3.24468300	2.10355500	-2.09225800
H	-2.09295300	2.41910500	-3.39921300
C	1.35678800	0.01118500	-3.41005200
H	0.40280100	-0.14238200	-3.92494400
H	1.95886100	0.67571500	-4.04277700
H	1.87489400	-0.94962800	-3.35298300
O	0.04009300	2.60450200	-2.81379500
H	-0.12826500	2.10644600	-0.69577000
C	1.27446200	3.33754500	-2.78343300
H	2.10813100	2.73777600	-3.15810400
H	1.11468600	4.19633200	-3.43600400
H	1.49883000	3.68340100	-1.76984800
O	1.62750800	3.75533900	0.91208200
C	0.78257200	2.92340600	1.19873800
C	-0.52825900	2.83925900	0.44631600
C	0.99662600	1.90480000	2.25990400
C	-1.61288300	2.09848200	1.04006100
C	0.01345400	1.04928300	2.63259800
C	-1.38483100	1.10733300	2.06502200
O	-2.26232100	0.36615100	2.51296200
Cl	2.57038400	1.91474000	2.98882100

Cl	0.25980600	-0.15065400	3.84939600
C	-0.87604200	4.09173500	-0.19591900
C	-2.95454800	2.32129900	0.65503700
N	-1.16898200	5.08772700	-0.71731400
N	-4.06453900	2.51815700	0.34768200
N	-5.98416500	-3.54867200	0.08577100
N	6.40592600	-3.13584000	-0.28195100
C	6.67879300	-3.71348400	1.02660900
H	5.83470900	-4.32110800	1.37332600
H	7.54915100	-4.36675500	0.95247900
H	6.88528300	-2.94873900	1.79058100
C	7.45655400	-3.16704000	-1.28951500
H	8.19781400	-3.91606300	-1.00763600
H	7.05367100	-3.44913300	-2.26922500
H	7.96808800	-2.19842700	-1.39696500
C	-7.35118400	-3.21362500	-0.30887700
H	-8.02189000	-4.00090100	0.03300200
H	-7.67572800	-2.26645800	0.13839400
H	-7.44217800	-3.13425400	-1.39846600
C	-5.74571300	-4.76972000	0.85281400
H	-6.69233500	-5.28899100	0.99695400
H	-5.06116800	-5.44362600	0.32441200
H	-5.32214500	-4.54548800	1.83918700

para-NMe_2-Ph (TS_D)

E(B3LYP/BS1) = -2603.585108 au

H(B3LYP/BS1) = -2602.971353 au

G(B3LYP/BS1) = -2603.099752 au

E(M06-2X/BS2//B3LYP/BS1) = -2603.385776 au

C	0.45303300	0.76827500	2.77754600
C	1.81993200	0.68137800	2.24600300
C	-0.55557300	-0.30641700	2.60176600
C	2.24616800	-0.45120600	1.57757700
H	1.58484000	-1.31201200	1.64184100
C	-0.86257800	-0.71781900	1.33057500
H	-0.32031300	-0.20909500	0.53466500
C	3.46545100	-0.70946100	0.85422800
C	4.32164800	0.27122200	0.28857100
C	3.83573300	-2.06307100	0.63349300
C	5.46682200	-0.06967900	-0.40520600
H	4.06069300	1.31997700	0.35235600
C	4.98177900	-2.42104600	-0.04613100
H	3.19506600	-2.84907700	1.02600500
C	5.84904400	-1.42878100	-0.58357300
H	6.06889700	0.72404100	-0.83008300
H	5.21013900	-3.47241500	-0.17038300
C	-1.76563000	-1.73205500	0.81817100
C	-2.70832100	-2.48489600	1.55946300
C	-1.72574700	-1.99447300	-0.57366600
C	-3.52814300	-3.42961500	0.96319600
H	-2.82680700	-2.32286300	2.62226000
C	-2.53248000	-2.93678900	-1.18490800

H	-1.02822000	-1.43294000	-1.19110200
C	-3.46303800	-3.69768300	-0.42928100
H	-4.23537100	-3.96308700	1.58681400
H	-2.44529800	-3.08296900	-2.25472200
C	2.70728700	1.88456900	2.47518400
H	3.75323600	1.58652300	2.58465200
H	2.64455500	2.59181700	1.63905400
H	2.39767300	2.41249800	3.37822900
C	-1.17936900	-0.88499800	3.85256300
H	-0.65789500	-0.52623200	4.74163400
H	-2.24052800	-0.62546400	3.95722900
H	-1.11426900	-1.97899000	3.83744000
O	0.41826200	1.44017400	4.00871200
H	0.01637100	1.77537800	1.77922500
C	-0.70840700	2.27785000	4.27926200
H	-0.57894100	2.63167400	5.30446000
H	-0.73331700	3.13310600	3.59633300
H	-1.65523800	1.73243000	4.20543300
O	-0.14554400	2.70447000	1.06986500
C	-0.81340800	2.59246800	-0.04465800
C	-0.11808300	2.70800500	-1.28967400
C	-2.24488400	2.41842200	-0.08706200
C	-0.78757200	2.61561600	-2.51198900
C	-2.91910900	2.32446800	-1.28196900
C	-2.22996600	2.40370600	-2.57924600
O	-2.83053400	2.30769700	-3.66222800
Cl	-3.08338900	2.37121500	1.43218400
Cl	-4.63411500	2.12132500	-1.35103400
C	1.29346800	2.92370600	-1.24158900
C	-0.09153200	2.71717300	-3.74907700
N	2.44235700	3.10621300	-1.21613300
N	0.48059800	2.79958500	-4.75997700
N	-4.26487400	-4.64419400	-1.01814400
N	6.99263400	-1.76657400	-1.25459400
C	7.84880200	-0.73021600	-1.82203400
H	8.20725000	-0.04166900	-1.04734700
H	8.71523900	-1.19954500	-2.28711200
H	7.32232900	-0.14537300	-2.58718400
C	7.34270900	-3.16861700	-1.45466400
H	6.58122500	-3.69466000	-2.04470000
H	8.28982500	-3.22633900	-1.99035400
H	7.45890900	-3.69089300	-0.49715600
C	-5.24815800	-5.36863300	-0.22442200
H	-5.99966800	-4.69626800	0.21223600
H	-5.76374900	-6.08584700	-0.86336100
H	-4.77173100	-5.92455200	0.59296500
C	-4.21705600	-4.84926800	-2.45958600
H	-3.21353500	-5.14746800	-2.78871100
H	-4.91047600	-5.64590700	-2.72981000
H	-4.50273100	-3.94370100	-3.01237500

para-NMe_2-Ph (2_D)

E(B3LYP/BS1) = -2603.626437 au
H(B3LYP/BS1) = -2603.005632 au
G(B3LYP/BS1) = -2603.138777 au
E(M06-2X/BS2//B3LYP/BS1) = -2603.412358 au

C	0.57017300	-1.01785400	2.74851500
C	1.87893400	-0.52535900	2.14251000
C	-0.04503600	-2.23384700	2.07262400
C	2.53988200	-1.26935100	1.21446300
H	2.15022200	-2.26737100	1.02217000
C	-0.96583000	-1.99433700	1.09160700
H	-1.14560600	-0.94119800	0.87427400
C	3.72881300	-0.94958500	0.44861500
C	4.12767900	0.36188300	0.08618200
C	4.53231600	-2.01481500	-0.03291100
C	5.26568400	0.59524400	-0.65934100
H	3.50861300	1.21119300	0.34971800
C	5.67935200	-1.80120600	-0.76764400
H	4.24146600	-3.03632200	0.19849700
C	6.09451900	-0.47809100	-1.09681600
H	5.51002100	1.61604600	-0.92535500
H	6.26050500	-2.65428400	-1.09458000
C	-1.72936900	-2.89117300	0.25462600
C	-1.85255900	-4.29606700	0.41930700
C	-2.45288600	-2.31937300	-0.82690600
C	-2.61307000	-5.06691500	-0.43585000
H	-1.36356100	-4.79375100	1.24583400
C	-3.21036600	-3.07308200	-1.69618400
H	-2.39955600	-1.24429800	-0.97582800
C	-3.31269200	-4.48499800	-1.53282400
H	-2.67812800	-6.13233500	-0.25426900
H	-3.73119700	-2.57614600	-2.50488300
C	2.29964600	0.82727200	2.65100700
H	3.37962200	0.98036900	2.58681800
H	1.80536700	1.62502900	2.08152000
H	1.99630000	0.93270300	3.69715500
C	0.42698900	-3.58159800	2.55302700
H	1.31453100	-3.47218600	3.18002800
H	-0.33666500	-4.07879800	3.16699400
H	0.66188100	-4.25494700	1.72164200
O	0.79282900	-1.22973300	4.14539000
H	-0.13311500	-0.17723500	2.62646200
C	-0.39182000	-1.15269400	4.92965600
H	-0.09181000	-1.31149300	5.96826800
H	-0.86739700	-0.16575300	4.83750600
H	-1.12409600	-1.92196200	4.64812000
O	-0.70934900	1.49108300	0.74151300
C	-1.27080500	2.50854000	0.28492500
C	-0.52523800	3.60688600	-0.30622700
C	-2.73382800	2.68252100	0.30472700
C	-1.15357900	4.74448900	-0.82561700
C	-3.34832300	3.79258300	-0.19967400

C	-2.59896900	4.90893500	-0.80750100
O	-3.16309700	5.91694800	-1.26972700
Cl	-3.63789100	1.37578600	1.01749900
Cl	-5.07739100	3.98405100	-0.16811000
C	0.89199700	3.47354300	-0.33248300
C	-0.39795100	5.80397300	-1.40323100
N	2.05266800	3.36750900	-0.35068000
N	0.22702200	6.66694100	-1.87513000
N	7.23193100	-0.24848800	-1.81499900
N	-4.05622300	-5.24712600	-2.38475500
C	-4.15580400	-6.69240900	-2.19322800
C	-4.77994200	-4.62736500	-3.49272200
C	8.04539400	-1.36431900	-2.29212900
C	7.63709200	1.11581900	-2.14620900
H	-5.52126700	-3.90587600	-3.12921600
H	-4.09371400	-4.10989400	-4.17312300
H	-4.77625100	-7.11341300	-2.98305200
H	-3.16876000	-7.16681200	-2.24032200
H	7.47426900	-2.01281000	-2.96717000
H	8.90259900	-0.97161900	-2.83720800
H	6.90101600	1.60489600	-2.79582800
H	7.75928500	1.72020300	-1.24052800
H	8.59183000	1.08587800	-2.66944000
H	8.41534600	-1.96991800	-1.45654200
H	-4.61434500	-6.93531000	-1.22720000
H	-5.30087500	-5.40155500	-4.05430000

para-NMe_2-Ph (2_A)

E(B3LYP/BS1) = -2603.636711 au

H(B3LYP/BS1) = -2603.014759 au

G(B3LYP/BS1) = -2603.13712 au

E(M06-2X/BS2//B3LYP/BS1) = -2603.466709 au

C	-0.35268400	-1.27815800	2.05622000
C	-1.77829900	-1.15165200	1.52110700
C	0.51753200	-0.02594100	2.05423700
C	-2.26254500	0.03242500	1.08343300
H	-1.56434300	0.86283600	1.05383600
C	0.85255600	0.54542100	0.87169400
H	0.44211800	0.08932300	-0.02683200
C	-3.59887100	0.40203100	0.60498300
C	-4.80475000	-0.26894000	0.89526600
C	-3.71274900	1.56220300	-0.19038100
C	-6.02920700	0.16891500	0.40577000
H	-4.80367700	-1.13803800	1.54154300
C	-4.92359800	2.00836300	-0.69835300
H	-2.81261800	2.12549500	-0.42789000
C	-6.12988000	1.32109500	-0.41234300
H	-6.91841700	-0.39018800	0.67167800
H	-4.93266100	2.89871900	-1.31569000
C	1.65183000	1.73774400	0.58216800
C	2.64857000	2.27808600	1.42046700
C	1.45924500	2.38633000	-0.65573400

C	3.37551100	3.40680600	1.06572000
H	2.89719700	1.78812900	2.35460000
C	2.16607700	3.52166700	-1.02149600
H	0.72477700	1.98602600	-1.35156800
C	3.14156000	4.08208100	-0.15828300
H	4.14198200	3.75899300	1.74543900
H	1.96577900	3.96998300	-1.98711500
C	-2.59278800	-2.42143300	1.62977700
H	-3.17849200	-2.44757700	2.55741600
H	-3.29083500	-2.51175100	0.79228600
H	-1.94407900	-3.29809200	1.62977800
C	0.83751600	0.58904600	3.39811600
H	0.08515300	0.30488900	4.13768600
H	1.81493900	0.27741200	3.78842700
H	0.85197800	1.68044200	3.32182600
O	-0.51864500	-1.86152500	3.30562200
H	3.30977500	-2.52065600	-3.94568000
C	0.57155600	-2.52141100	3.96202300
H	0.86538000	-3.41740500	3.41066900
H	1.44092700	-1.87425400	4.08890300
H	0.18077800	-2.80283400	4.94203700
O	3.76882300	-2.31521000	-3.11056200
C	2.89979500	-2.34298800	-2.08516200
C	3.39599500	-2.08278200	-0.80023700
C	1.52981400	-2.63063200	-2.22959200
C	2.52835500	-2.09499700	0.32055700
C	0.67248400	-2.63566700	-1.12633100
C	1.14717400	-2.35012200	0.18112600
O	0.32911000	-2.44758100	1.23642700
Cl	0.95310100	-2.98516400	-3.83704600
Cl	-1.00082000	-3.02808300	-1.34293900
C	4.78959300	-1.81430400	-0.64423200
C	3.09664600	-1.86824100	1.61152900
N	5.92492000	-1.59538200	-0.51623100
N	3.62085000	-1.69853700	2.63632500
N	3.83401200	5.22671800	-0.49643700
N	-7.34601700	1.76408500	-0.89185700
C	-8.53918800	0.95359800	-0.69649700
H	-8.74834200	0.80489600	0.36995600
H	-9.39546600	1.46839300	-1.13405500
H	-8.45508700	-0.03726500	-1.16761100
C	-7.39061900	2.86532700	-1.84256600
H	-6.85168900	2.63763600	-2.77459900
H	-8.43064700	3.07840900	-2.09282400
H	-6.95678900	3.77730700	-1.41455300
C	3.68805400	5.79236700	-1.83011500
H	4.27788000	6.70762200	-1.89490900
H	4.02895000	5.10548500	-2.61953800
H	2.64326700	6.05393700	-2.03492000
C	4.94852200	5.66840300	0.33023600
H	5.76544600	4.93190100	0.36470300

H	5.34495300	6.60024100	-0.07518300
H	4.62318200	5.86368500	1.35879200

meta-CN-Ph (TS_A)

E(B3LYP/BS1) = -2704.619659 au

H(B3LYP/BS1) = -2704.158766 au

G(B3LYP/BS1) = -2704.279529 au

E(M06-2X/BS2//B3LYP/BS1) = -2704.462108 au

C	0.74087300	-2.17252900	-1.27322300
C	2.08978300	-1.82611200	-0.70504000
C	-0.18706900	-1.14600800	-1.77949500
C	2.69327000	-0.66527400	-1.06083900
H	2.20339700	-0.04467100	-1.80640100
C	-0.36718800	-0.01916100	-1.00432300
H	0.31569000	0.10657200	-0.17208200
C	3.99065700	-0.14854700	-0.60295400
C	4.44614900	-0.28805600	0.71850200
C	4.78535300	0.56926800	-1.51282200
C	5.68470300	0.24683200	1.10471100
H	3.82592400	-0.77308000	1.46289400
C	6.02482400	1.09516500	-1.12545800
H	4.44095200	0.71182400	-2.53194300
C	6.48858600	0.93407200	0.18705000
H	7.44495300	1.34420200	0.48878500
C	-1.26253600	1.11836500	-1.19342300
C	-2.47208900	1.07451800	-1.91392500
C	-0.91266100	2.32810300	-0.55917600
C	-3.27942600	2.21478500	-2.02234600
H	-2.81333000	0.15557800	-2.36950100
C	-1.71762300	3.46708000	-0.67909600
H	0.00286100	2.38525200	0.01990400
C	-2.90850600	3.42169300	-1.41537600
H	-3.53592500	4.30033200	-1.50556500
C	2.70827900	-2.89067300	0.16823900
H	3.79657100	-2.80778500	0.20034000
H	2.32958200	-2.83006800	1.19549300
H	2.45098400	-3.87992500	-0.21930200
C	-0.90695000	-1.40828400	-3.07694200
H	-0.31401000	-2.08247800	-3.69906100
H	-1.89273100	-1.86698100	-2.93431400
H	-1.05481200	-0.47259700	-3.62307400
O	0.82536800	-3.37272800	-1.95459300
H	0.04970900	-2.44457200	-0.12191500
C	-0.26569000	-4.31070300	-1.92139400
H	0.08041400	-5.17185800	-2.49376700
H	-0.47438700	-4.60861300	-0.89063200
H	-1.17191700	-3.90961400	-2.38008800
O	-0.58016000	-2.64590000	0.92607500
C	-1.39453900	-1.69389000	1.24231500
C	-0.96338400	-0.64565800	2.14086600
C	-2.78535900	-1.69198500	0.82379800
C	-1.82805000	0.34082000	2.57210600

C	-3.65639100	-0.72103400	1.23820100
C	-3.23848200	0.37973100	2.13152200
O	-4.00470600	1.26532000	2.50444400
Cl	-3.29692500	-3.00010600	-0.19221000
Cl	-5.32243200	-0.71459900	0.77719500
C	0.39529800	-0.68604300	2.58997600
C	-1.41081800	1.36026000	3.47609500
N	1.50131500	-0.71659900	2.94714900
N	-1.07061200	2.19454400	4.21239200
C	-4.50870600	2.14146400	-2.76014400
C	-1.32190900	4.68992400	-0.04015600
C	6.82394300	1.81072000	-2.07876500
C	6.13000300	0.09662200	2.46094700
N	-5.50226100	2.08033100	-3.36056100
N	-0.99911300	5.68115600	0.47414300
N	7.46969200	2.38953800	-2.85337600
N	6.49170200	-0.02723300	3.55904000

meta-CN-Ph (TS_B)

E(B3LYP/BS1) = -2704.65677 au

H(B3LYP/BS1) = -2704.189748 au

G(B3LYP/BS1) = -2704.319632 au

E(M06-2X/BS2//B3LYP/BS1) = -2704.49673 au

C	0.09253900	1.58994900	1.68898400
C	1.45228600	1.02955600	1.70922300
C	-1.08878800	0.65746100	1.88852700
C	1.62446300	-0.19085600	1.11046000
H	0.73955100	-0.65936400	0.68815600
C	-1.89681300	0.26613800	0.88855600
H	-1.66796200	0.59134600	-0.12052500
C	2.84094400	-0.99083800	0.96372300
C	3.93835500	-0.92677600	1.84088200
C	2.88609100	-1.91676300	-0.09599300
C	5.05997200	-1.74293100	1.63799400
H	3.91718900	-0.28012300	2.70763100
C	4.01442300	-2.71961000	-0.30222400
H	2.04670200	-2.00160000	-0.77587400
C	5.11408900	-2.63711900	0.56124600
H	5.98487800	-3.26317400	0.40723500
C	-3.07573000	-0.62051800	0.97106300
C	-4.01387000	-0.54291700	2.00995000
C	-3.29586500	-1.54530800	-0.06167400
C	-5.12783500	-1.39712200	2.03262900
H	-3.90486500	0.19748400	2.79295900
C	-4.40632700	-2.40060500	-0.03473900
H	-2.59689000	-1.60927500	-0.88904600
C	-5.33080200	-2.33734700	1.01604700
H	-6.19111700	-2.99576000	1.03549200
C	2.55691900	1.89531600	2.26148400
H	2.65675800	1.74160900	3.34413500
H	3.51531400	1.68120700	1.78733200
H	2.32860300	2.95208100	2.11624900

