Electronic Supplementary Information (ESI)

Theoretical Study of the Activation Mechanism Involving Bifunctional Tertiary