C	-1.20881200	0.21708200	3.33603000
H	-0.21845200	0.00632500	3.75112600
H	-1.66149700	0.99332000	3.96450900
H	-1.81382000	-0.68767800	3.42383500
O	0.00975100	2.78427800	2.32405400
H	0.12019800	1.98166300	0.25230300
C	-1.23671100	3.51213900	2.29316600
H	-2.04543100	2.93515300	2.74624800
H	-1.04953800	4.41601200	2.87092200
H	-1.49319800	3.77260900	1.26247000
O	-1.63726000	3.43079500	-1.45984700
C	-0.84642100	2.53254200	-1.66629400
C	0.50046300	2.49795600	-0.93521300
C	-1.14101700	1.39270900	-2.57184600
C	1.53520800	1.66492400	-1.48349300
C	-0.19778000	0.46687400	-2.87162300
C	1.22928200	0.56907600	-2.38325800
O	2.07240800	-0.23279300	-2.78080100
Cl	-2.74620100	1.35468400	-3.21509500
Cl	-0.52541100	-0.87379200	-3.89828800
C	0.90463800	3.82569400	-0.49664100
C	2.90430500	1.90294400	-1.20633200
N	1.23367000	4.87887000	-0.13631200
N	4.03319000	2.10749500	-0.99352600
C	-4.60101100	-3.34724800	-1.09571900
C	-6.07357200	-1.29636600	3.10721900
C	4.03877300	-3.64315100	-1.40047100
C	6.16356300	-1.66845700	2.55262700
N	-6.83660200	-1.21255800	3.98059200
N	-4.75724800	-4.11429400	-1.95544500
N	4.05686400	-4.39253200	-2.28905600
N	7.05612900	-1.60752500	3.29508600

meta-CN-Ph (TS_D)

E(B3LYP/BS1) = -2704.604548 au

H(B3LYP/BS1) = -2704.14549 au

G(B3LYP/BS1) = -2704.271006 au

E(M06-2X/BS2//B3LYP/BS1) = -2704.438352 au

C	0.07663600	-0.63899700	2.53940800
C	1.48121700	-0.85945800	2.13745700
C	-1.03461000	-1.46358200	1.94418600
C	1.76296200	-1.59598200	1.00567100
H	0.94986000	-2.17069800	0.57281900
C	-1.40736700	-1.22211000	0.66340500
H	-0.88368100	-0.42850500	0.13489400
C	3.04279400	-1.76487600	0.32818600
C	4.03104500	-0.76282900	0.26402500
C	3.27184500	-2.97553900	-0.35559900
C	5.22676000	-0.98926000	-0.43009200
H	3.86087300	0.21065600	0.70739800
C	4.47352300	-3.20051500	-1.03657600
H	2.51247400	-3.75030200	-0.34417000

C	5.46523800	-2.21032300	-1.07557200
H	6.39387100	-2.38045800	-1.60717800
C	-2.40419500	-1.91385100	-0.16487300
C	-3.54953100	-2.54699600	0.34574800
C	-2.21908900	-1.90215900	-1.55919000
C	-4.46135900	-3.17779600	-0.51417700
H	-3.76408100	-2.52920400	1.40567600
C	-3.12605600	-2.54060300	-2.41434100
H	-1.35613300	-1.39843600	-1.98212400
C	-4.25594100	-3.18931200	-1.89882900
H	-4.96139300	-3.67977900	-2.55881100
C	2.53198200	-0.21585100	3.00351700
H	3.52227200	-0.62806400	2.80741000
H	2.56375700	0.86726600	2.83692200
H	2.28767000	-0.37348000	4.05602700
C	-1.59001100	-2.55122200	2.83552300
H	-0.85421700	-2.83216600	3.59320100
H	-2.49648900	-2.23865200	3.36816700
H	-1.84410600	-3.43892400	2.24872300
O	-0.02643200	-0.40174700	3.90072900
H	-0.00658200	0.56111500	2.01090000
C	-1.16684000	0.32575900	4.38053600
H	-1.12071700	0.26195500	5.46800800
H	-1.09665600	1.37057700	4.06367700
H	-2.10752100	-0.10367000	4.02565200
O	0.30750500	1.84716100	1.71421500
C	-0.11495100	2.57883600	0.74128400
C	0.85927500	3.26111300	-0.06666000
C	-1.50999300	2.79781200	0.43056300
C	0.48504700	4.08396300	-1.12759100
C	-1.89290900	3.60756100	-0.61171500
C	-0.91748000	4.30078000	-1.46847100
O	-1.25899500	5.02608700	-2.41654200
Cl	-2.68079300	2.03267200	1.46044000
Cl	-3.55559100	3.88822300	-0.98598000
C	2.23317200	3.02653000	0.24503500
C	1.45618900	4.73795800	-1.93776100
N	3.35063000	2.82108500	0.49695500
N	2.25309400	5.27139600	-2.59782100
C	4.68899200	-4.45070800	-1.70784600
C	6.21832500	0.04708600	-0.49142600
C	-2.89901500	-2.52570800	-3.83137500
C	-5.62609700	-3.81161100	0.03521300
N	-2.71259500	-2.51399400	-4.97894100
N	-6.56787000	-4.32490500	0.48411800
N	4.86147600	-5.46453100	-2.25006200
N	7.02460100	0.88307600	-0.54085100

meta-CN-Ph (2_D)

E(B3LYP/BS1) = -2704.61722 au

H(B3LYP/BS1) = -2704.151557 au

G(B3LYP/BS1) = -2704.279425 au

E(M06-2X/BS2//B3LYP/BS1) = -2704.442688 au

C	-2.08743900	1.37656100	2.50509800
C	-2.35734900	0.07529400	1.75540200
C	-1.86544200	2.34516800	1.33804300
C	-3.57702100	-0.03402500	1.12394200
H	-4.27931100	0.77571600	1.29850600
C	-0.60645500	2.31682100	0.75315200
H	0.10005000	1.60739700	1.17788000
C	-4.12715400	-1.12962700	0.34238400
C	-3.35855300	-2.02320100	-0.43450400
C	-5.53303100	-1.25885000	0.32825800
C	-3.99002700	-3.03535900	-1.16772100
H	-2.28328200	-1.91661400	-0.52128000
C	-6.15310700	-2.28273000	-0.39274200
H	-6.14093000	-0.56331400	0.89706600
C	-5.38486600	-3.18308200	-1.14472600
H	-5.86236500	-3.97309100	-1.71227400
C	-0.04062600	3.09426500	-0.32553700
C	-0.70386700	4.11030600	-1.05315400
C	1.30579800	2.80063200	-0.66048000
C	-0.04198700	4.79563800	-2.07502200
H	-1.72614800	4.37881400	-0.83738900
C	1.95777300	3.49213300	-1.68305200
H	1.82344600	2.01550100	-0.11759600
C	1.29065200	4.49619900	-2.40044300
H	1.79554400	5.03417100	-3.19420800
C	-1.29326500	-0.97169800	1.83451200
H	-1.65344200	-1.95451000	1.52965100
H	-0.41612100	-0.72655800	1.22091000
H	-0.93889900	-1.03530600	2.87065400
C	-3.01173600	3.21562500	0.92264900
H	-3.88645100	3.02485900	1.54457000
H	-2.73929300	4.27050100	1.05951000
H	-3.28218100	3.07632200	-0.12892400
O	-3.16877400	1.70724300	3.33556500
H	-1.16410700	1.27287700	3.08888100
C	-2.86468000	2.72246800	4.29764800
H	-3.76378700	2.84765300	4.90275700
H	-2.03015400	2.41229000	4.93905800
H	-2.61532100	3.67745800	3.81820800
O	1.76730600	-0.00804200	0.76474400
C	2.66497700	-0.84420900	0.50591900
C	2.42412700	-2.00121300	-0.33440000
C	4.03071800	-0.71454200	1.03179800
C	3.42297300	-2.93818500	-0.61829200
C	5.00933300	-1.62764500	0.75853900
C	4.77425400	-2.81076200	-0.09182000
O	5.66650900	-3.63974400	-0.34120800
Cl	4.32192200	0.67667300	2.03682100
Cl	6.61876200	-1.47098200	1.39308800
C	1.10834300	-2.13573200	-0.86080600

C	3.16117500	-4.06796500	-1.44389200
N	0.02502900	-2.22794400	-1.27964000
N	2.93855100	-4.99057700	-2.11966400
C	3.32088300	3.17603000	-2.00468500
C	-0.73409500	5.82195300	-2.80210900
C	-7.58271300	-2.40746300	-0.37216000
C	-3.21009700	-3.93760700	-1.96763100
N	-2.59896900	-4.68027000	-2.62008800
N	-8.74067100	-2.50700700	-0.35360300
N	4.42462400	2.92352500	-2.26658600
N	-1.29630500	6.65259600	-3.38931100

meta-CN-Ph (2_A)

E(B3LYP/BS1) = -2704.671256 au

H(B3LYP/BS1) = -2704.203673 au

G(B3LYP/BS1) = -2704.323101 au

E(M06-2X/BS2//B3LYP/BS1) = -2704.538256 au

C	-0.30983300	-0.57061800	2.12541700
C	-1.76782600	-0.67043800	1.62583400
C	0.44213700	0.71021600	1.73508300
C	-2.32199400	0.32441900	0.90562900
H	-1.72762800	1.20837800	0.70202100
C	0.74343900	0.93212400	0.43827900
H	0.40446800	0.21087600	-0.30034600
C	-3.69684500	0.41040100	0.37929000
C	-4.42245300	-0.69251400	-0.09692100
C	-4.29663600	1.67874700	0.30057400
C	-5.72256000	-0.53298500	-0.60270900
H	-3.97635900	-1.67869600	-0.10628800
C	-5.59702300	1.83593200	-0.19804800
H	-3.74895400	2.55255900	0.63852600
C	-6.32618200	0.72886200	-0.65130200
H	-7.33028900	0.84839800	-1.04036100
C	1.44151800	2.08702800	-0.15537300
C	2.48806900	2.76972100	0.48363300
C	1.07389900	2.49481200	-1.44840700
C	3.12084400	3.85583500	-0.14131300
H	2.84277400	2.44453800	1.45361700
C	1.70316900	3.58295100	-2.06830800
H	0.28594200	1.96624100	-1.97517000
C	2.73058900	4.27834800	-1.41743400
H	3.22015700	5.11802900	-1.89613800
C	-2.51946400	-1.88697400	2.11614400
H	-3.58908900	-1.67947900	2.20442600
H	-2.39385000	-2.74291200	1.44643700
H	-2.14656400	-2.18355700	3.09744100
C	0.66916300	1.71536000	2.83938900
H	-0.13679300	1.65399400	3.57427700
H	1.60953100	1.54034400	3.37527400
H	0.69982000	2.73232500	2.44043800
O	-0.42365500	-0.74239000	3.50027000
H	3.66775400	-3.32560600	-3.13960100

C	0.68977100	-1.16759000	4.29811500
H	1.07253200	-2.12849600	3.94784000
H	1.49820200	-0.43441100	4.31224800
H	0.28218900	-1.27901600	5.30430100
O	4.06640400	-2.84553600	-2.39035400
C	3.14395300	-2.60051800	-1.44746500
C	3.55583800	-1.91845800	-0.29366300
C	1.79683900	-2.99389600	-1.54827200
C	2.63088000	-1.62843300	0.74009700
C	0.88158400	-2.69787200	-0.53358300
C	1.27406100	-1.99610400	0.63362500
O	0.38895000	-1.83607000	1.64251100
Cl	1.32175600	-3.86191300	-2.98090600
Cl	-0.76136400	-3.21914500	-0.69538900
C	4.92508300	-1.52947400	-0.17945400
C	3.12570800	-0.95326500	1.89750800
N	6.04002900	-1.21182900	-0.08644600
N	3.58833600	-0.40275800	2.81188700
C	-6.43748300	-1.67959800	-1.08630700
C	-6.18503000	3.14393100	-0.24992900
C	1.29497300	3.98513900	-3.38403400
C	4.18896900	4.53640100	0.53386300
N	5.05257400	5.08843100	1.08303000
N	0.96184500	4.30897900	-4.45002700
N	-6.65956900	4.20482500	-0.29032000
N	-7.01421800	-2.61086000	-1.47685000

meta-OMe-Ph (TS_A)

E(B3LYP/BS1) = -2793.747087 au

H(B3LYP/BS1) = -2793.146251 au

G(B3LYP/BS1) = -2793.271286 au

E(M06-2X/BS2//B3LYP/BS1) = -2793.572843 au

C	0.47043500	-2.41701800	-0.89314200
C	1.84430300	-2.05586200	-0.39954200
C	-0.42711000	-1.43223500	-1.51009100
C	2.50367100	-1.00512000	-0.95058400
H	2.01687900	-0.49310900	-1.77755000
C	-0.52886700	-0.19196300	-0.89579900
H	0.20457200	0.00265800	-0.12146400
C	3.83860400	-0.48553600	-0.62811200
C	4.36698200	-0.49262600	0.67316700
C	4.58615500	0.08676900	-1.67204000
C	5.63536700	0.04576900	0.91454500
H	3.79503700	-0.86235500	1.51514700
C	5.85798800	0.60825600	-1.42457700
H	4.19381200	0.12059800	-2.68346900
C	6.39686700	0.59136600	-0.12897800
H	7.37747600	1.00275900	0.06338200
C	-1.39024000	0.94308500	-1.16575500
C	-2.61197100	0.86338900	-1.87212600
C	-0.97777400	2.18157800	-0.61559700
C	-3.38814000	2.01439500	-2.03601200

H	-2.96506200	-0.08405000	-2.24639800
C	-1.75563200	3.32776400	-0.80587500
H	-0.04117800	2.22986500	-0.07417000
C	-2.96149500	3.24036400	-1.50931500
H	-3.57182700	4.12632000	-1.64631900
C	2.42020700	-3.00032600	0.62772300
H	3.51187700	-2.99921500	0.60738800
H	2.09968800	-2.72953700	1.64122700
H	2.07066800	-4.01831000	0.43277900
C	-1.21614800	-1.84673700	-2.72405400
H	-0.68411000	-2.63827300	-3.25667700
H	-2.21481600	-2.22671400	-2.47497400
H	-1.34790000	-0.99560700	-3.39705800
O	0.50418000	-3.69610900	-1.44489000
H	-0.20255700	-2.53081700	0.26619800
C	-0.58322900	-4.60306600	-1.20857800
H	-0.31703100	-5.51902300	-1.73840100
H	-0.68216400	-4.81035900	-0.13908700
H	-1.53277200	-4.22408700	-1.59472400
O	-0.86197000	-2.57351800	1.35740300
C	-1.63714700	-1.54962300	1.49851900
C	-1.17521000	-0.37776200	2.20199700
C	-3.01869300	-1.55352900	1.05109900
C	-1.98081800	0.73554500	2.37107300
C	-3.83014700	-0.46290500	1.21159300
C	-3.35706500	0.78406900	1.84428000
O	-4.06136700	1.78846700	1.95562200
Cl	-3.60025700	-3.01989700	0.32507100
Cl	-5.48794400	-0.46096700	0.70782300
C	0.15322300	-0.41185000	2.73320300
C	-1.52321300	1.88657200	3.07426900
N	1.23051900	-0.43503800	3.17097600
N	-1.14672700	2.82972000	3.64380900
O	6.50767900	1.12249100	-2.50773200
O	6.05270700	0.00220500	2.21190100
O	-4.57904800	2.05057000	-2.68894800
O	-1.43533000	4.56564800	-0.34894800
C	7.80542100	1.68265400	-2.32476400
H	8.12210400	2.02514700	-3.31091300
H	7.78037900	2.53473600	-1.63480100
H	8.51633900	0.93415200	-1.95450900
C	7.32661800	0.54980200	2.54075800
H	7.37633400	1.61929100	2.30304200
H	7.43906500	0.41280100	3.61714000
H	8.13586400	0.02255000	2.02115000
C	-0.22149700	4.73172100	0.38630600
H	-0.23982000	4.15518000	1.31781700
H	0.64917100	4.44237000	-0.21370500
H	-0.16361100	5.79564400	0.61899800
C	-5.07998500	0.84501400	-3.26614700
H	-5.27040100	0.08612000	-2.49848800

H	-6.01953600	1.11777700	-3.74798700
H	-4.38717500	0.44565000	-4.01621300

meta-OMe-Ph (TS_B)

E(B3LYP/BS1) = -2793.733821 au

H(B3LYP/BS1) = -2793.132117 au

G(B3LYP/BS1) = -2793.258568 au

E(M06-2X/BS2//B3LYP/BS1) = -2793.561601 au

C	0.19660500	1.73705800	-1.66688300
C	-1.18558600	1.26011600	-1.80780100
C	1.33362100	0.73897100	-1.80531300
C	-1.48022900	0.06674300	-1.18820000
H	-0.62972000	-0.45885600	-0.76069900
C	2.03385700	0.26363300	-0.76017200
H	1.72924600	0.57269100	0.23495600
C	-2.72616200	-0.67680600	-1.06840700
C	-4.00978000	-0.14657300	-1.30211400
C	-2.60311600	-2.02278100	-0.66392200
C	-5.13626200	-0.95933400	-1.14889400
H	-4.16879900	0.89149100	-1.55153000
C	-3.73340000	-2.82985600	-0.52911700
H	-1.62811600	-2.45401200	-0.46297500
C	-5.01154000	-2.30535300	-0.77250200
H	-5.88885200	-2.92672600	-0.66232300
C	3.16168100	-0.69118000	-0.76171100
C	4.18208400	-0.63967300	-1.72489600
C	3.21499500	-1.63791600	0.27556200
C	5.24058800	-1.55710400	-1.65760800
H	4.16623200	0.13013300	-2.48411200
C	4.27301600	-2.55406000	0.32418900
H	2.42728300	-1.65526000	1.01889800
C	5.28294900	-2.51496700	-0.64182500
H	6.10555100	-3.22035700	-0.59541100
C	-2.17221800	2.12557800	-2.54985500
H	-2.86331600	1.50050800	-3.12137000
H	-2.77039900	2.74489800	-1.87044800
H	-1.65360600	2.79392900	-3.23786100
C	1.53439700	0.32617000	-3.25258300
H	0.56546900	0.15590200	-3.73362100
H	2.05139300	1.09656300	-3.83760100
H	2.11901900	-0.59346800	-3.31547500
O	0.40091600	2.93972500	-2.27696800
H	0.11407200	2.11455300	-0.26392200
C	1.69395000	3.56371700	-2.15745000
H	2.46857000	2.97067500	-2.64879600
H	1.59025400	4.52809000	-2.65365100
H	1.95226400	3.71351800	-1.10525400
O	1.89794000	3.32268500	1.62849900
C	0.98349400	2.53039400	1.74894400
C	-0.29044100	2.67454000	0.92078900
C	1.05765200	1.35241400	2.65273500
C	-1.46158200	1.96809100	1.36281500

C	-0.01450100	0.55046600	2.85898400
C	-1.37545100	0.83572400	2.26399200
O	-2.34303600	0.15334400	2.59240400
Cl	2.58842200	1.10806100	3.42448200
Cl	0.05933300	-0.83028000	3.88616800
C	-0.49303200	4.04297600	0.47433200
C	-2.75763900	2.38920600	0.98156100
N	-0.66503100	5.13233300	0.11158900
N	-3.82352500	2.75574900	0.67712400
O	4.41075600	-3.52011500	1.27624000
O	6.28310300	-1.58971600	-2.53637200
O	-6.33054500	-0.35096200	-1.38755800
O	-3.50047900	-4.11694100	-0.15157900
C	3.41892800	-3.61417100	2.29601500
H	3.36488400	-2.69300900	2.88831300
H	2.43091900	-3.83379300	1.87389400
H	3.73060400	-4.43985600	2.93727300
C	6.30032100	-0.64953300	-3.60740800
H	5.42080700	-0.76167000	-4.25284600
H	6.35038200	0.38102800	-3.23586300
H	7.20135700	-0.87064800	-4.18134100
C	-7.53086400	-1.10382000	-1.22595500
H	-8.34458700	-0.41397500	-1.45301700
H	-7.56827700	-1.95124400	-1.92086000
H	-7.63862000	-1.46807400	-0.19736500
C	-4.61357100	-4.99008800	0.03029900
H	-5.28522500	-4.62265000	0.81521200
H	-5.17603800	-5.12066500	-0.90190000
H	-4.19051400	-5.94819600	0.33471000

meta-OMe-Ph (TS_D)

E(B3LYP/BS1) = -2793.730791 au

H(B3LYP/BS1) = -2793.131718 au

G(B3LYP/BS1) = -2793.262341 au

E(M06-2X/BS2//B3LYP/BS1) = -2793.547519 au

C	0.49049100	-0.09483000	2.68936500
C	1.84720600	-0.26534100	2.14146700
C	-0.64153900	-0.98395100	2.28327400
C	2.08632400	-1.20472600	1.15646000
H	1.28723100	-1.91685800	0.97265900
C	-1.03123600	-0.97451200	0.97748300
H	-0.48632300	-0.29861700	0.32065400
C	3.27784100	-1.44684700	0.36274700
C	4.24567300	-0.45948700	0.07375000
C	3.42001700	-2.74730300	-0.17703500
C	5.34594300	-0.78623300	-0.72433000
H	4.10656800	0.55285600	0.42203800
C	4.53274100	-3.06228500	-0.95908600
H	2.66161300	-3.48961100	0.03941600
C	5.49661000	-2.08399100	-1.23078800
H	6.35610800	-2.32698600	-1.84605200

C	-2.04336400	-1.76112700	0.26810600
C	-3.12551500	-2.41356200	0.88560300
C	-1.91787200	-1.83058500	-1.13276600
C	-4.04516900	-3.12960600	0.11288300
H	-3.30347100	-2.35194800	1.94971000
C	-2.83316400	-2.55920700	-1.89492600
H	-1.10190100	-1.32737500	-1.64157000
C	-3.90738200	-3.21887700	-1.27976700
H	-4.62092900	-3.77704300	-1.86879600
C	2.91876500	0.63534500	2.70897700
H	3.90298300	0.16908800	2.63367000
H	2.95239600	1.59204100	2.17383000
H	2.70855300	0.85294700	3.75682600
C	-1.23441800	-1.86336800	3.36022500
H	-0.55583900	-1.92958500	4.21347700
H	-2.19495200	-1.48629600	3.73283100
H	-1.41277600	-2.87080000	2.97137300
O	0.52399400	0.26079300	4.03721600
H	0.24827900	1.10365300	2.02845200
C	-0.53872100	1.07070500	4.55259800
H	-0.36211800	1.14125900	5.62718100
H	-0.50850700	2.06943100	4.10649200
H	-1.52142700	0.62316400	4.37617600
O	0.35208100	2.28446600	1.57681300
C	-0.28513500	2.77806200	0.56504400
C	0.47796200	3.38610200	-0.48868700
C	-1.72548500	2.80779700	0.44980800
C	-0.13569000	3.95109500	-1.60573600
C	-2.34382900	3.35988900	-0.64688100
C	-1.58753100	3.96073200	-1.75657600
O	-2.14109700	4.45284000	-2.75306800
Cl	-2.64360000	2.16616400	1.77544700
Cl	-4.06406100	3.40991100	-0.79556900
C	1.90035300	3.37147000	-0.35830300
C	0.62714000	4.53422800	-2.65699400
N	3.05964100	3.36501500	-0.25933900
N	1.25379600	5.01071600	-3.51468500
O	4.77179800	-4.28531400	-1.50784300
O	6.32717100	0.08790500	-1.07523600
O	-5.06189000	-3.71353200	0.80952900
O	-2.60573600	-2.57135800	-3.23885700
C	3.82651600	-5.32801500	-1.27658200
H	4.21658900	-6.20238800	-1.79909100
H	3.73425900	-5.55288300	-0.20735500
H	2.84079800	-5.07047100	-1.68197900
C	6.27338800	1.41706700	-0.55507000
H	6.31258100	1.41376900	0.54088700
H	7.15617700	1.92246800	-0.94895500
H	5.37073800	1.94326400	-0.88417900
C	-6.05030900	-4.44890900	0.09266100
H	-5.60988100	-5.30418400	-0.43389200

H	-6.75341800	-4.81052100	0.84424800
H	-6.58097900	-3.81206100	-0.62530300
C	-3.51116900	-3.28177400	-4.08001500
H	-3.13647900	-3.15039900	-5.09601900
H	-3.53051100	-4.35061100	-3.83521000
H	-4.52638200	-2.87285500	-4.01115300

meta-OMe-Ph (2_D)

E(B3LYP/BS1) = -2793.753652 au

H(B3LYP/BS1) = -2793.148711 au

G(B3LYP/BS1) = -2793.285528 au

E(M06-2X/BS2//B3LYP/BS1) = -2793.558947 au

C	-1.11085900	0.55210400	2.65517000
C	-1.82466200	-0.61111100	1.97427100
C	-1.21277400	1.85015300	1.86605800
C	-2.85076000	-0.36507800	1.11086800
H	-3.17896500	0.66783500	1.01710900
C	-0.31744100	1.97821400	0.82227900
H	0.36554900	1.13911100	0.69874000
C	-3.64027800	-1.30335500	0.32192500
C	-3.11909500	-2.50808200	-0.17880500
C	-4.97391900	-0.93219600	0.01736700
C	-3.92621100	-3.35163400	-0.95549400
H	-2.08454800	-2.78943900	-0.02658700
C	-5.76897700	-1.78500300	-0.73977600
H	-5.35874500	0.00651000	0.39640300
C	-5.25050600	-3.00170200	-1.23026200
H	-5.90265700	-3.62975400	-1.82417200
C	-0.13478100	3.02158100	-0.15494200
C	-0.78764500	4.27925400	-0.15911000
C	0.79673100	2.71759900	-1.18247600
C	-0.50790300	5.18012600	-1.17857100
H	-1.47305400	4.54695300	0.62744600
C	1.06292500	3.62993200	-2.21029900
H	1.30948600	1.76196400	-1.18327500
C	0.41133900	4.86306300	-2.21202500
H	0.58342400	5.60808200	-2.97867600
C	-1.30074600	-1.95926400	2.37570500
H	-2.04208700	-2.74991900	2.24583000
H	-0.41169600	-2.21501300	1.78497800
H	-0.99707000	-1.93071000	3.42788200
C	-2.26329600	2.83551600	2.27621900
H	-2.91179300	2.40263000	3.03970600
H	-1.80505500	3.73710800	2.70640700
H	-2.87078500	3.16081600	1.42448400
O	-1.59037500	0.64707900	3.98599800
H	-0.04440300	0.26982500	2.67169400
C	-0.67443300	1.26500300	4.88992900
H	-1.14125400	1.22921300	5.87631600
H	0.27929600	0.72130200	4.91804800
H	-0.47934500	2.31251800	4.62419800
O	1.51143500	-0.75519000	0.69931800

C	2.61912900	-1.25726300	0.40724300
C	2.73464000	-2.57453800	-0.19172800
C	3.89169900	-0.55836700	0.64474600
C	3.97095500	-3.13841600	-0.52370500
C	5.10041600	-1.10675100	0.32290400
C	5.22786600	-2.44280800	-0.29014800
O	6.33012700	-2.93850700	-0.58466800
Cl	3.76003900	1.01998300	1.36906200
Cl	6.59769700	-0.27040200	0.61059800
C	1.51571700	-3.27224600	-0.42765600
C	4.05627700	-4.43172700	-1.11301800
N	0.51470500	-3.83916100	-0.61469800
N	4.11847800	-5.49061000	-1.59532300
O	1.95948300	3.22930300	-3.14295700
O	-1.05601600	6.41006800	-1.29367700
O	-7.06428800	-1.54617300	-1.07628200
O	-3.32883900	-4.48675000	-1.40328300
C	2.27893800	4.12480900	-4.21025100
H	2.71927500	5.05307800	-3.82865800
H	3.00986300	3.59975100	-4.82534200
H	1.39207000	4.35600800	-4.81128700
C	-2.00354600	6.83586800	-0.31075500
H	-1.54721200	6.87142200	0.68463800
H	-2.30782200	7.83834700	-0.61140200
H	-2.87618800	6.17345600	-0.29527700
C	-7.66761600	-0.33304400	-0.62849900
H	-7.14408300	0.54237700	-1.03029500
H	-8.68971800	-0.35277000	-1.00823300
H	-7.68419600	-0.27902600	0.46632300
C	-4.08614700	-5.38259800	-2.21597800
H	-4.42028700	-4.89591700	-3.13980000
H	-3.40989200	-6.20235800	-2.46059300
H	-4.95434000	-5.77475200	-1.67336600

meta-OMe-Ph (2_A)

E(B3LYP/BS1) = -2793.789956 au

H(B3LYP/BS1) = -2793.182581 au

G(B3LYP/BS1) = -2793.308373 au

E(M06-2X/BS2//B3LYP/BS1) = -2793.638101 au

C	-0.25189100	-1.01635400	2.13270100
C	-1.70081800	-1.00054500	1.61424200
C	0.56595000	0.25915600	1.91062900
C	-2.21824800	0.10593100	1.04218900
H	-1.58168500	0.98151500	0.97072900
C	0.86601800	0.63697900	0.64882000
H	0.47442200	0.02944700	-0.16343800
C	-3.58151800	0.33622200	0.52721700
C	-4.38105400	-0.66686500	-0.04180600
C	-4.07325000	1.65176900	0.57536500
C	-5.65549400	-0.35756500	-0.53002400
H	-4.02602800	-1.68352800	-0.14980600
C	-5.35163000	1.95056800	0.09788800

H	-3.47249000	2.45346600	0.99361100
C	-6.15929600	0.94828400	-0.45932300
H	-7.14537100	1.18021600	-0.83565800
C	1.61473300	1.81567900	0.17573800
C	2.67169000	2.39595300	0.89293000
C	1.26729800	2.34362800	-1.07890500
C	3.34993800	3.50217100	0.36864000
H	3.01309400	1.98474400	1.83436200
C	1.94107800	3.45616300	-1.58937600
H	0.46601100	1.90431900	-1.66489600
C	2.98899200	4.04954500	-0.87021000
H	3.51517900	4.90519300	-1.26868800
C	-2.49877800	-2.24853700	1.92408300
H	-3.54672400	-2.00027700	2.11338200
H	-2.47201000	-2.96912700	1.10100000
H	-2.09492100	-2.74486900	2.80752300
C	0.85970500	1.09695100	3.13394800
H	0.07503900	0.96159600	3.88237300
H	1.81226900	0.83044300	3.60772600
H	0.91350500	2.15544900	2.86777000
O	-0.38062500	-1.37366800	3.47011000
H	3.64248100	-3.11050000	-3.48218200
C	0.71760100	-1.92055600	4.20962800
H	1.07810400	-2.84034000	3.74390800
H	1.54482700	-1.21644700	4.31421900
H	0.30496000	-2.14534200	5.19507400
O	4.05990300	-2.76754100	-2.67064300
C	3.14560100	-2.64015500	-1.69490100
C	3.57922200	-2.16033400	-0.45134200
C	1.78647900	-2.96841300	-1.84809500
C	2.66324900	-2.00207200	0.61901300
C	0.88099700	-2.80291300	-0.79624200
C	1.29351700	-2.30288800	0.46587800
O	0.41618600	-2.25555600	1.48595500
Cl	1.28366000	-3.58850200	-3.39732700
Cl	-0.77909200	-3.23605100	-1.03015200
C	4.96104400	-1.84135200	-0.28468000
C	3.18347300	-1.54052000	1.86671800
N	6.08693600	-1.58213300	-0.14994400
N	3.67633300	-1.17339700	2.85443900
O	-6.34431500	-1.40529400	-1.07146800
O	-5.73440400	3.25643300	0.20993400
O	4.36651200	3.98370900	1.14102700
O	1.51234800	3.89878900	-2.80706500
C	-7.64483200	-1.16671300	-1.60093400
H	-7.61634400	-0.44300400	-2.42473100
H	-7.99370500	-2.12944200	-1.97759700
H	-8.33418000	-0.80881100	-0.82643000
C	-7.02246700	3.63350500	-0.26716200
H	-7.10751600	4.70469400	-0.07817300
H	-7.12300900	3.44553400	-1.34313300

H	-7.81994900	3.10581900	0.27016800
C	2.16326200	5.02226500	-3.39369700
H	1.66147300	5.19129000	-4.34759400
H	2.06242500	5.91667400	-2.76694700
H	3.22646500	4.82137700	-3.57311100
C	5.11951500	5.09572300	0.66558500
H	4.48736700	5.98277100	0.53697200
H	5.87004700	5.29522800	1.43182000
H	5.62035500	4.86479300	-0.28243800

meta-Me-Ph (TS_A)

E(B3LYP/BS1) = -2492.924712 au

H(B3LYP/BS1) = -2492.347392 au

G(B3LYP/BS1) = -2492.468616 au

E(M06-2X/BS2//B3LYP/BS1) = -2492.736351 au

C	-0.93059100	2.21627100	-0.80271100
C	-2.25361600	1.74272300	-0.27052500
C	-0.00812200	1.32520900	-1.51750300
C	-2.87686400	0.68533400	-0.85308300
H	-2.40196200	0.25847400	-1.73407200
C	0.19791800	0.06120500	-0.98078100
H	-0.48480700	-0.21826400	-0.18602000
C	-4.15622600	0.06285000	-0.50126200
C	-4.63322500	-0.03581500	0.81892400
C	-4.91739000	-0.51765400	-1.53615800
C	-5.84833000	-0.66780200	1.10380300
H	-4.03015600	0.33945800	1.63907400
C	-6.13877600	-1.14182400	-1.28215400
H	-4.54294400	-0.47057600	-2.55647500
C	-6.58912400	-1.20734700	0.04514900
H	-7.53257000	-1.70632600	0.25954400
C	1.11580300	-0.99911300	-1.34048300
C	2.29043700	-0.83740600	-2.11724100
C	0.84405000	-2.27980800	-0.80335700
C	3.14340700	-1.90959100	-2.36182900
H	2.55972300	0.13620100	-2.50526900
C	1.67776800	-3.37418400	-1.04489500
H	-0.05225800	-2.41770200	-0.20348000
C	2.82143100	-3.16900900	-1.82324100
H	3.48746600	-4.00791800	-2.01390100
C	-2.83284200	2.58705900	0.83886800
H	-3.92328700	2.52900900	0.86076800
H	-2.45668900	2.27038300	1.81950200
H	-2.54520700	3.63305100	0.69832300
C	0.69780600	1.85346800	-2.73805000
H	0.10161400	2.64631200	-3.19541400
H	1.68792200	2.26847400	-2.51195400
H	0.83813400	1.05268000	-3.46879300
O	-1.06591300	3.52109100	-1.27639100
H	-0.21414700	2.30550100	0.32616300
C	-0.02302500	4.47686100	-1.03344000
H	-0.36332200	5.40261700	-1.50024600

H	0.11041700	4.63244300	0.04111200
H	0.92906000	4.17579500	-1.47770400
O	0.49835800	2.32697500	1.39415500
C	1.34033100	1.34849000	1.43292900
C	0.98918200	0.10770700	2.08010000
C	2.69287300	1.46721300	0.91686600
C	1.86720100	-0.96222400	2.13010900
C	3.57618700	0.42261800	0.96359600
C	3.21518400	-0.88812900	1.53749000
O	3.98623400	-1.84898300	1.55260800
Cl	3.14509700	3.01017200	0.26042500
Cl	5.20099100	0.55830800	0.37652000
C	-0.30788400	0.02313100	2.67906000
C	1.52037200	-2.18584800	2.77266000
N	-1.35900600	-0.04995700	3.17171400
N	1.24001700	-3.18966900	3.29156000
C	4.40312100	-1.73462100	-3.17691000
H	5.29407000	-1.95524200	-2.57699000
H	4.41573000	-2.41719400	-4.03490900
H	4.49607800	-0.71271000	-3.55553700
C	1.35332500	-4.73071300	-0.46401800
H	1.31250600	-4.68873700	0.63066300
H	0.37621900	-5.08681300	-0.81127300
H	2.10412600	-5.47415500	-0.74670900
C	-6.35597500	-0.75605800	2.52503300
H	-7.02421900	0.08349500	2.75800400
H	-6.92394600	-1.67746500	2.69070200
H	-5.53259700	-0.72643600	3.24579900
C	-6.96274600	-1.73260500	-2.40307200
H	-7.32923400	-2.73257600	-2.14476600
H	-7.84338800	-1.11293700	-2.61586300
H	-6.38228900	-1.81060900	-3.32747500

meta-Me-Ph (TS_B)

E(B3LYP/BS1) = -2492.911863 au

H(B3LYP/BS1) = -2492.334011 au

G(B3LYP/BS1) = -2492.457043 au

E(M06-2X/BS2//B3LYP/BS1) = -2492.724775 au

C	0.06488100	-1.21088600	-1.92052200
C	1.39175700	-0.58569500	-1.94487200
C	-1.16561000	-0.32084500	-1.96177300
C	1.55296500	0.52845200	-1.14889100
H	0.64327400	0.89739200	-0.68003000
C	-1.94274300	-0.07685800	-0.89122800
H	-1.63505200	-0.49697000	0.06120700
C	2.70986100	1.36414500	-0.88126900
C	4.05225500	1.01027000	-1.13891700
C	2.45109500	2.62238000	-0.28692600
C	5.09761200	1.88735500	-0.84143800
H	4.29521300	0.03280500	-1.53183700
C	3.47453400	3.51979300	0.00634900
H	1.42282800	2.89522100	-0.06243300

C	4.79318500	3.13445200	-0.27968300
H	5.60573700	3.81946800	-0.04457200
C	-3.16364700	0.74822300	-0.80474800
C	-4.14552900	0.77123100	-1.80760000
C	-3.37816100	1.50097100	0.36453700
C	-5.30354200	1.54737500	-1.67116300
H	-4.03081800	0.14828700	-2.68937300
C	-4.51833900	2.29093300	0.52390900
H	-2.63520300	1.47157700	1.15841100
C	-5.47140800	2.30150400	-0.50502100
H	-6.37273800	2.90021200	-0.38621000
C	2.47489600	-1.23039000	-2.77190100
H	3.11058300	-0.46304300	-3.22181800
H	3.11968000	-1.88425000	-2.17203400
H	2.03928200	-1.83486500	-3.56815900
C	-1.37278100	0.27598600	-3.34247500
H	-0.41356700	0.59218100	-3.76558100
H	-1.81251800	-0.44185300	-4.04573800
H	-2.03248700	1.14460400	-3.29330700
O	-0.00116400	-2.32868100	-2.70263500
H	0.15373700	-1.77258500	-0.58581900
C	-1.22530800	-3.08630500	-2.71779700
H	-2.04728500	-2.50707500	-3.14470300
H	-1.01508700	-3.95357200	-3.34300300
H	-1.48743200	-3.41271600	-1.70750300
O	-1.52708900	-3.39488100	1.09770600
C	-0.69777700	-2.53823500	1.33783500
C	0.59266400	-2.45008400	0.53007400
C	-0.90001900	-1.49737200	2.38005300
C	1.68375100	-1.69947300	1.08977600
C	0.08369500	-0.62656700	2.71049000
C	1.47405800	-0.70210400	2.12040100
O	2.36479600	0.02495600	2.55448900
Cl	-2.45572200	-1.50493300	3.14123200
Cl	-0.14084200	0.60036900	3.89892000
C	0.93325300	-3.72054600	-0.08756900
C	3.02008400	-1.93925300	0.69142000
N	1.21593100	-4.72961700	-0.58748200
N	4.12198400	-2.15469400	0.37071500
C	-6.34310900	1.57558500	-2.76843100
H	-6.11613500	2.35501200	-3.50787500
H	-6.38421400	0.62216200	-3.30551200
H	-7.34033600	1.78701600	-2.36923800
C	-4.72266200	3.12116800	1.77032300
H	-4.04532000	2.81170800	2.57220000
H	-4.53684100	4.18481200	1.57231900
H	-5.75064500	3.03885900	2.14080600
C	3.18464300	4.86879200	0.62178200
H	3.45514000	5.68196800	-0.06298000
H	2.12390500	4.97601900	0.86684400
H	3.76252300	5.01748800	1.54135700

C	6.53023400	1.50369300	-1.13227100
H	6.65375300	0.41665800	-1.15792800
H	6.85259500	1.89502500	-2.10598100
H	7.21253900	1.90889200	-0.37791100

meta-Me-Ph (TS_D)

E(B3LYP/BS1) = -2492.90768 au

H(B3LYP/BS1) = -2492.332218 au

G(B3LYP/BS1) = -2492.45855 au

E(M06-2X/BS2//B3LYP/BS1) = -2492.710239 au

C	0.52882300	-0.78767600	2.47774000
C	1.88956700	-0.49919400	1.99466000
C	-0.33370000	-1.82389200	1.83622600
C	2.38200900	-1.13318400	0.87048600
H	1.81606000	-1.98977600	0.51408100
C	-0.67423700	-1.65704000	0.52456600
H	-0.29175300	-0.75596700	0.04766200
C	3.59425500	-0.86791700	0.11663600
C	4.20069600	0.40365700	0.01792100
C	4.15969800	-1.93776000	-0.61597700
C	5.34444900	0.60092100	-0.75746600
H	3.74727600	1.25837900	0.50682600
C	5.31140400	-1.77172400	-1.38202100
H	3.68459300	-2.91499600	-0.56869900
C	5.89179600	-0.49459000	-1.44134500
H	6.78158600	-0.34637000	-2.05062000
C	-1.43563800	-2.50132500	-0.39402900
C	-2.31824100	-3.53225600	-0.01038900
C	-1.29066600	-2.23286200	-1.77295100
C	-3.01344900	-4.28322000	-0.96232700
H	-2.50061200	-3.73488300	1.03708200
C	-1.96337600	-2.97398500	-2.74402400
H	-0.62923500	-1.42728900	-2.08396300
C	-2.82243800	-3.99784700	-2.32059500
H	-3.36508600	-4.57723700	-3.06548400
C	2.68377300	0.51179900	2.78817600
H	3.75534300	0.38483400	2.62523200
H	2.41407200	1.53644600	2.50666900
H	2.47050800	0.39860500	3.85252100
C	-0.72884800	-3.00621000	2.69056300
H	-0.10034300	-3.05838300	3.58215400
H	-1.77271700	-2.95790100	3.02472700
H	-0.61399600	-3.93667900	2.12506900
O	0.44983000	-0.70667400	3.86797400
H	-0.00248900	0.42352200	2.03502500
C	-0.79077900	-0.29515000	4.45293500
H	-0.65142300	-0.37938900	5.53206800
H	-1.01253700	0.74339800	4.18894300
H	-1.62417200	-0.93428800	4.14561900
O	-0.19529400	1.65419300	1.81442300
C	-0.90256800	2.15109200	0.85186600
C	-0.28402400	3.10034500	-0.03042000

C	-2.29991000	1.85050000	0.63781800
C	-0.98491900	3.68316700	-1.08529800
C	-3.00311300	2.41784800	-0.39816800
C	-2.38702300	3.36604700	-1.33935800
O	-3.01431700	3.87325200	-2.28327600
Cl	-3.06568900	0.78318000	1.77236700
Cl	-4.67518700	2.07437800	-0.66257300
C	1.09150400	3.40999000	0.20002500
C	-0.36057500	4.60540400	-1.97230500
N	2.21199200	3.66745000	0.37982500
N	0.15258500	5.35918800	-2.69608100
C	-3.95004500	-5.39158500	-0.53785700
H	-4.88422900	-5.36574200	-1.10971800
H	-3.49709800	-6.37725400	-0.70598800
H	-4.19904500	-5.32020600	0.52537300
C	-1.77347500	-2.68832900	-4.21596100
H	-1.23228500	-1.75069200	-4.37462300
H	-1.20265300	-3.48875300	-4.70369800
H	-2.73589000	-2.61836700	-4.73559400
C	5.92554300	-2.92897100	-2.13513000
H	5.27008500	-3.80497600	-2.12474900
H	6.12353000	-2.66359800	-3.17998100
H	6.88474600	-3.22455800	-1.69167800
C	5.98342600	1.96726600	-0.85523100
H	5.27973100	2.75578700	-0.57154400
H	6.85278400	2.04421700	-0.18926100
H	6.33683500	2.17106900	-1.87174000

meta-Me-Ph (2_D)

E(B3LYP/BS1) = -2492.933112 au

H(B3LYP/BS1) = -2492.350816 au

G(B3LYP/BS1) = -2492.480104 au

E(M06-2X/BS2//B3LYP/BS1) = -2492.723518 au

C	-2.47582100	1.39340600	2.25059700
C	-2.61291500	0.02056500	1.60888300
C	-2.28368600	2.28318200	1.01749600
C	-3.82741200	-0.29875400	1.04417900
H	-4.63009000	0.41246700	1.22159200
C	-0.99626900	2.37521700	0.52049100
H	-0.24176500	1.82060900	1.07555700
C	-4.23441800	-1.48552000	0.32453600
C	-3.35004300	-2.32127800	-0.40013400
C	-5.61884200	-1.79050100	0.30869900
C	-3.82152200	-3.43755400	-1.08778600
H	-2.29885500	-2.06903800	-0.47684500
C	-6.11108100	-2.91048200	-0.35310300
H	-6.30488100	-1.13808300	0.84312700
C	-5.19702600	-3.72448400	-1.04377800
H	-5.56880100	-4.59698500	-1.57782800
C	-0.44997100	3.09531300	-0.60135700
C	-1.18473100	3.89726100	-1.51454400
C	0.95641000	2.98387600	-0.78664300

C	-0.55072100	4.55698400	-2.56089900
H	-2.25487600	4.00568100	-1.41337100
C	1.61154800	3.63550900	-1.82487300
H	1.51928800	2.35572400	-0.10233300
C	0.84353000	4.41956200	-2.70180800
H	1.34112900	4.93697800	-3.51986100
C	-1.41133200	-0.87584800	1.69108500
H	-1.68746800	-1.92532700	1.57514000
H	-0.64779600	-0.64422200	0.93881100
H	-0.93059200	-0.74958100	2.66806400
C	-3.50294600	2.94296200	0.43942700
H	-4.38174200	2.72945300	1.04891300
H	-3.36609700	4.03118600	0.42402100
H	-3.70038500	2.62266300	-0.58885100
O	-3.61051900	1.70798900	3.02300000
H	-1.57199800	1.41779800	2.87322100
C	-3.43574600	2.86410300	3.84177100
H	-4.35538700	2.97568200	4.41911700
H	-2.58771800	2.73366200	4.52736200
H	-3.27395400	3.77022900	3.24338400
O	1.70124600	0.14143900	0.77005000
C	2.67794700	-0.58849800	0.49551200
C	2.58577100	-1.69374400	-0.44198800
C	4.00505900	-0.38478700	1.10022700
C	3.68199000	-2.50880400	-0.74656500
C	5.07592100	-1.17890100	0.80518800
C	4.99136000	-2.30398300	-0.14608700
O	5.96880600	-3.02481200	-0.41477400
Cl	4.12166700	0.93794200	2.22677200
Cl	6.63698500	-0.92906500	1.52985600
C	1.31584100	-1.91451400	-1.04602700
C	3.56452900	-3.58583100	-1.67012100
N	0.27572400	-2.09204600	-1.54115400
N	3.45979500	-4.46542300	-2.42724800
C	3.10410100	3.51038000	-2.01638000
H	3.54919000	2.86011000	-1.25839400
H	3.34150300	3.09479400	-3.00275200
H	3.59293900	4.48986600	-1.95318100
C	-1.32861800	5.40741500	-3.53641400
H	-0.96285500	6.44108600	-3.53643200
H	-1.22226600	5.02900300	-4.56005700
H	-2.39416500	5.42478600	-3.29083200
C	-7.58250400	-3.25021500	-0.34085400
H	-7.96702900	-3.38148400	-1.35885400
H	-7.76516600	-4.18932300	0.19567000
H	-8.16896300	-2.46590000	0.14630900
C	-2.88157900	-4.32406200	-1.87035700
H	-1.87385900	-3.90148300	-1.90505200
H	-2.81679000	-5.32105200	-1.41674600
H	-3.23347600	-4.46271700	-2.89921800

meta-Me-Ph (2_A)

E(B3LYP/BS1) = -2492.96664 au
H(B3LYP/BS1) = -2492.382923 au
G(B3LYP/BS1) = -2492.50504 au
E(M06-2X/BS2//B3LYP/BS1) = -2492.800214 au

C	-0.47048500	-0.38967400	2.07157500
C	-1.88730700	-0.61617000	1.51817700
C	0.22157700	0.91435200	1.66872500
C	-2.49454600	0.32272700	0.76261600
H	-1.95075400	1.24241000	0.57219100
C	0.53208600	1.12289400	0.36990100
H	0.23442600	0.35840400	-0.34430900
C	-3.84936900	0.31742500	0.18202600
C	-4.52402400	-0.83962400	-0.24272900
C	-4.48333700	1.56185500	-0.00487000
C	-5.80316900	-0.77061400	-0.80919300
H	-4.03802100	-1.80638700	-0.16840700
C	-5.76182800	1.66102000	-0.55586400
H	-3.96082300	2.46828000	0.29431100
C	-6.40884800	0.48202900	-0.95400700
H	-7.39996900	0.54471900	-1.40004800
C	1.17470100	2.28669200	-0.26451500
C	2.14590500	3.08170500	0.36623100
C	0.82869900	2.58457900	-1.59728700
C	2.73898000	4.16467900	-0.29509200
H	2.47903400	2.83378700	1.36854900
C	1.39414900	3.66451900	-2.27657400
H	0.09815300	1.95862800	-2.10565400
C	2.34963800	4.44520500	-1.60905700
H	2.81123300	5.28078100	-2.13228900
C	-2.56293100	-1.88049900	2.00327800
H	-3.63986900	-1.72526200	2.11396600
H	-2.41714600	-2.71727400	1.31340100
H	-2.15536700	-2.17865700	2.97031300
C	0.37969600	1.95993600	2.74891100
H	-0.41833800	1.86336300	3.48932900
H	1.33323900	1.87366400	3.28376000
H	0.33845600	2.96330500	2.31718700
O	-0.61908300	-0.54476700	3.44549600
H	3.87785400	-2.93515300	-3.00627500
C	0.49586900	-0.84790600	4.29202400
H	0.96951100	-1.78403500	3.98830300
H	1.24101300	-0.05062000	4.30650600
H	0.06565400	-0.96103500	5.28908200
O	4.21935500	-2.41870100	-2.25309100
C	3.25095600	-2.23044700	-1.34136000
C	3.57378000	-1.50922800	-0.18377000
C	1.94031300	-2.72211300	-1.47905700
C	2.59688500	-1.27897700	0.81769100
C	0.97451500	-2.48803700	-0.49626600
C	1.27411500	-1.74961800	0.67802000
O	0.35150100	-1.63764700	1.65105800

Cl	1.57604200	-3.63213500	-2.92016600
Cl	-0.61972500	-3.13151100	-0.70422900
C	4.90642800	-1.01929200	-0.03203800
C	3.00816200	-0.56590700	1.98508200
N	5.99216400	-0.62047700	0.09097100
N	3.41568300	0.00939900	2.91047700
C	-6.51899500	-2.03028000	-1.24232000
H	-5.81292900	-2.79491100	-1.58325300
H	-7.09186200	-2.46551000	-0.41262000
H	-7.22538400	-1.83041100	-2.05466100
C	-6.44002500	3.00260300	-0.71638100
H	-5.72450300	3.82590000	-0.62587100
H	-6.93529100	3.08643200	-1.69036200
H	-7.21208700	3.15094500	0.04994700
C	3.77108100	5.01871900	0.40591200
H	3.29368400	5.81850600	0.98754100
H	4.37263000	4.42686800	1.10390400
H	4.44803000	5.49634500	-0.30970300
C	0.98887400	3.99250000	-3.69546400
H	0.42855700	3.17035200	-4.15139600
H	0.35185900	4.88586600	-3.72932200
H	1.86324000	4.19883900	-4.32318900

Table 2

TS_A for **X=H, X'=H**

E(B3LYP/BS1) = -1231.983491 au

H(B3LYP/BS1) = -1231.507269 au

G(B3LYP/BS1) = -1231.593567 au

E(M06-2X/BS2//B3LYP/BS1) = -1231.822362 au

C	-0.83660400	1.79969100	-0.72574100
C	-2.09254800	1.24554500	-0.12584300
C	0.20230500	0.98029100	-1.33158500
C	-2.57465300	0.04559900	-0.53604800
H	-2.04215000	-0.44353800	-1.34910000
C	0.58777600	-0.17837800	-0.67298100
H	-0.04616900	-0.47699600	0.15487400
C	-3.76212700	-0.68722600	-0.07770500
C	-4.25778700	-0.64123200	1.24106200
C	-4.42121500	-1.52695200	-0.99979900
C	-5.38366400	-1.37797900	1.60809300
H	-3.74175100	-0.05385200	1.99229900
C	-5.55042800	-2.25568200	-0.63484700
H	-4.04108100	-1.59533900	-2.01629300
C	-6.04059300	-2.18070300	0.67230200
H	-5.74280000	-1.33158300	2.63268500
H	-6.04517800	-2.88707200	-1.36789900
H	-6.91803600	-2.75234000	0.96159500
C	1.62948400	-1.14668500	-0.96946900
C	2.76684800	-0.91141200	-1.77806200
C	1.52539700	-2.41365700	-0.34461400
C	3.71952900	-1.90796700	-1.97841000

H	2.92405600	0.05594900	-2.23529100
C	2.47444100	-3.40837000	-0.55288100
H	0.67233700	-2.61200900	0.29864500
C	3.57796100	-3.16002500	-1.37460500
H	4.58444900	-1.70061200	-2.60231100
H	2.35930900	-4.37417100	-0.06908400
H	4.32499500	-3.93204800	-1.53573200
C	-2.77759000	2.15623200	0.86677700
H	-3.84794000	1.95127400	0.93761400
H	-2.34261600	2.05251500	1.86938200
H	-2.64583800	3.19863200	0.56287400
C	0.85598100	1.47764200	-2.59898600
H	0.18538800	2.16460500	-3.11961900
H	1.79968400	2.00622200	-2.41778400
H	1.07774400	0.63651400	-3.26212400
O	-1.09480600	3.04571600	-1.30782200
H	-0.09308000	2.06997700	0.48655200
C	-0.15950300	4.10803100	-1.08464600
H	-0.53642200	4.95969600	-1.65439900
H	-0.11309800	4.36772400	-0.02240200
H	0.84620000	3.85829800	-1.43815500
O	0.55174600	2.20973900	1.44334600
C	1.56714900	1.37753400	1.48691400
C	1.50160600	0.19234500	2.30354700
C	2.81246900	1.70013800	0.83948800
C	2.58288400	-0.62127100	2.44594900
C	3.89795300	0.88864200	0.96420300
C	3.85369300	-0.33886200	1.76797500
O	4.84088900	-1.08961100	1.87831800
H	0.56229300	-0.01464600	2.80999400
H	2.54846100	-1.50740600	3.07323700
H	4.84247600	1.12531600	0.48275100
H	2.85354500	2.61641800	0.25643100

TS_B for **X=H, X'=H**

E(B3LYP/BS1) = -1231.972488 au

H(B3LYP/BS1) = -1231.495576 au

G(B3LYP/BS1) = -1231.583443 au

E(M06-2X/BS2//B3LYP/BS1) = -1231.809696 au

C	-0.16450200	-1.60120300	-1.12442400
C	1.18793900	-1.14771700	-1.31569000
C	-1.33593000	-0.66386400	-1.31438200
C	1.52663300	0.08014900	-0.76802500
H	0.68849500	0.69499900	-0.45108300
C	-1.91905400	0.00520300	-0.30158500
H	-1.48791400	-0.11014200	0.68836800
C	2.79665600	0.81111900	-0.79246800
C	4.07773000	0.22237500	-0.85998600
C	2.72729000	2.21903800	-0.71847300
C	5.22596900	1.01111800	-0.88885400
H	4.18602900	-0.85505100	-0.85661800
C	3.87534800	3.00657800	-0.75715500

H	1.75303100	2.69522800	-0.64367900
C	5.13262400	2.40518900	-0.84759100
H	6.20053000	0.53289700	-0.93562400
H	3.78852600	4.08854900	-0.70972600
H	6.03153200	3.01471900	-0.87278000
C	-3.05938300	0.94133400	-0.33833300
C	-4.17324200	0.78155900	-1.18357300
C	-3.06145200	2.02549500	0.56114500
C	-5.23034100	1.69221500	-1.15266700
H	-4.23189700	-0.07649000	-1.84457400
C	-4.11354100	2.93867800	0.58664200
H	-2.22185300	2.15138600	1.24025100
C	-5.20214600	2.77821900	-0.27524500
H	-6.08280900	1.54519600	-1.81035100
H	-4.08676500	3.77263300	1.28277800
H	-6.02640000	3.48570000	-0.25350000
C	2.18283700	-2.11690400	-1.90707300
H	2.96177200	-1.58261000	-2.45660900
H	2.67602600	-2.72283000	-1.13431100
H	1.68583600	-2.80891800	-2.58885900
C	-1.73380900	-0.54914600	-2.77503900
H	-0.83985600	-0.53754000	-3.40768100
H	-2.34868600	-1.39564000	-3.10585600
H	-2.29872800	0.36725400	-2.95976500
O	-0.38563300	-2.88685300	-1.56623900
H	0.01579900	-1.77267400	0.42520600
C	-1.57458400	-3.53667600	-1.09723000
H	-2.48055300	-3.04124600	-1.46012400
H	-1.53004700	-4.55219000	-1.49312800
H	-1.59038100	-3.56395400	-0.00169400
O	-1.45342300	-2.67286800	2.65718600
C	-0.62403700	-1.77993400	2.51059000
C	0.54275000	-1.93760200	1.56380900
C	-0.74703600	-0.48508500	3.21610800
C	1.63254700	-1.01515800	1.66588900
C	0.23302400	0.43490000	3.15001200
C	1.52748600	0.19603400	2.43725200
O	2.45451000	1.01093800	2.59301500
H	0.15618900	1.38504600	3.67317600
H	-1.65535900	-0.33041600	3.79253400
H	2.62279500	-1.29818300	1.32960700
H	0.81239100	-2.99093800	1.44043500

TS_D for **X=H, X'=H**

E(B3LYP/BS1) = -1231.966277 au

H(B3LYP/BS1) = -1231.487473 au

G(B3LYP/BS1) = -1231.582497 au

E(M06-2X/BS2//B3LYP/BS1) = -1231.785791 au

C	0.60376500	0.63417900	1.48268300
C	1.96829000	1.05587800	1.02250500
C	0.26812600	-0.85134200	1.38532300
C	2.57669200	0.33895200	0.01839300

H	1.99412800	-0.48107400	-0.39462500
C	-0.48911400	-1.28380100	0.35631000
H	-0.88134900	-0.51958500	-0.31235800
C	3.87235700	0.51040900	-0.60949100
C	4.97624100	1.17896700	-0.02542900
C	4.05474600	-0.08171400	-1.88485300
C	6.18388500	1.28056500	-0.70661300
H	4.90253100	1.57954500	0.97768300
C	5.25767800	0.03754200	-2.56828200
H	3.22663500	-0.62072900	-2.33701000
C	6.32794000	0.72353900	-1.98266500
H	7.02206200	1.78799600	-0.23834300
H	5.36803200	-0.40845400	-3.55217200
H	7.27321800	0.81051700	-2.51033200
C	-0.90306300	-2.65256300	0.00086900
C	-0.13471900	-3.80306300	0.26264200
C	-2.12544100	-2.81519300	-0.68163300
C	-0.58893000	-5.06679700	-0.11626800
H	0.83703200	-3.71042900	0.73462600
C	-2.58242500	-4.07793400	-1.05208700
H	-2.72363900	-1.93631400	-0.90996100
C	-1.81620700	-5.21172300	-0.76707000
H	0.02397000	-5.94001200	0.09055700
H	-3.53343700	-4.17720600	-1.56827300
H	-2.16721000	-6.19735000	-1.05991800
C	2.49455100	2.33511900	1.60658100
H	3.01467700	2.14611900	2.55561400
H	3.18244600	2.84300700	0.92866500
H	1.66530000	3.00648600	1.84492100
C	0.85209200	-1.70686500	2.48455600
H	0.88552700	-1.14601900	3.42300200
H	0.27064400	-2.61842500	2.64248900
H	1.88507100	-2.00046600	2.25155200
O	0.37731800	1.17384300	2.76596700
H	-0.07494500	1.20688800	0.73251700
C	-0.97666900	1.17519600	3.21186000
H	-0.96205600	1.58048700	4.22526200
H	-1.59342200	1.81610300	2.57059600
H	-1.40073400	0.16429300	3.22923300
O	-1.05846600	2.03606200	-0.35597000
C	-2.34373100	2.00414700	-0.53065000
C	-2.92073000	2.86707400	-1.52952500
C	-3.23256800	1.15162100	0.20560900
C	-4.26914100	2.87672000	-1.76543500
C	-4.58377400	1.16224600	-0.03338500
C	-5.18870400	2.02421700	-1.03212600
O	-6.43192600	2.03189600	-1.24931500
H	-2.80811900	0.49129600	0.95450700
H	-5.25001900	0.51341700	0.52957300
H	-4.69550400	3.53384300	-2.51943200
H	-2.24313400	3.50941100	-2.08473300

2_D for **X=H, X'=H**

E(B3LYP/BS1) = -1231.965279 au

H(B3LYP/BS1) = -1231.484374 au

G(B3LYP/BS1) = -1231.579059 au

E(M06-2X/BS2//B3LYP/BS1) = -1231.786145 au

C	-0.83020000	-0.08674700	1.93853600
C	-1.47647100	-0.92431900	0.83839100
C	-0.89684400	1.33683700	1.37799200
C	-2.82822000	-0.77680800	0.64471500
H	-3.34899000	-0.16010800	1.37305600
C	0.07381600	1.67171800	0.44870700
H	0.79352000	0.88761600	0.20770600
C	-3.70442700	-1.39212200	-0.33730800
C	-3.29534500	-1.78386500	-1.63408800
C	-5.06834300	-1.55217500	0.00843400
C	-4.20596000	-2.34091100	-2.52494400
H	-2.27712800	-1.60616600	-1.95910700
C	-5.97058500	-2.12621100	-0.87843800
H	-5.40340300	-1.23299400	0.99167500
C	-5.54149000	-2.52679300	-2.14892300
H	-3.87807500	-2.62306700	-3.52101400
H	-7.00884300	-2.25494200	-0.58751300
H	-6.24661400	-2.96701800	-2.84789000
C	0.31385000	2.88892600	-0.28491600
C	-0.40377700	4.10900600	-0.15260200
C	1.38305600	2.83998200	-1.22582100
C	-0.07139500	5.20808900	-0.93036500
H	-1.21356300	4.20090000	0.55663900
C	1.70093800	3.94283800	-2.00462200
H	1.93402900	1.90724100	-1.32397000
C	0.97712800	5.13240400	-1.85930900
H	-0.62774700	6.13355000	-0.81718300
H	2.51464400	3.88466200	-2.72122600
H	1.22947800	6.00040400	-2.46145600
C	-0.56362700	-1.86576200	0.11963600
H	-1.10067700	-2.57684600	-0.50811800
H	0.19223800	-1.34442800	-0.49228800
H	0.00999500	-2.42913700	0.86853300
C	-2.01814000	2.22035600	1.84197100
H	-2.66621000	1.68913700	2.54000300
H	-1.61129400	3.09154800	2.37198000
H	-2.62082900	2.59709600	1.00915200
O	-1.51281500	-0.26472200	3.15978400
H	0.21976400	-0.39063400	2.04394200
C	-0.78990200	0.22253400	4.29030900
H	-1.39261200	-0.01576100	5.16877600
H	0.18744100	-0.27144700	4.37309800
H	-0.63679900	1.30876500	4.24318700
O	2.08481200	-0.35992500	-0.97169000
C	3.15453900	-1.00271800	-0.67542300
C	3.25480800	-2.43513200	-0.83743500

C	4.32989500	-0.33643100	-0.16184200
C	4.39708100	-3.12353300	-0.51861200
C	5.47255800	-1.02346600	0.15722400
C	5.58062100	-2.46320200	0.00200100
O	6.63475900	-3.09868500	0.29969400
H	4.45332300	-4.20257200	-0.64919100
H	2.38277100	-2.95311800	-1.23185700
H	4.27348100	0.74300000	-0.03417600
H	6.34666700	-0.50398600	0.54533800

2_A for **X=H, X'=H**

E(B3LYP/BS1) = -1232.036133 au

H(B3LYP/BS1) = -1231.55336 au

G(B3LYP/BS1) = -1231.64128 au

E(M06-2X/BS2//B3LYP/BS1) = -1231.893526 au

C	-0.23186000	-1.15924100	0.98636700
C	-1.65492800	-1.28836200	0.39525100
C	0.23865900	0.29032900	1.18634200
C	-2.44430100	-0.20902800	0.23800100
H	-2.04966700	0.75229900	0.55556500
C	0.61250600	1.00103100	0.10323500
H	0.54361800	0.50093500	-0.86096000
C	-3.82298900	-0.13490200	-0.28292400
C	-4.32474300	-0.96030000	-1.30717000
C	-4.67780900	0.85639300	0.23931100
C	-5.63632600	-0.81981700	-1.76356800
H	-3.67817400	-1.69583500	-1.77294000
C	-5.98969800	0.99194100	-0.21015100
H	-4.30331900	1.52045300	1.01495000
C	-6.47756200	0.14945700	-1.21322000
H	-5.99779000	-1.46584000	-2.55938300
H	-6.63002500	1.75865900	0.21802700
H	-7.49831700	0.25584500	-1.57007000
C	1.07195600	2.39688700	0.00809100
C	1.80343800	3.05551600	1.01529000
C	0.80466100	3.10485700	-1.18111700
C	2.21917300	4.37726300	0.84984500
H	2.07867600	2.52376000	1.91931800
C	1.21215600	4.42718200	-1.34269600
H	0.26196300	2.60697800	-1.98123300
C	1.91924800	5.07216600	-0.32387500
H	2.78811900	4.86177500	1.63893200
H	0.98364200	4.95295400	-2.26591200
H	2.24383600	6.10145400	-0.44911200
C	-2.07028300	-2.71077400	0.09976300
H	-3.15612500	-2.82700000	0.14903600
H	-1.74223700	-3.02932500	-0.89708000
H	-1.61434500	-3.39083000	0.82323700
C	0.10847800	0.85269400	2.58182500
H	-0.73895900	0.39404400	3.09776100
H	0.99554200	0.65857200	3.19997600
H	-0.03862500	1.93555100	2.55620600

O	-0.33686100	-1.86301500	2.21789200
H	5.90937300	-1.81259800	-2.59473600
C	0.83857700	-2.36353500	2.84575000
H	1.41291900	-3.00613300	2.17123800
H	1.48480500	-1.56258300	3.22552800
H	0.48917600	-2.95729000	3.69381400
O	5.83926700	-1.49911400	-1.67873700
C	4.53355300	-1.59149700	-1.27035200
C	4.22932000	-1.17282200	0.02796700
C	3.51092000	-2.07982300	-2.09031600
C	2.92211600	-1.24356200	0.50989600
C	2.20323900	-2.13813400	-1.61133000
C	1.89449100	-1.72813000	-0.30895500
O	0.57568700	-1.92631300	0.05683600
H	1.40402300	-2.51244200	-2.24354900
H	3.73064000	-2.40922800	-3.10345800
H	5.02521400	-0.79297000	0.66138800
H	2.71935600	-0.90839600	1.51797000

TS_A for **X=Cl, X'=Cl**

E(B3LYP/BS1) = -3070.350347 au

H(B3LYP/BS1) = -3069.907589 au

G(B3LYP/BS1) = -3070.00697 au

E(M06-2X/BS2//B3LYP/BS1) = -3070.225522 au

C	1.35765700	2.10939900	0.27233000
C	2.61277900	1.40702100	-0.15520700
C	0.43509000	1.55825600	1.26704200
C	3.20210800	0.50825300	0.67442500
H	2.75124700	0.37681500	1.65553800
C	0.10018600	0.21887200	1.15386700
H	0.68730000	-0.34843300	0.43966400
C	4.41787100	-0.28622000	0.46847600
C	4.84980700	-0.75451500	-0.78914600
C	5.17534700	-0.64432300	1.60359400
C	6.00875800	-1.52084200	-0.90504700
H	4.25975700	-0.54895800	-1.67504700
C	6.33828000	-1.40045500	1.48514000
H	4.84521500	-0.31247400	2.58495400
C	6.76279600	-1.83920200	0.22730000
H	6.31880000	-1.87795500	-1.88326200
H	6.91034300	-1.65381500	2.37339500
H	7.66641200	-2.43474000	0.13231100
C	-0.83590900	-0.60124900	1.90299900
C	-1.92649300	-0.11420500	2.66219200
C	-0.67494200	-2.00518000	1.80819800
C	-2.78843700	-0.99279100	3.31181900
H	-2.12322900	0.94791700	2.72229600
C	-1.53282300	-2.87895500	2.46705400
H	0.14741400	-2.40194300	1.21933800
C	-2.59485800	-2.37502500	3.22307000
H	-3.62374100	-0.59721700	3.88212000
H	-1.38001000	-3.95087500	2.38439200

H	-3.27277400	-3.05374500	3.73238400
C	3.17657700	1.86092600	-1.48069900
H	4.25793200	1.71619200	-1.53069600
H	2.72030100	1.31502900	-2.31615100
H	2.96466500	2.92330200	-1.62960500
C	-0.13389200	2.48836800	2.30873900
H	0.54006300	3.33498500	2.45790600
H	-1.11746600	2.88882400	2.03496700
H	-0.24890600	1.96130400	3.26001500
O	1.58339700	3.48341900	0.29102100
H	0.53509500	1.86276500	-0.83084500
C	0.56579100	4.37659100	-0.18402100
H	0.96127900	5.38100900	-0.02364700
H	0.38592800	4.21752100	-1.25156500
H	-0.37353600	4.26450400	0.36225400
O	-0.22315500	1.60581900	-1.74885200
C	-1.09623700	0.69701300	-1.44824100
C	-0.86208600	-0.69958400	-1.76210900
C	-2.39736300	1.04146800	-0.91071500
C	-1.79497900	-1.66298500	-1.49792700
C	-3.33945200	0.08831700	-0.63888700
C	-3.09754600	-1.34525100	-0.88189300
O	-3.93351500	-2.21120700	-0.62028100
Cl	-2.72103200	2.73216700	-0.65849000
Cl	-4.91416700	0.48756900	-0.02453000
Cl	-1.54288600	-3.33397500	-1.89756600
Cl	0.66078700	-1.08790700	-2.51176300

TS_B for **X=Cl, X'=Cl**

E(B3LYP/BS1) = -3070.33312 au

H(B3LYP/BS1) = -3069.889902 au

G(B3LYP/BS1) = -3069.990277 au

E(M06-2X/BS2//B3LYP/BS1) = -3070.204583 au

C	0.51821700	-1.95485900	0.14734000
C	-0.84775900	-1.94721600	0.70430900
C	1.66746400	-1.35855400	0.93911300
C	-1.29057900	-0.77210200	1.24820000
H	-0.55458200	0.02928600	1.31450900
C	2.64056200	-0.67209300	0.30106800
H	2.49276900	-0.46484600	-0.75453400
C	-2.57101800	-0.44423200	1.87268200
C	-3.80571600	-1.02236300	1.50954300
C	-2.57052000	0.54335400	2.88218300
C	-4.98044200	-0.65591700	2.16405100
H	-3.85480700	-1.72899900	0.69019500
C	-3.74298700	0.89683400	3.54251800
H	-1.63262500	1.01997400	3.15575500
C	-4.95369500	0.29303300	3.18875500
H	-5.92206900	-1.10743200	1.86494500
H	-3.71543200	1.64728300	4.32737500
H	-5.87178200	0.57206000	3.69798900
C	3.90017400	-0.11501400	0.82525800

C	4.66715500	-0.71613500	1.84162400
C	4.39407400	1.06311000	0.22894700
C	5.86417800	-0.13931400	2.26696700
H	4.35011100	-1.65664800	2.27792800
C	5.58346800	1.64378000	0.66298900
H	3.82764200	1.52461500	-0.57565900
C	6.32215300	1.04632200	1.68830000
H	6.44425400	-0.62427600	3.04731500
H	5.93823600	2.55875000	0.19660400
H	7.25337800	1.49406500	2.02402900
C	-1.65095700	-3.22094200	0.62136900
H	-2.43019800	-3.23605700	1.38576900
H	-2.13150700	-3.34490000	-0.35568600
H	-0.99606300	-4.08409200	0.76597700
C	1.68614100	-1.69610000	2.41703400
H	0.68377600	-1.64696000	2.84743300
H	2.05530200	-2.71729300	2.58535400
H	2.33259600	-1.01062900	2.96955300
O	0.75642900	-3.12098200	-0.52616500
H	0.25874000	-0.97968200	-0.93640600
C	2.08120100	-3.51396000	-0.91563400
H	2.74398200	-3.58655500	-0.05004200
H	1.95385200	-4.49567700	-1.37293100
H	2.50003200	-2.82006700	-1.64800600
O	1.73800500	1.11328300	-2.32379800
C	0.61536100	1.02681800	-1.86425700
C	-0.19991700	-0.26282900	-1.97656700
C	-0.01239000	2.15367300	-1.12590400
C	-1.60811500	-0.12631900	-1.86020000
C	-1.33449500	2.14906300	-0.85166900
C	-2.25025900	1.01600700	-1.26825200
O	-3.46677400	1.13356400	-1.11290400
Cl	1.03734800	3.48004600	-0.74382500
Cl	-2.11278700	3.46430400	-0.05408600
Cl	0.41578800	-1.29936500	-3.30979100
Cl	-2.67415500	-1.38811000	-2.41542300

TS_D for **X=Cl, X'=Cl**

E(B3LYP/BS1) = -3070.331687 au

H(B3LYP/BS1) = -3069.890662 au

G(B3LYP/BS1) = -3069.995962 au

E(M06-2X/BS2//B3LYP/BS1) = -3070.193975 au

C	-1.45104000	0.90112900	1.95080800
C	-2.46679600	-0.05788000	1.45689700
C	-1.11409100	2.13651400	1.18011600
C	-3.09166400	0.15109100	0.24741900
H	-2.94176600	1.12528300	-0.20978900
C	-0.57792800	1.98169800	-0.06711200
H	-0.42450100	0.95342000	-0.39044400
C	-3.99755000	-0.71131600	-0.49395300
C	-4.01084900	-2.12323700	-0.41233900
C	-4.89315600	-0.09290000	-1.39918000

C	-4.90011400	-2.87092600	-1.17844200
H	-3.29919400	-2.63706700	0.22225200
C	-5.78940400	-0.84224200	-2.15239300
H	-4.88176400	0.98988100	-1.49325300
C	-5.79930900	-2.23690800	-2.04230000
H	-4.88708700	-3.95480100	-1.10827900
H	-6.47543900	-0.34334700	-2.83078300
H	-6.49351600	-2.82608400	-2.63457500
C	-0.20019900	2.95814900	-1.08511100
C	0.02540400	4.33391000	-0.85610400
C	-0.02139100	2.47343400	-2.40162600
C	0.38867200	5.17945800	-1.90196300
H	-0.04840700	4.74400900	0.14212800
C	0.33086900	3.32216600	-3.44545900
H	-0.17235400	1.41500900	-2.59779800
C	0.53492600	4.68339800	-3.20031300
H	0.56520400	6.23209700	-1.69955300
H	0.45248900	2.92283200	-4.44828400
H	0.81577000	5.34926400	-4.01127400
C	-2.74847900	-1.24437300	2.34696500
H	-3.76079700	-1.62312700	2.19165600
H	-2.04127100	-2.05852400	2.14874900
H	-2.63538100	-0.96021800	3.39418500
C	-1.42739000	3.46087900	1.83345000
H	-2.10551200	3.31699500	2.67718500
H	-0.53091400	3.96761000	2.21220300
H	-1.90096100	4.13672100	1.11378600
O	-1.54521000	1.05952300	3.33526500
H	-0.39263300	0.09962600	1.77025400
C	-0.35015700	1.36796900	4.06183400
H	-0.65992100	1.49009200	5.10118000
H	0.36759100	0.54633700	3.98116900
H	0.11695400	2.29406400	3.71257400
O	0.42247300	-0.94410200	1.78092900
C	1.41931500	-1.13193100	0.97593400
C	1.50744200	-2.37312200	0.24549000
C	2.49412800	-0.19247000	0.79381200
C	2.54093900	-2.63400100	-0.62267500
C	3.53394100	-0.44269400	-0.07378700
C	3.62409100	-1.67741500	-0.85242200
O	4.55699900	-1.90194700	-1.64451900
Cl	2.45898800	1.25754000	1.75974500
Cl	4.83237500	0.68764300	-0.29459100
Cl	0.22400800	-3.52471900	0.50228100
Cl	2.63157300	-4.11447300	-1.52402100

2_D for **X=Cl, X'=Cl**

E(B3LYP/BS1) = -3070.35119 au

H(B3LYP/BS1) = -3069.903004 au

G(B3LYP/BS1) = -3070.012288 au

E(M06-2X/BS2//B3LYP/BS1) = -3070.202274 au

C	1.95612700	-0.14984400	1.48382600

C	2.76880600	0.74520300	0.56149200
C	2.19814200	-1.49527500	0.79055300
C	4.10793100	0.90561800	0.86160700
H	4.43773000	0.38987600	1.75871800
C	1.26777000	-1.85537700	-0.16875800
H	0.41887300	-1.18049700	-0.26226800
C	5.14216800	1.69862700	0.24252600
C	5.01949000	2.43644400	-0.96477100
C	6.39690600	1.72914100	0.91137200
C	6.09495500	3.15890300	-1.46319500
H	4.09135600	2.43739900	-1.51732900
C	7.46623300	2.45534100	0.40965800
H	6.51066500	1.16904200	1.83520100
C	7.31919900	3.17582700	-0.78194500
H	5.98356900	3.71356600	-2.38983900
H	8.41369000	2.46323300	0.93956200
H	8.15349500	3.74606700	-1.17954300
C	1.18127300	-3.00751200	-1.03009300
C	2.19243700	-3.98569700	-1.22472300
C	-0.03454600	-3.15332000	-1.75472000
C	1.98508000	-5.04963200	-2.09103100
H	3.14304600	-3.90245900	-0.71711400
C	-0.23749900	-4.22310000	-2.61273300
H	-0.81136600	-2.40597700	-1.62101100
C	0.77259600	-5.17820900	-2.78312400
H	2.77038200	-5.78538900	-2.23493200
H	-1.17466600	-4.31689800	-3.15243300
H	0.61965500	-6.01684000	-3.45592100
C	2.03804700	1.37634100	-0.59162700
H	2.14310000	2.46752800	-0.53680600
H	2.43719100	1.05905600	-1.56127100
H	0.97159500	1.14335200	-0.56658000
C	3.40442000	-2.29358400	1.19861600
H	3.85275000	-1.87506500	2.10128100
H	3.11065600	-3.32692800	1.41500400
H	4.17109200	-2.32751200	0.41680600
O	2.42612700	-0.08709500	2.80814100
H	0.89531400	0.11923700	1.42598400
C	1.59151000	-0.78412500	3.73318700
H	2.02045700	-0.61694800	4.72293900
H	0.56583500	-0.39345100	3.70734400
H	1.56693300	-1.86238900	3.52749700
O	-1.15044500	0.29236100	-0.03379400
C	-2.38485300	0.53019700	0.00771900
C	-3.06036600	1.34358300	-0.99376700
C	-3.24971300	0.01357600	1.05895700
C	-4.40761300	1.60555300	-0.95040300
C	-4.59736100	0.27332700	1.10511200
C	-5.27877600	1.08979100	0.10309900
O	-6.50391700	1.32616800	0.14352300
Cl	-2.46566200	-0.97052700	2.27433900

Cl	-5.61210600	-0.35975800	2.37775000
Cl	-5.19252900	2.58477000	-2.16502400
Cl	-2.04615400	1.97373400	-2.27172700

2_A for **X=Cl, X'=Cl**

E(B3LYP/BS1) = -3070.38915 au

H(B3LYP/BS1) = -3069.939976 au

G(B3LYP/BS1) = -3070.038952 au

E(M06-2X/BS2//B3LYP/BS1) = -3070.285527 au

C	-0.90470100	0.18824100	1.81248500
C	-2.24570700	-0.34543100	1.26681200
C	-0.36971600	1.46866100	1.15747500
C	-2.93889400	0.33885700	0.33404800
H	-2.51259500	1.27097400	-0.02302900
C	-0.01303500	1.44299800	-0.14489900
H	-0.17409400	0.51630900	-0.68969400
C	-4.25322000	0.03686100	-0.26047600
C	-4.77253300	-1.26045400	-0.43660100
C	-5.02597600	1.12085800	-0.72554400
C	-6.02216900	-1.45832000	-1.02555200
H	-4.18745600	-2.12328000	-0.14122200
C	-6.27779000	0.92442300	-1.30394900
H	-4.63494700	2.13018300	-0.62028000
C	-6.78456600	-0.36960100	-1.45387000
H	-6.39714000	-2.47005300	-1.15590200
H	-6.85535600	1.78002800	-1.64365600
H	-7.75807700	-0.52771100	-1.90974300
C	0.52199000	2.52324200	-0.99179100
C	1.34081300	3.56541000	-0.51616700
C	0.23508100	2.48694600	-2.37137300
C	1.82391200	4.54687100	-1.38236800
H	1.63011300	3.59267100	0.52834000
C	0.70947300	3.47233200	-3.23413500
H	-0.37576200	1.67699200	-2.76303600
C	1.50451200	4.51114100	-2.74147000
H	2.45982500	5.33752800	-0.99325700
H	0.46446700	3.42668500	-4.29182900
H	1.88134700	5.27786300	-3.41270200
C	-2.76512900	-1.57896700	1.97407600
H	-3.85366100	-1.53663100	2.07788700
H	-2.51890300	-2.49896900	1.43549200
H	-2.32830400	-1.65579200	2.97054900
C	-0.41039600	2.72763800	1.99259700
H	-1.24656100	2.68664300	2.69509600
H	0.50140400	2.87564300	2.58437400
H	-0.53134300	3.60800700	1.35624800
O	-1.17439700	0.33903400	3.17847900
H	3.98455100	-2.52835100	-2.51977100
C	-0.13812600	0.36502300	4.16306900
H	0.47206000	-0.53843800	4.11634300
H	0.50368500	1.24506400	4.07194300
H	-0.66461300	0.40469800	5.11939700

O	4.25401500	-1.90097900	-1.82452000
C	3.21779200	-1.68403100	-0.98954800
C	3.40528400	-0.81135300	0.09148100
C	1.96446900	-2.29383600	-1.13776400
C	2.36333900	-0.54822800	0.98809300
C	0.91980700	-2.02642000	-0.24627500
C	1.08357200	-1.12742900	0.82945200
O	0.09252200	-0.95826600	1.74310700
Cl	1.76527400	-3.40290800	-2.47703900
Cl	-0.60251400	-2.83702400	-0.46471700
Cl	2.66858600	0.49522100	2.34385200
Cl	4.97781400	-0.08358200	0.27702700

TS_A for **X=CN, X'=H**

E(B3LYP/BS1) = -1416.471388 au

H(B3LYP/BS1) = -1415.994569 au

G(B3LYP/BS1) = -1416.089469 au

E(M06-2X/BS2//B3LYP/BS1) = -1416.304453 au

C	1.11097100	2.10081000	0.18535600
C	2.29354800	1.25773000	-0.19740600
C	0.09707800	1.64655700	1.14309100
C	2.75719700	0.31130400	0.65767000
H	2.27836900	0.24938300	1.63275500
C	-0.37867800	0.35176100	1.00115900
H	0.17409200	-0.27110900	0.30581300
C	3.87215900	-0.62512400	0.47594200
C	4.21325100	-1.19786800	-0.76588700
C	4.60879900	-1.01648100	1.61311500
C	5.27001200	-2.10185800	-0.86644300
H	3.62399900	-0.96793900	-1.64682900
C	5.67130000	-1.91019200	1.50885600
H	4.34391000	-0.60289800	2.58313700
C	6.00923300	-2.45392800	0.26575000
H	5.51044700	-2.53968800	-1.83130600
H	6.23184500	-2.18878300	2.39690600
H	6.83348500	-3.15678700	0.18293800
C	-1.43987000	-0.36111700	1.68570900
C	-2.49262600	0.23887300	2.41924400
C	-1.45727400	-1.77191900	1.54479500
C	-3.48664100	-0.54145700	3.00182400
H	-2.55300000	1.31440800	2.51406600
C	-2.44770700	-2.54706900	2.13627000
H	-0.66778000	-2.25382300	0.97452600
C	-3.46836300	-1.93336100	2.86861900
H	-4.28773000	-0.05976100	3.55473500
H	-2.43059800	-3.62644200	2.01957000
H	-4.24894700	-2.53434400	3.32580400
C	2.93070200	1.61915200	-1.51785500
H	2.41636700	1.13074900	-2.35518300
H	2.86325000	2.69926100	-1.67826600
H	3.98365100	1.33125500	-1.55197000
C	-0.41093400	2.62566800	2.17058100

H	0.33543200	3.40400900	2.34342000
H	-1.34384900	3.11805700	1.87026700
H	-0.60434000	2.11096100	3.11599200
O	1.48764900	3.44406200	0.23772000
H	0.34397500	1.98460100	-0.92568100
C	0.58973600	4.43743300	-0.27804100
H	1.06968800	5.39737800	-0.08065400
H	0.45235800	4.30769500	-1.35554000
H	-0.38569600	4.41508200	0.21742800
O	-0.42453000	1.84813000	-1.90115400
C	-1.47485700	1.15043000	-1.59009100
C	-1.51996400	-0.26420000	-1.88825300
C	-2.65207200	1.75844900	-1.02725600
C	-2.65073500	-1.01587000	-1.61200900
C	-3.76693600	1.03500800	-0.74080000
C	-3.85075600	-0.40278300	-0.99029000
O	-4.85185800	-1.07875600	-0.72234300
C	-0.36328000	-0.85459100	-2.49183800
C	-2.71981400	-2.40428300	-1.92580600
N	0.58195600	-1.33049100	-2.97484100
N	-2.78552000	-3.53878500	-2.17912900
H	-4.65141000	1.50149500	-0.31887100
H	-2.61352400	2.82824400	-0.84509000

TS_B for **X=CN, X'=H**

E(B3LYP/BS1) = -1416.458315 au

H(B3LYP/BS1) = -1415.981012 au

G(B3LYP/BS1) = -1416.077963 au

E(M06-2X/BS2//B3LYP/BS1) = -1416.294668 au

C	0.26049400	0.83744800	-1.51590100
C	-1.03027600	0.15281700	-1.62954000
C	1.52712400	0.00854500	-1.39921300
C	-1.21764000	-0.93161700	-0.80156500
H	-0.34109500	-1.24049300	-0.23677900
C	2.19832700	-0.16243200	-0.24591900
H	1.77549000	0.27358800	0.65355400
C	-2.35942900	-1.81002800	-0.60305900
C	-3.68568800	-1.54558600	-1.01715000
C	-2.10996300	-3.02280900	0.08331800
C	-4.69880600	-2.46999100	-0.77756800
H	-3.93756400	-0.60880400	-1.49288500
C	-3.12288100	-3.94685100	0.31068700
H	-1.10123500	-3.23543400	0.42731500
C	-4.42361300	-3.67438800	-0.12382200
H	-5.71188900	-2.24556800	-1.09832300
H	-2.90242500	-4.87450500	0.83055100
H	-5.21982100	-4.39131700	0.05498500
C	3.43850400	-0.92377900	-0.00146000
C	4.51788900	-0.95667700	-0.90314000
C	3.57083500	-1.61045900	1.22076400
C	5.67401800	-1.67886800	-0.60466400
H	4.46941600	-0.38877100	-1.82617800

C	4.72184900	-2.33880900	1.51399800
H	2.75615300	-1.57702100	1.93978600
C	5.77782100	-2.37888700	0.59917500
H	6.49870100	-1.68575800	-1.31202300
H	4.79746000	-2.87022400	2.45864000
H	6.67876100	-2.94087200	0.82872400
C	-2.06547600	0.72008600	-2.56853300
H	-2.60600900	-0.09032100	-3.06568700
H	-2.80389900	1.33763900	-2.04297300
H	-1.59401200	1.34156800	-3.33023100
C	1.90217400	-0.62295400	-2.72821500
H	1.00516600	-0.98596100	-3.24051300
H	2.39227800	0.08808100	-3.40460700
H	2.57932200	-1.46673700	-2.58018800
O	0.35265800	1.92813400	-2.33062000
H	0.01500500	1.44973400	-0.19492600
C	1.53298600	2.74872200	-2.25039900
H	2.42266600	2.19987800	-2.56799500
H	1.34694900	3.58156600	-2.92794700
H	1.67112800	3.12225900	-1.23181000
O	1.48886500	3.19770700	1.52690500
C	0.68426300	2.30597100	1.74451500
C	-0.53945400	2.11969900	0.83637100
C	0.85000800	1.33220900	2.83666600
C	-1.62833500	1.32086100	1.34524800
C	-0.10686200	0.43561900	3.13499400
C	-1.42643700	0.38938300	2.44623900
O	-2.30437300	-0.37779100	2.85599300
C	-0.90757300	3.34956400	0.15240300
C	-2.94099000	1.46207700	0.83824300
N	-1.20657300	4.32900800	-0.39504900
N	-4.02812800	1.59262100	0.43083500
H	1.78104500	1.39702400	3.39190100
H	0.01691900	-0.27855300	3.94403200

TS_D for **X=CN, X'=H**

E(B3LYP/BS1) = -1416.459557 au

H(B3LYP/BS1) = -1415.984027 au

G(B3LYP/BS1) = -1416.086465 au

E(M06-2X/BS2//B3LYP/BS1) = -1416.280033 au

C	0.91485800	0.05114000	1.88794400
C	1.82781500	1.09143300	1.36088900
C	1.07815400	-1.38937700	1.49322700
C	2.76219100	0.76751500	0.40102300
H	2.91013000	-0.29263800	0.21559000
C	0.78850300	-1.72964500	0.20587000
H	0.44536600	-0.91627400	-0.43247100
C	3.64770000	1.62451200	-0.36782200
C	3.39515600	2.98340100	-0.67062300
C	4.82423700	1.03684300	-0.89342700
C	4.29461400	3.71891700	-1.43584200
H	2.47744000	3.45358500	-0.34008000

C	5.72722000	1.77903900	-1.64490400
H	5.02331900	-0.01230900	-0.69120300
C	5.46739200	3.12671200	-1.91674600
H	4.07718200	4.75785500	-1.66597100
H	6.62902900	1.30915700	-2.02633200
H	6.16728500	3.70814500	-2.50989600
C	0.89767500	-3.00451400	-0.50305200
C	0.98115900	-4.27304100	0.11132700
C	0.89063900	-2.95621500	-1.91541300
C	1.07694500	-5.43117400	-0.65748900
H	0.93955900	-4.36504600	1.18863700
C	0.99715900	-4.11325700	-2.68032200
H	0.80832300	-1.99125600	-2.40913400
C	1.09411300	-5.35874600	-2.05294100
H	1.13198300	-6.39679500	-0.16277000
H	0.99825000	-4.04553800	-3.76446000
H	1.17159900	-6.26540800	-2.64614000
C	1.62579900	2.48469300	1.90392200
H	2.54645700	3.06898600	1.85032000
H	0.84950100	3.01603600	1.33880100
H	1.29787500	2.43816600	2.94321800
C	1.59755200	-2.32788600	2.55741300
H	2.03351100	-1.76130500	3.38318100
H	0.81175400	-2.96735500	2.97855200
H	2.36444700	-2.98939900	2.14124100
O	0.63560100	0.26145100	3.24168900
H	-0.13756200	0.45620100	1.25067100
C	-0.61611700	-0.22111800	3.73731600
H	-0.59343300	-0.06277800	4.81661900
H	-1.44476500	0.34961200	3.30358900
H	-0.75783200	-1.28760700	3.53329700
O	-1.14106300	1.17996300	0.63209200
C	-2.29137300	0.68471100	0.31677200
C	-3.24981100	1.54084200	-0.33196500
C	-2.67566000	-0.67829300	0.57299200
C	-4.51330100	1.06191900	-0.69484700
C	-3.90382500	-1.15117800	0.22164800
C	-4.90735200	-0.32295500	-0.43211400
O	-6.03302500	-0.76012700	-0.75237300
C	-2.86938100	2.89304400	-0.59002300
C	-5.46620200	1.90474600	-1.33451800
N	-2.56317500	3.99576600	-0.80248500
N	-6.24883800	2.59049300	-1.85794000
H	-1.94978600	-1.32865700	1.04866600
H	-4.18280200	-2.18188900	0.41802000

2_D for **X=CN, X'=H**

E(B3LYP/BS1) = -1416.471294 au

H(B3LYP/BS1) = -1415.989476 au

G(B3LYP/BS1) = -1416.093203 au

E(M06-2X/BS2//B3LYP/BS1) = -1416.286701 au

C	2.58478500	-0.64753400	1.89379300

C	2.16577500	0.66752400	1.24976700
C	2.62548200	-1.59163200	0.68788100
C	3.10694200	1.33070900	0.49320700
H	4.11202900	0.91768600	0.52096300
C	1.41081600	-2.10658900	0.26821100
H	0.54219000	-1.78946900	0.84262400
C	2.99391100	2.55707700	-0.26722300
C	1.78647400	3.04737500	-0.82597100
C	4.18771700	3.28517400	-0.50775600
C	1.78001300	4.22902600	-1.55691600
H	0.86395300	2.48651700	-0.73465900
C	4.17013900	4.47399000	-1.22338900
H	5.12409600	2.90777700	-0.10600300
C	2.96326400	4.95347300	-1.74796300
H	0.84920500	4.58356700	-1.98911300
H	5.09171800	5.02557600	-1.38242700
H	2.94752800	5.87894600	-2.31611600
C	1.07418200	-3.00987500	-0.80334800
C	1.99152600	-3.63732100	-1.69005600
C	-0.31162600	-3.29660900	-0.96540000
C	1.53824300	-4.49537700	-2.68077200
H	3.05360300	-3.46146000	-1.60363700
C	-0.75464500	-4.15349800	-1.96155100
H	-1.02045800	-2.81012100	-0.30148200
C	0.16802900	-4.75804200	-2.82367800
H	2.25208100	-4.96730000	-3.34889700
H	-1.81598900	-4.35353900	-2.07210400
H	-0.17544200	-5.43162200	-3.60328300
C	0.77184800	1.13278600	1.54099400
H	0.64986700	2.19903400	1.34658400
H	0.00978300	0.59364700	0.96127600
H	0.54563500	0.94363500	2.59757700
C	3.95851700	-1.84602700	0.04618600
H	4.74551300	-1.29036000	0.55711700
H	4.20945300	-2.91196800	0.12144900
H	3.96545100	-1.58160800	-1.01602200
O	3.81492700	-0.50736900	2.56509000
H	1.80338200	-0.97176300	2.59345600
C	4.12014900	-1.60262300	3.42897600
H	5.06231600	-1.35398300	3.92086500
H	3.33603300	-1.73358000	4.18657700
H	4.24065200	-2.54231100	2.87427900
O	-1.73520400	-0.87016100	0.68481400
C	-2.95138700	-0.54352800	0.71343600
C	-3.44322000	0.67443400	0.08822100
C	-3.95441400	-1.36920400	1.37537300
C	-4.80323300	1.02639800	0.13100700
C	-5.26794000	-1.03058900	1.41906500
C	-5.79065600	0.18749300	0.80373800
O	-7.00377700	0.49042500	0.84968700
C	-2.49085200	1.49705500	-0.57673200

C	-5.27419500	2.21980300	-0.48442900
N	-1.70365900	2.16455100	-1.11999200
N	-5.66011800	3.19802400	-0.98834600
H	-5.99661400	-1.66116800	1.92153300
H	-3.59097400	-2.28053600	1.84306700

2_A for **X=CN, X'=H**

E(B3LYP/BS1) = -1416.533224 au

H(B3LYP/BS1) = -1416.049514 au

G(B3LYP/BS1) = -1416.146407 au

E(M06-2X/BS2//B3LYP/BS1) = -1416.387153 au

C	-0.51954700	0.17487800	1.52548200
C	0.32916100	-1.09110800	1.33833200
C	-1.96191600	0.09408900	1.01031000
C	-0.06887900	-2.03449100	0.46094700
H	-1.03033700	-1.88487700	-0.02687800
C	-2.38119100	0.87197600	-0.00681600
H	-1.63784700	1.51322700	-0.47205900
C	0.59642600	-3.29102100	0.07138100
C	1.99289400	-3.44849800	-0.01224200
C	-0.21465800	-4.38566100	-0.28841700
C	2.55230800	-4.66402400	-0.40812500
H	2.64586800	-2.60958700	0.20054700
C	0.34410800	-5.60220600	-0.67396700
H	-1.29603400	-4.27668500	-0.25342900
C	1.73307800	-5.74777400	-0.73167300
H	3.63285800	-4.76029600	-0.47133000
H	-0.30351000	-6.43463300	-0.93549200
H	2.17205500	-6.69328200	-1.03780500
C	-3.71391000	0.97490900	-0.62962100
C	-4.93044300	0.75948300	0.04615600
C	-3.77398000	1.35535400	-1.98575100
C	-6.15075900	0.88889300	-0.61849900
H	-4.93070400	0.52218200	1.10335900
C	-4.99154700	1.47533100	-2.65161000
H	-2.84725300	1.55007200	-2.52044900
C	-6.18845700	1.23781000	-1.97003600
H	-7.07608500	0.72379100	-0.07306300
H	-5.00721600	1.76026100	-3.70015000
H	-7.14056300	1.33580300	-2.48414300
C	1.58514500	-1.16246000	2.17323400
H	1.90361200	-2.19787300	2.31605500
H	2.41912600	-0.62247200	1.70453800
H	1.41542200	-0.70726400	3.15033000
C	-2.83159000	-0.87135900	1.78578300
H	-2.23419900	-1.67636700	2.21953500
H	-3.34261300	-0.37091500	2.61835700
H	-3.59988100	-1.31644000	1.14697600
O	-0.53530700	0.43611000	2.90640000
H	3.81323300	0.97498300	-3.80259400
C	-1.11379200	1.67419600	3.33432100
H	-0.48111200	2.51892300	3.04836500

H	-2.11968300	1.81815300	2.92483500
H	-1.16987000	1.60961300	4.42259100
O	4.05239200	1.49584800	-3.01780200
C	3.07739900	1.40254700	-2.08384100
C	3.26668400	2.10041600	-0.87931300
C	1.90220900	0.66060200	-2.26565600
C	2.27953800	2.02733300	0.13886600
C	0.93054000	0.60530700	-1.27575200
C	1.10534300	1.27844400	-0.05615100
O	0.16844400	1.34154400	0.92542600
C	4.45334700	2.87039400	-0.68866800
C	2.46556200	2.72688300	1.37154800
N	5.42075400	3.49787800	-0.53196000
N	2.62601000	3.29841600	2.37222500
H	0.02087500	0.04653100	-1.45119900
H	1.74384200	0.13361900	-3.20227900

TS_A for **X=CN, X'=CN**

E(B3LYP/BS1) = -1600.947897 au
H(B3LYP/BS1) = -1600.470816 au
G(B3LYP/BS1) = -1600.575068 au
E(M06-2X/BS2//B3LYP/BS1) = -1600.773626 au

C	1.19361900	2.09886600	0.19479400
C	2.46158900	1.38323000	-0.17589300
C	0.25709400	1.55127000	1.19494100
C	3.02059200	0.49979900	0.69543200
H	2.54888600	0.40503800	1.67110900
C	-0.06840500	0.20726100	1.07561300
H	0.52208000	-0.34561300	0.35261000
C	4.23260200	-0.30422100	0.53722800
C	4.67391500	-0.81970600	-0.69961900
C	4.97348300	-0.62367400	1.69550700
C	5.82827200	-1.59644300	-0.77306100
H	4.09044800	-0.64800600	-1.59708900
C	6.13353300	-1.38798600	1.61718300
H	4.63321900	-0.25427900	2.65960800
C	6.56789800	-1.87443500	0.37993300
H	6.14700400	-1.99333800	-1.73269300
H	6.69556000	-1.61166400	2.51942200
H	7.46927800	-2.47740200	0.31700600
C	-1.00645500	-0.62534200	1.79772900
C	-2.09443100	-0.15305000	2.57462500
C	-0.85555200	-2.02913700	1.65231900
C	-2.96761300	-1.04647600	3.18429300
H	-2.27766100	0.90814500	2.67801800
C	-1.72525800	-2.91641800	2.27404100
H	-0.02963400	-2.41205400	1.05957200
C	-2.78664200	-2.42725900	3.04146800
H	-3.80141500	-0.66602200	3.76614000
H	-1.58313100	-3.98598500	2.15511400
H	-3.47499000	-3.11699800	3.52057500
C	3.06537900	1.80036400	-1.49419900

H	4.14819600	1.65883900	-1.50268200
H	2.64146800	1.22561200	-2.32730100
H	2.85416900	2.85675400	-1.68176400
C	-0.31122100	2.48256200	2.23049300
H	0.36548000	3.32707500	2.37824500
H	-1.29128700	2.88791700	1.94891200
H	-0.43484600	1.95899200	3.18244400
O	1.42713800	3.47185500	0.22317600
H	0.46017200	1.88385800	-0.85790900
C	0.42340200	4.37205700	-0.27387600
H	0.81318600	5.37315300	-0.08415600
H	0.28382200	4.22841000	-1.34942200
H	-0.53482800	4.25200200	0.23626600
O	-0.36164200	1.65388500	-1.88826100
C	-1.21467900	0.72598000	-1.62497600
C	-0.95149900	-0.65359000	-1.97957000
C	-2.49643400	1.01894900	-1.02209800
C	-1.85980300	-1.66243900	-1.71153800
C	-3.41888400	0.02425500	-0.74309700
C	-3.15320000	-1.39338300	-1.05031400
O	-3.95936400	-2.28758600	-0.79183100
C	0.29038900	-0.93505000	-2.63440100
C	-1.59932900	-3.01585400	-2.07792200
N	1.30068200	-1.16144500	-3.16348500
N	-1.38932900	-4.12146200	-2.37287000
C	-4.68360900	0.32311200	-0.15651900
N	-5.71720200	0.56129200	0.32163600
C	-2.79166200	2.38562800	-0.71965900
N	-3.03940700	3.49120400	-0.45811600

TS_B for **X=CN, X'=CN**

E(B3LYP/BS1) = -1600.92925 au

H(B3LYP/BS1) = -1600.451565 au

G(B3LYP/BS1) = -1600.556842 au

E(M06-2X/BS2//B3LYP/BS1) = -1600.759618 au

C	-3.23148800	-1.91463200	0.43329900
C	-2.00661700	-2.39434300	-0.14622300
C	-3.83326300	-0.61058900	0.18016000
C	-1.51131900	-1.71501800	-1.24177300
H	-2.15979600	-0.96138800	-1.67755500
C	-3.01366600	0.48587200	0.25196200
H	-1.97260000	0.29466800	0.50385700
C	-0.26421100	-1.89423300	-1.95617400
C	0.90155700	-2.46811300	-1.39694800
C	-0.20575700	-1.41399100	-3.28610400
C	2.06411800	-2.57881200	-2.15233600
H	0.91132800	-2.78451900	-0.36169700
C	0.95087100	-1.54869700	-4.04420000
H	-1.08578100	-0.94608500	-3.71899100
C	2.08876700	-2.13361100	-3.47844100
H	2.95631300	-3.00082200	-1.70009300

H	0.97307600	-1.18885900	-5.06830600
H	2.99821800	-2.22817300	-4.06476400
C	-3.30275200	1.90487100	0.07746500
C	-4.58853600	2.48311500	-0.02828500
C	-2.17854700	2.76162000	0.01471500
C	-4.73335800	3.85561700	-0.20823900
H	-5.47941900	1.87634900	0.05315600
C	-2.33067900	4.13077300	-0.18084100
H	-1.18558500	2.33339400	0.11982600
C	-3.60899400	4.68307300	-0.29432700
H	-5.72940000	4.28276300	-0.28024900
H	-1.44993700	4.76336800	-0.24040300
H	-3.73144400	5.75256900	-0.44094200
C	-1.39734300	-3.65673200	0.42039000
H	-0.81662800	-4.18336400	-0.33922300
H	-0.73812600	-3.42975100	1.26738800
H	-2.17978300	-4.32739300	0.77978300
C	-5.31121300	-0.59727400	-0.16537700
H	-5.67087100	-1.60264900	-0.39747800
H	-5.94026200	-0.19015100	0.63365900
H	-5.46888500	0.01481000	-1.05897000
O	-3.82845900	-2.78341800	1.22606800
H	4.07423200	-0.49416600	2.76696100
C	-4.82920600	-2.39884100	2.20002600
H	-5.82459100	-2.49811100	1.76612300
H	-4.70688100	-3.10493100	3.02059700
H	-4.65215200	-1.37750800	2.54082800
O	5.82884700	0.47703600	1.00342000
C	4.61558500	0.56448900	1.03431900
C	3.75862800	-0.52707700	1.71119200
C	3.90293700	1.71827800	0.43885500
C	2.25003800	-0.36569700	1.61254100
C	2.53627600	1.76289500	0.40040700
C	1.61863600	0.70989700	0.96484100
O	0.38322900	0.88883400	0.83292700
C	4.19338200	-1.83394600	1.18362900
C	1.44928100	-1.33810200	2.23852700
N	4.49801800	-2.87105100	0.76036300
N	0.80279800	-2.15937500	2.76721300
C	1.87834600	2.88176600	-0.20770100
C	4.71872700	2.75224300	-0.11679100
N	1.35810500	3.79758700	-0.70001300
N	5.38805500	3.59162700	-0.56388100

TS_D for **X=CN, X'=CN**

E(B3LYP/BS1) = -1600.93064 au

H(B3LYP/BS1) = -1600.455444 au

G(B3LYP/BS1) = -1600.564444 au

E(M06-2X/BS2//B3LYP/BS1) = -1600.752056 au

C	-1.25448900	0.88222600	1.97515100
C	-2.34214700	0.02818700	1.45809300
C	-0.75731700	2.07589500	1.23875300

C	-2.97030500	0.33636600	0.27115100
H	-2.75992300	1.31743800	-0.14619700
C	-0.32382800	1.90452500	-0.04895400
H	-0.37939700	0.88856100	-0.43638500
C	-3.94756500	-0.42905300	-0.48665100
C	-4.04045100	-1.84009700	-0.47736500
C	-4.82914500	0.28679300	-1.33114000
C	-4.99292900	-2.49423300	-1.25346300
H	-3.34033000	-2.42709100	0.10514800
C	-5.78847300	-0.36946400	-2.09382600
H	-4.75706400	1.37070300	-1.36972500
C	-5.87727000	-1.76511800	-2.05520800
H	-5.04073200	-3.57933700	-1.23999500
H	-6.46265200	0.20315500	-2.72424700
H	-6.62091200	-2.28142900	-2.65544800
C	0.17085400	2.85873900	-1.03712600
C	0.66964900	4.14963300	-0.75210300
C	0.17502500	2.43643900	-2.38713500
C	1.12447700	4.97879300	-1.77505600
H	0.73809700	4.49927500	0.26913100
C	0.61934300	3.27101400	-3.40689300
H	-0.18753800	1.44038600	-2.62830700
C	1.09429000	4.55092400	-3.10507100
H	1.51192100	5.96361900	-1.52983700
H	0.60142500	2.92290500	-4.43568900
H	1.44784700	5.20428800	-3.89751200
C	-2.71691700	-1.16548500	2.30674100
H	-3.75948100	-1.44846300	2.14746900
H	-2.08943400	-2.03390100	2.07340900
H	-2.57333600	-0.93168000	3.36277600
C	-0.77910600	3.39697600	1.96830200
H	-1.43249400	3.33963100	2.84113800
H	0.21718500	3.69790300	2.31504600
H	-1.14667800	4.18789500	1.30680500
O	-1.30942400	0.99088600	3.36248400
H	-0.22742300	-0.05567500	1.73025300
C	-0.08140300	1.08366500	4.09676400
H	-0.37034900	1.28036800	5.13046200
H	0.46601100	0.13665400	4.04388700
H	0.55882400	1.89240200	3.73565400
O	0.42982400	-1.11196100	1.65470500
C	1.44970600	-1.34701100	0.89906700
C	1.48567300	-2.61131700	0.20169200
C	2.57203300	-0.46093000	0.73739800
C	2.54403700	-2.96178000	-0.62309500
C	3.64073900	-0.80158400	-0.08996000
C	3.68664500	-2.06679600	-0.82589100
O	4.63554300	-2.36481300	-1.56854200
C	0.36440200	-3.48242100	0.37702600
C	2.56348000	-4.20502400	-1.32089000
N	-0.54895100	-4.18912000	0.51196800

N	2.58025100	-5.21898100	-1.89064200
C	2.60883200	0.76100400	1.47696800
C	4.75787500	0.06947600	-0.24735700
N	2.67130800	1.75286600	2.08069900
N	5.66947900	0.78058600	-0.37724400

2_D for **X=CN, X'=CN**

E(B3LYP/BS1) = -1600.957721 au

H(B3LYP/BS1) = -1600.475657 au

G(B3LYP/BS1) = -1600.589032 au

E(M06-2X/BS2//B3LYP/BS1) = -1600.767993 au

C	-3.14684000	-1.06542100	-1.78377200
C	-2.87207900	0.32579700	-1.23510600
C	-2.97024000	-1.90117700	-0.50996700
C	-3.90715000	0.96318900	-0.58224100
H	-4.86529400	0.45180600	-0.61662000
C	-1.67456600	-2.25957900	-0.18388900
H	-0.90899200	-1.91621000	-0.87745300
C	-3.95125600	2.25216900	0.06767700
C	-2.81767800	2.96425900	0.53819600
C	-5.23475700	2.82139200	0.28412000
C	-2.97022200	4.19316200	1.16653100
H	-1.82289400	2.54702000	0.45422500
C	-5.37801100	4.05615800	0.89927000
H	-6.11353200	2.27871500	-0.05306900
C	-4.24379600	4.74994400	1.34072600
H	-2.09177000	4.71755600	1.52983900
H	-6.36725500	4.47944100	1.04382300
H	-4.35263400	5.71382300	1.82915300
C	-1.13702300	-3.03676400	0.90329900
C	-1.88474600	-3.63139300	1.95634800
C	0.27380400	-3.22862400	0.89799100
C	-1.24773100	-4.37277900	2.94002300
H	-2.95747800	-3.51578200	2.00741200
C	0.90153400	-3.97251900	1.88519300
H	0.86219500	-2.76249600	0.11464400
C	0.14338200	-4.55006000	2.91064800
H	-1.83313300	-4.81963200	3.73764100
H	1.97877700	-4.10377500	1.85971300
H	0.63091700	-5.13469900	3.68516200
C	-1.50202100	0.89177400	-1.47829300
H	-1.54847500	1.97756300	-1.59505600
H	-0.79200800	0.67925800	-0.67040800
H	-1.07620300	0.46835000	-2.39326600
C	-4.20079800	-2.22941500	0.28486200
H	-5.09211400	-1.83045000	-0.20029400
H	-4.32038200	-3.31821500	0.34862100
H	-4.15084400	-1.84327600	1.30798800
O	-4.42800500	-1.14711000	-2.35654500
H	-2.37788800	-1.33160900	-2.51984900
C	-4.64835200	-2.35551500	-3.08502600
H	-5.64978000	-2.27928900	-3.51219700

H	-3.91326800	-2.46422600	-3.89347400
H	-4.59924900	-3.23958300	-2.43629500
O	1.47308900	-0.33461700	-0.30076100
C	2.61221900	0.17586400	-0.26723000
C	2.83399200	1.57183800	0.10768900
C	3.81762600	-0.58445400	-0.59743600
C	4.10054400	2.14129600	0.13458200
C	5.08436800	-0.01720100	-0.57021700
C	5.30625900	1.38375200	-0.20563900
O	6.44113100	1.89389000	-0.18368400
C	1.67691500	2.33314000	0.45185900
C	4.28748700	3.50778200	0.50160700
N	0.73140500	2.95026400	0.73457800
C	6.24341800	-0.78274300	-0.89870100
C	3.62922800	-1.95553800	-0.94689900
N	7.18626600	-1.40986300	-1.16719100
N	3.46549700	-3.07466200	-1.22274000
N	4.43548000	4.62260600	0.80112800

2_A for **X=CN, X'=CN**

E(B3LYP/BS1) = -1600.992258 au

H(B3LYP/BS1) = -1600.508761 au

G(B3LYP/BS1) = -1600.613037 au

E(M06-2X/BS2//B3LYP/BS1) = -1600.842862 au

C	-0.77888300	0.39502200	1.88494100
C	-2.14108100	-0.05132500	1.34771100
C	-0.08726900	1.55573900	1.17432800
C	-2.70738300	0.56957100	0.29071600
H	-2.19078500	1.42485500	-0.13257600
C	0.27247300	1.42030800	-0.12280400
H	0.01849400	0.48607000	-0.61734600
C	-3.99504900	0.27504100	-0.36367800
C	-4.50048700	-1.02703000	-0.53983000
C	-4.73363300	1.35092400	-0.89452200
C	-5.71493300	-1.23748800	-1.19408800
H	-3.92433600	-1.88030700	-0.19823200
C	-5.95216300	1.14091700	-1.53652800
H	-4.34640600	2.36171300	-0.79004900
C	-6.45024800	-0.15662800	-1.68580100
H	-6.08288500	-2.25139500	-1.32650400
H	-6.50970500	1.98807600	-1.92674400
H	-7.39671200	-0.32417400	-2.19240300
C	0.91602700	2.38892500	-1.02540700
C	1.81796500	3.38438900	-0.60266100
C	0.64352000	2.28375800	-2.40453400
C	2.39811800	4.25725500	-1.52330900
H	2.09778600	3.45631400	0.44189200
C	1.21368000	3.16388300	-3.32096500
H	-0.03203700	1.50640200	-2.75335000
C	2.09251600	4.15842600	-2.88247100
H	3.09793400	5.01234400	-1.17605100
H	0.97853800	3.06962800	-4.37750000

H	2.54455900	4.84202500	-3.59560600
C	-2.82210100	-1.13315800	2.15654300
H	-3.90388500	-1.10420800	2.00813300
H	-2.47206700	-2.13258200	1.88270700
H	-2.61336800	-0.99112100	3.21858300
C	0.01417500	2.85550400	1.94058100
H	-0.78427600	2.92350700	2.68323200
H	0.96712800	2.95990300	2.47351200
H	-0.07133200	3.70552200	1.25842300
O	-0.95723600	0.57678900	3.23816300
H	3.69179700	-3.30206100	-2.37540000
C	0.15042600	0.57521700	4.15013900
H	0.63428100	-0.40361700	4.15588500
H	0.88636000	1.34610500	3.91853500
H	-0.29277400	0.77488300	5.12704800
O	3.98772400	-2.58683300	-1.78288000
C	3.01587100	-2.20983800	-0.94099900
C	3.31868200	-1.19026700	-0.01881600
C	1.72895000	-2.77739100	-0.91566400
C	2.34749200	-0.73744600	0.90187200
C	0.75540100	-2.31594900	0.00189400
C	1.03477600	-1.27819600	0.92181800
O	0.11719100	-0.93267100	1.82703500
C	4.63334100	-0.62953200	-0.02668900
C	2.73846200	0.26322600	1.84461700
N	5.70225600	-0.17255400	-0.03306600
N	3.12029900	1.06356800	2.59694800
C	-0.52630400	-2.94758900	0.00141900
C	1.43782900	-3.82679600	-1.83913400
N	-1.54375400	-3.50922000	-0.03676500
N	1.26423200	-4.67364800	-2.61808700

Table 3
ortho-CN-Ph (TS_A)
E(B3LYP/BS1) = -2704.612335 au
H(B3LYP/BS1) = -2704.151802 au
G(B3LYP/BS1) = -2704.270963 au
E(M06-2X/BS2//B3LYP/BS1) = -2704.455576 au

C	-0.25471800	-0.19334500	0.96890300
C	-1.09409800	-1.42610900	0.95457600
C	-0.96881400	1.14569000	0.96825100
C	-2.22865900	-1.40318100	0.20262500
H	-2.47201500	-0.47655300	-0.31219500
C	-0.99059100	1.90155000	-0.14365000
H	-0.48413200	1.54337200	-1.03574700
C	-3.25247900	-2.44929000	0.06392300
C	-2.99285000	-3.78932500	-0.30954700
C	-4.61274200	-2.09319000	0.25402400
C	-4.03501200	-4.72462200	-0.44134100
C	-5.64683100	-3.03003000	0.12286800
C	-5.35464700	-4.34832700	-0.21797100

H	-6.15306400	-5.07478500	-0.32137100
C	-1.68614200	3.19941300	-0.31304500
C	-1.34765800	4.35602700	0.42114800
C	-2.69360300	3.33152100	-1.29486900
C	-2.00218900	5.58009800	0.19609900
C	-3.34641800	4.55343700	-1.51764900
C	-2.99947400	5.67479400	-0.76867900
H	-3.50170500	6.62043500	-0.94052100
C	-0.65351700	-2.57121900	1.82557400
H	-1.44336700	-3.31685700	1.92799800
H	0.23616300	-3.06478100	1.42271600
H	-0.39134800	-2.19754100	2.82019100
C	-1.70299400	1.47650200	2.25086000
H	-2.27613700	0.60881400	2.59265600
H	-1.01436000	1.75467800	3.05565900
H	-2.39875600	2.30527200	2.10259500
O	0.86150500	-0.34249700	1.73842000
H	0.36269200	-0.29701600	-0.28221500
C	1.50192700	0.76672200	2.40662600
H	1.10992400	0.82794500	3.42553100
H	2.56384700	0.52410600	2.43803300
H	1.33852800	1.70974100	1.88425000
O	1.13612200	-0.27139400	-1.17864000
C	2.38341300	-0.32100600	-0.81939800
C	3.16715200	0.88479700	-0.76496800
C	3.04970400	-1.57792500	-0.54992200
C	4.51054900	0.85431200	-0.43552100
C	4.37516400	-1.62466800	-0.20927000
C	5.20210000	-0.40891100	-0.10915200
O	6.39238700	-0.42846400	0.20476200
Cl	2.09130100	-3.00879600	-0.71898000
Cl	5.19302400	-3.11654300	0.10766400
C	2.52836100	2.12103700	-1.09944200
C	5.30017900	2.03944800	-0.40680300
N	2.01716400	3.12999900	-1.36889600
N	5.94684100	3.00676200	-0.38031100
H	-6.67173400	-2.71848700	0.29227600
H	-3.79625700	-5.74131800	-0.73398500
H	-4.12220000	4.61331700	-2.27317100
H	-1.71505700	6.44925100	0.77776500
C	-4.94750300	-0.74795200	0.62355100
C	-1.67090300	-4.23055300	-0.64468400
C	-3.07667600	2.18328100	-2.06496800
C	-0.29587200	4.31486800	1.39551900
N	-5.22995100	0.33940300	0.92602000
N	-0.62532000	-4.64322000	-0.94342600
N	0.55282600	4.30726100	2.19121500
N	-3.39150100	1.25078600	-2.68551900

ortho-CN-Ph (2_A)

E(B3LYP/BS1) = -2704.667107 au

H(B3LYP/BS1) = -2704.20015 au

G(B3LYP/BS1) = -2704.317153 au

E(M06-2X/BS2//B3LYP/BS1) = -2704.545791 au

C	-0.49185600	-0.30758900	1.68798400
C	-1.80083600	-0.89021700	1.09940600
C	-0.03829100	1.05431800	1.12466300
C	-2.68114300	-0.06910300	0.49994100
H	-2.40483900	0.96977300	0.35004800
C	0.15760500	1.17159900	-0.20418800
H	-0.07556000	0.31774900	-0.83486500
C	-4.07876400	-0.36859100	0.11836000
C	-4.47252100	-1.39019300	-0.77338500
C	-5.11061200	0.45327000	0.63459800
C	-5.82553000	-1.59753500	-1.10128400
C	-6.45820500	0.24727300	0.30416700
C	-6.81438800	-0.78412100	-0.56056400
H	-6.08556800	-2.39378400	-1.79034600
H	-7.21609100	0.89502500	0.73126800
H	-7.85531700	-0.94633800	-0.81763500
C	0.55254100	2.37535900	-0.96536700
C	1.69572600	3.15731300	-0.68349600
C	-0.21451800	2.75852000	-2.09352500
C	2.02406200	4.28323000	-1.46114400
C	0.11646300	3.88033600	-2.86771500
C	1.23283600	4.64680600	-2.54440900
H	2.91006800	4.85678900	-1.21145100
H	-0.50605500	4.14418300	-3.71576900
H	1.49051700	5.51481800	-3.14105700
C	-2.09762900	-2.31049300	1.50977400
H	-3.16202600	-2.53716400	1.41552800
H	-1.53969600	-3.03007200	0.90531100
H	-1.80753900	-2.46021600	2.55322100
C	0.04104700	2.20413400	2.09476500
H	-0.81696400	2.17704100	2.77194300
H	0.94695400	2.16604800	2.70964000
H	0.03930900	3.16163300	1.56952200
O	-0.83859300	-0.24981200	3.04280600
H	5.01779800	-1.82967000	-2.45724000
C	0.12434800	-0.34869900	4.09867600
H	0.66142500	-1.29735700	4.05169800
H	0.83699000	0.47740300	4.09448400
H	-0.46932600	-0.30795200	5.01395300
O	5.17933100	-1.47395500	-1.56367900
C	4.04150900	-1.45048400	-0.85446100
C	4.10420900	-0.97795100	0.46411500
C	2.79848600	-1.88359900	-1.34918700
C	2.93643300	-0.91836700	1.26399500
C	1.64624500	-1.82511100	-0.55881600
C	1.68235800	-1.31041800	0.75973500
O	0.58786800	-1.34474900	1.56948300
Cl	2.75499000	-2.50073100	-2.97660600
Cl	0.14917200	-2.40086000	-1.20356300

C	5.36833200	-0.56314700	0.98222100
C	3.09819800	-0.49236000	2.61825000
N	6.40019500	-0.22779700	1.40111400
N	3.31524800	-0.16335300	3.71193000
C	-3.50327900	-2.22433000	-1.42087400
C	-4.78024500	1.51625300	1.54018300
C	2.60222300	2.79721900	0.36659300
C	-1.37631000	1.99899800	-2.45620400
N	-2.76362600	-2.92305300	-1.98479600
N	-4.52830100	2.38272300	2.27467300
N	3.37725100	2.54006900	1.19525700
N	-2.32000600	1.39188900	-2.76405100

ortho-Cl-Ph (TS_A)

E(B3LYP/BS1) = -4174.004808 au

H(B3LYP/BS1) = -4173.580957 au

G(B3LYP/BS1) = -4173.692836 au

E(M06-2X/BS2//B3LYP/BS1) = -4173.889607 au

C	0.83389300	0.74248400	-1.79997500
C	2.07487100	-0.05164600	-1.50607300
C	0.20437500	1.57700500	-0.74217800
C	2.85947400	0.31855700	-0.46556700
H	2.54535700	1.16386600	0.13854800
C	-0.17851900	0.94278400	0.40484200
H	0.05743300	-0.11451200	0.49080800
C	4.19803600	-0.20626000	-0.12399600
C	4.46942900	-1.53391500	0.26457100
C	5.30283600	0.67264500	-0.10849200
C	5.74935100	-1.96515900	0.61064700
C	6.58930100	0.26837400	0.23106300
C	6.80856100	-1.06154800	0.58795000
H	7.80708600	-1.39164500	0.85622300
C	-0.74115000	1.53365000	1.63155300
C	-1.89704800	2.34404100	1.69633000
C	-0.13714000	1.24062400	2.87850300
C	-2.38368300	2.86061900	2.89616000
C	-0.60337900	1.74602000	4.08620200
C	-1.73006500	2.56662000	4.08913800
H	-2.10593900	2.96714300	5.02508200
C	2.43603400	-1.11147000	-2.51390500
H	3.47911600	-1.41797400	-2.41741100
H	1.80538000	-1.99790600	-2.37925000
H	2.27297600	-0.73829600	-3.52882500
C	0.12630000	3.06627700	-0.96352300
H	0.98941600	3.39825400	-1.54842400
H	-0.77658200	3.37416300	-1.49896400
H	0.12388200	3.58936100	-0.00377400
O	0.95860200	1.27558100	-3.06113200
H	-0.13949600	-0.25150500	-1.94649400
C	-0.19498800	1.65324700	-3.83085700
H	0.18547000	2.28315500	-4.63572500
H	-0.66159000	0.75677000	-4.24613600

H	-0.92532700	2.20738400	-3.24122600
O	-0.97074700	-1.09275100	-2.22169400
C	-1.93476100	-1.25621800	-1.36618800
C	-1.81768200	-2.24852000	-0.32894900
C	-3.19620000	-0.55113400	-1.47572500
C	-2.83883700	-2.47675800	0.57852300
C	-4.21767900	-0.76743100	-0.58855400
C	-4.09852300	-1.71521400	0.53376900
O	-4.99431600	-1.89356100	1.36085500
Cl	-3.38637700	0.52786100	-2.82020600
Cl	-5.74159700	0.04203300	-0.72061200
C	-0.64688400	-3.07017300	-0.31592100
C	-2.73016500	-3.47335200	1.58996500
N	0.27034100	-3.78465200	-0.30986500
N	-2.64249200	-4.28436500	2.42037900
H	7.40406600	0.98316200	0.21201900
H	5.90518100	-2.99680000	0.90519200
H	-0.08831800	1.50187500	5.00811200
H	-3.27728400	3.47401800	2.88962200
Cl	3.15953500	-2.69506800	0.38123700
Cl	5.06563000	2.35794600	-0.56590000
Cl	-2.85002200	2.67191800	0.25763600
Cl	1.29526500	0.21963700	2.92825200

ortho-Cl-Ph (2_A)

E(B3LYP/BS1) = -4174.06279 au

H(B3LYP/BS1) = -4173.63113 au

G(B3LYP/BS1) = -4173.744137 au

E(M06-2X/BS2//B3LYP/BS1) = -4173.980627 au

C	-0.42588400	0.53370200	1.76652000
C	-1.82522900	0.01975500	1.38961700
C	0.14273000	1.58484500	0.79603400
C	-2.38356200	0.32027400	0.20617200
H	-1.79802200	0.84559200	-0.54358000
C	0.89174200	1.28366500	-0.27868200
H	1.11131700	0.24750500	-0.50895700
C	-3.77610000	-0.00189100	-0.20090000
C	-4.04805200	-0.85183200	-1.29148300
C	-4.91014000	0.57480900	0.40704200
C	-5.33731900	-1.15077000	-1.72424400
C	-6.21335000	0.29522900	-0.00261700
C	-6.42361000	-0.57687100	-1.06738900
H	-5.48367800	-1.82290600	-2.56217800
H	-7.04862800	0.76541900	0.50377900
H	-7.43449400	-0.80140700	-1.39254900
C	1.42008500	2.23654200	-1.28894100
C	2.32496500	3.28154200	-1.01156700
C	1.08363800	2.07898100	-2.64983900
C	2.82981200	4.12366900	-2.00249700
C	1.57204100	2.90178000	-3.65981000
C	2.44782800	3.93340600	-3.32737400
H	3.52240300	4.91272600	-1.73257400

H	1.26671600	2.73718400	-4.68691400
H	2.83743200	4.58533900	-4.10266000
C	-2.52449900	-0.75494300	2.47908800
H	-3.35828800	-1.33341300	2.07357500
H	-1.82866700	-1.44122200	2.96792100
H	-2.91478400	-0.08105400	3.24795100
C	-0.36759600	2.98348900	1.06782100
H	-1.43984100	2.95806700	1.28463500
H	0.12479700	3.44680300	1.92817700
H	-0.20615500	3.62779300	0.20121900
O	-0.61662600	1.07633600	3.03438400
H	3.73252400	-4.23458800	-1.47978900
C	0.52873600	1.47060800	3.80060200
H	1.02480900	0.59528600	4.22566600
H	1.24952800	2.03753800	3.20622000
H	0.13819100	2.10080400	4.60190900
O	4.14091100	-3.49722700	-0.98927900
C	3.21526600	-2.84608200	-0.26851000
C	3.64279500	-1.76958000	0.52276200
C	1.85384200	-3.20056300	-0.23884100
C	2.70899900	-1.03059400	1.28894500
C	0.93301400	-2.47702000	0.52695300
C	1.33260200	-1.33073400	1.25752900
O	0.47186100	-0.65708700	2.05389900
Cl	1.37034300	-4.59028300	-1.17033800
Cl	-0.70134600	-3.02698700	0.63753700
C	5.03173800	-1.44085300	0.54596900
C	3.20638500	-0.00010900	2.14447400
N	6.16306400	-1.17111800	0.56530700
N	3.67532200	0.79654700	2.84985100
Cl	-2.70858900	-1.59007200	-2.16591900
Cl	-4.72257400	1.74929000	1.70936300
Cl	-0.02812600	0.79194100	-3.11074100
Cl	2.91274600	3.54597100	0.62650900

ortho-Me-Ph (TS_A)

E(B3LYP/BS1) = -2492.901086 au
H(B3LYP/BS1) = -2492.324119 au
G(B3LYP/BS1) = -2492.439458 au
E(M06-2X/BS2//B3LYP/BS1) = -2492.715334 au

C	1.04706500	1.84492400	0.36723400
C	2.27736500	1.33972800	-0.33388900
C	0.37620200	1.01937700	1.39801900
C	3.06733600	0.43020800	0.29391700
H	2.73907300	0.09938200	1.27678800
C	-0.02227800	-0.24225500	1.02470900
H	0.26979700	-0.54142800	0.02124800
C	4.40657600	-0.05078600	-0.10255100
C	4.67009300	-0.70617800	-1.33011000
C	5.45328100	0.12291800	0.84610600
C	5.97585100	-1.14115300	-1.59754100
C	6.74050300	-0.31531600	0.53318800

C	7.00674500	-0.94214200	-0.68518500
H	8.01211600	-1.28548500	-0.91374000
C	-0.64138100	-1.31132300	1.81601900
C	-1.76104200	-1.12436400	2.67239400
C	-0.09060100	-2.62173800	1.65779100
C	-2.25249400	-2.22032100	3.39377900
C	-0.60712400	-3.67656100	2.40756500
C	-1.67794000	-3.48085000	3.28127800
H	-2.07469000	-4.31502900	3.85317100
C	2.64083400	2.04374700	-1.61571300
H	3.69742500	1.91052600	-1.85668200
H	2.04555700	1.66035000	-2.45331300
H	2.43450300	3.11457700	-1.52935200
C	0.27013800	1.57232900	2.79604900
H	1.14132000	2.19974000	3.00811700
H	-0.61961500	2.18882400	2.95778700
H	0.23297200	0.75404200	3.51961500
O	1.23453400	3.18981000	0.63482300
H	0.09982200	1.81542600	-0.62102100
C	0.11271300	4.07631000	0.76369000
H	0.53468000	5.03260400	1.07569500
H	-0.38663800	4.18565400	-0.20198400
H	-0.60616900	3.73352800	1.51025100
O	-0.75326000	1.88426000	-1.52633500
C	-1.72229900	1.02582100	-1.43832100
C	-1.62588500	-0.24857600	-2.10096300
C	-2.97441800	1.33245500	-0.77493100
C	-2.65062700	-1.18108600	-2.04717300
C	-3.99882100	0.42370600	-0.71423000
C	-3.89677600	-0.92060100	-1.30988000
O	-4.79662300	-1.76017500	-1.23276900
Cl	-3.14595900	2.92814200	-0.11055700
Cl	-5.50894300	0.78561000	0.05412700
C	-0.46541200	-0.49662000	-2.89999400
C	-2.55417200	-2.43308800	-2.71870100
N	0.44976000	-0.70121900	-3.58781500
N	-2.47499400	-3.45903700	-3.26328900
H	7.54173400	-0.16492900	1.25222900
H	6.17512200	-1.65531400	-2.53463700
H	-0.16839900	-4.66504100	2.30266100
H	-3.11516000	-2.07588800	4.03922000
C	5.19849200	0.79777300	2.17518700
H	4.76309800	1.79592400	2.04988400
H	4.49874500	0.22271900	2.79631900
H	6.12920700	0.90256600	2.74007700
C	3.59275300	-1.00339100	-2.34624800
H	2.60371300	-1.08431200	-1.89195400
H	3.52887300	-0.22203900	-3.11304500
H	3.80701800	-1.94305300	-2.86576100
C	1.06359400	-2.89302200	0.71947900
H	0.79827700	-2.68601800	-0.32529000

H	1.94278000	-2.28274600	0.95338700
H	1.36167700	-3.94335900	0.77665400
C	-2.51895700	0.17763500	2.79705100
H	-2.27495900	0.70001500	3.72986000
H	-2.31915900	0.85953200	1.97034400
H	-3.59583300	-0.01929300	2.81660700

ortho-Me-Ph (2_A)

E(B3LYP/BS1) = -2492.953613 au
H(B3LYP/BS1) = -2492.369999 au
G(B3LYP/BS1) = -2492.482917 au
E(M06-2X/BS2//B3LYP/BS1) = -2492.800149 au

C	-0.61959500	0.59572700	1.68238400
C	-2.00482600	0.07894100	1.27070100
C	-0.03973000	1.70460700	0.78800700
C	-2.56933100	0.42688000	0.10024200
H	-1.96934200	1.00341000	-0.60193700
C	0.79933200	1.48935400	-0.24347200
H	1.05508600	0.46436400	-0.48935200
C	-3.94541800	0.09391100	-0.36243000
C	-4.09979400	-0.62233500	-1.57765200
C	-5.09513000	0.53524500	0.33655600
C	-5.38179700	-0.93671800	-2.03622600
C	-6.36514700	0.20904500	-0.16382400
C	-6.51499100	-0.53075000	-1.33153400
H	-5.49018200	-1.50230200	-2.95863600
H	-7.24504000	0.55362900	0.37468400
H	-7.50704900	-0.77765200	-1.70056100
C	1.39467500	2.48703200	-1.17302600
C	2.16327300	3.59275500	-0.73313300
C	1.24367700	2.25257400	-2.56621100
C	2.71193900	4.46231500	-1.68885200
C	1.80020500	3.14636800	-3.48352600
C	2.52696200	4.25558100	-3.05101600
H	3.30454300	5.30752200	-1.34678300
H	1.66442200	2.96693400	-4.54719700
H	2.95979200	4.94260300	-3.77335100
C	-2.68475800	-0.77647500	2.31247100
H	-3.51922100	-1.33025000	1.87540900
H	-1.97731800	-1.48994500	2.74251500
H	-3.06770200	-0.16769300	3.13774300
C	-0.63218500	3.06640500	1.08700700
H	-1.71519800	2.98678800	1.22286700
H	-0.23142200	3.51222000	2.00331000
H	-0.43954000	3.75447700	0.26127800
O	-0.82318400	1.06029400	2.98091200
H	3.61997500	-4.07379200	-1.67046100
C	0.30736500	1.44532900	3.77029200
H	0.84877800	0.56453100	4.12240000
H	0.99561100	2.09301200	3.22103800
H	-0.10544200	1.99066700	4.62133100
O	4.01959900	-3.35415400	-1.14761500

C	3.07973900	-2.72307200	-0.42653100
C	3.49131400	-1.67200800	0.40553700
C	1.71671900	-3.07230400	-0.43823100
C	2.54236900	-0.95646700	1.17508300
C	0.78102000	-2.37214900	0.33144700
C	1.16491800	-1.25323400	1.11294400
O	0.29761200	-0.60853100	1.92057300
Cl	1.25007100	-4.42696700	-1.42885800
Cl	-0.85736000	-2.92451600	0.38179000
C	4.87929300	-1.34349300	0.46498400
C	3.02010000	0.06466000	2.05207500
N	6.00971900	-1.07378000	0.51446000
N	3.47096400	0.86459200	2.76603500
C	0.48008000	1.05244900	-3.07639000
H	0.95422200	0.10819900	-2.77734400
H	-0.54362600	1.02714400	-2.68799700
H	0.42561500	1.06217100	-4.16890100
C	2.46692500	3.86773800	0.72307000
H	1.71829600	4.52715300	1.17897900
H	2.50236400	2.95225400	1.31800100
H	3.43437300	4.37161700	0.81740000
C	-5.02599300	1.38132700	1.58943400
H	-5.07572200	0.76617500	2.49649600
H	-4.10316500	1.96406100	1.64469300
H	-5.87317800	2.07415300	1.62670800
C	-2.90074100	-1.04184000	-2.39670500
H	-2.43093800	-0.17651300	-2.88267400
H	-2.13060000	-1.52260500	-1.78646100
H	-3.19427200	-1.73804600	-3.18833000

ortho-NH_2-Ph (TS_A)

E(B3LYP/BS1) = -2557.074 au

H(B3LYP/BS1) = -2556.542438 au

G(B3LYP/BS1) = -2556.655328 au

E(M06-2X/BS2//B3LYP/BS1) = -2556.934362 au

C	1.04173300	1.99818600	0.28743500
C	2.31313300	1.47611700	-0.31115000
C	0.32304500	1.23432000	1.32813800
C	3.03309500	0.52829900	0.36033400
H	2.62145600	0.23041700	1.32597600
C	-0.05845000	-0.05829200	1.01158500
H	0.32796500	-0.42885700	0.06478900
C	4.33133100	-0.05744600	0.04440800
C	4.65862300	-0.63575700	-1.22245000
C	5.30030100	-0.13465400	1.09786800
C	5.91678500	-1.23159400	-1.41641100
C	6.54120600	-0.75168800	0.87827800
C	6.83511200	-1.28478200	-0.37320000
H	7.79909900	-1.75986900	-0.53670800
C	-0.79097100	-1.05523900	1.75709200
C	-1.96870700	-0.79514800	2.53645600

C	-0.37302200	-2.42364800	1.59860000
C	-2.63147800	-1.85454300	3.17629500
C	-1.06799700	-3.45657700	2.23520900
C	-2.18097300	-3.16009600	3.01988100
H	-2.71248100	-3.96796500	3.51547500
C	2.79520800	2.18406700	-1.55149000
H	3.87315200	2.06885700	-1.67786600
H	2.30950400	1.79074600	-2.45285300
H	2.55667700	3.24895500	-1.48428000
C	0.14065400	1.87565700	2.68026800
H	0.99929600	2.52247300	2.88561500
H	-0.75733500	2.49621000	2.76849600
H	0.06814700	1.10670800	3.45252500
O	1.19053600	3.36616000	0.50754500
H	0.17284500	1.88982600	-0.73259000
C	0.04286700	4.22270300	0.44251900
H	0.40909600	5.21968600	0.69294600
H	-0.37451300	4.22188500	-0.56782100
H	-0.73326600	3.93282200	1.15535200
O	-0.67400400	1.83773400	-1.69270200
C	-1.59100100	0.93320500	-1.53741800
C	-1.39251300	-0.40341600	-2.02596900
C	-2.88028700	1.22341300	-0.94158300
C	-2.35278800	-1.39753600	-1.87378700
C	-3.84422600	0.25794000	-0.79364800
C	-3.64001100	-1.13741300	-1.21809100
O	-4.49079700	-2.01992400	-1.06421000
Cl	-3.17419900	2.87172700	-0.46387900
Cl	-5.39184000	0.60394900	-0.09015900
C	-0.17282600	-0.67526600	-2.72042900
C	-2.13653400	-2.71783400	-2.36031600
N	0.80977700	-0.90125600	-3.30055200
N	-1.95731100	-3.79918300	-2.75360700
H	7.27142300	-0.78446400	1.68185700
H	6.14997000	-1.67270400	-2.38149100
H	-0.72210100	-4.48061200	2.13023100
H	-3.52159700	-1.64484600	3.76214600
N	3.75566600	-0.62854100	-2.26831700
N	5.06738500	0.47536100	2.31932800
N	0.71444400	-2.71901200	0.78966500
N	-2.48521500	0.48142600	2.65215900
H	1.49268200	-2.07256500	0.79836100
H	1.03101900	-3.68022300	0.83476700
H	-2.27942300	1.12453000	1.89971200
H	-3.45681000	0.52852300	2.93495500
H	3.92721900	-1.31120400	-2.99586200
H	2.77141900	-0.56195800	-2.04555800
H	5.59141200	0.11182300	3.10481300
H	4.12085900	0.73415300	2.55931100

ortho-NH_2-Ph (2_A)

E(B3LYP/BS1) = -2557.117613 au

H(B3LYP/BS1) = -2556.579146 au
G(B3LYP/BS1) = -2556.689606 au
E(M06-2X/BS2//B3LYP/BS1) = -2557.014347 au

C	-0.62169300	0.08027200	1.80403100
C	-1.92974200	-0.49852600	1.23531400
C	-0.11262400	1.35407300	1.12034200
C	-2.69728800	0.20805100	0.38288900
H	-2.33274000	1.18628800	0.06950400
C	0.29671000	1.30121200	-0.16741300
H	0.23366600	0.33415400	-0.66672500
C	-4.05070900	-0.15215400	-0.11416300
C	-4.28095900	-1.26195600	-0.96384300
C	-5.13702200	0.70434100	0.20021100
C	-5.57089800	-1.51281100	-1.46421800
C	-6.41952900	0.44151600	-0.31088700
C	-6.62196100	-0.66220200	-1.13464500
H	-5.73270200	-2.36869400	-2.11441300
H	-7.24416400	1.10019000	-0.05100200
H	-7.61499200	-0.85971900	-1.53097300
C	0.72951600	2.39124800	-1.06689500
C	1.77545400	3.30497100	-0.76858500
C	0.12363200	2.44911100	-2.35329800
C	2.14378900	4.28179300	-1.71402800
C	0.51426300	3.42181400	-3.28520200
C	1.51668600	4.33035200	-2.95321600
H	2.94118700	4.97905200	-1.47052000
H	0.02409000	3.46423100	-4.25420500
H	1.81120800	5.09031000	-3.67269200
C	-2.40934500	-1.77608200	1.89085600
H	-3.18864300	-1.54929300	2.62824200
H	-2.83624700	-2.45666700	1.15012000
H	-1.59695700	-2.28870400	2.40624900
C	-0.29706000	2.65062700	1.87456700
H	-1.23874300	2.63471700	2.43132200
H	0.49279800	2.84467300	2.61180800
H	-0.31510500	3.49261300	1.17755400
O	-0.94642100	0.24145800	3.15130800
H	4.58691200	-2.72455400	-2.14736900
C	0.06557800	0.34937600	4.15946500
H	0.69002100	-0.54634100	4.18253100
H	0.69770200	1.22940800	4.02689300
H	-0.48487400	0.43721900	5.09821600
O	4.77452500	-2.03661000	-1.48225600
C	3.69475200	-1.81940800	-0.71554400
C	3.79734400	-0.85642600	0.29812100
C	2.47773400	-2.51186800	-0.86186100
C	2.69030700	-0.57796100	1.13779400
C	1.38443200	-2.22948600	-0.03847600
C	1.45556900	-1.23349500	0.96742200
O	0.42026500	-1.04271500	1.80960800
Cl	2.39517000	-3.73245500	-2.10096700

Cl	-0.08412800	-3.12561800	-0.22534900
C	5.03575300	-0.16768000	0.47037700
C	2.87057800	0.36900400	2.19071100
N	6.04407800	0.39464500	0.61205500
N	3.07326600	1.13947100	3.03845100
N	-3.24174000	-2.13899100	-1.29075100
N	-4.96025500	1.77424400	1.08237000
N	2.53474700	3.19105800	0.39222400
N	-0.83724000	1.49752500	-2.71176500
H	3.03989400	4.02817400	0.65616700
H	2.10135400	2.75096400	1.18984300
H	-1.37380000	1.74611800	-3.53516400
H	-1.45184200	1.19137400	-1.96762700
H	-4.01264300	2.12025000	1.17040300
H	-5.61723800	2.53497700	0.95317900
H	-2.31400300	-1.73596200	-1.22405900
H	-3.36839900	-2.61650500	-2.17621500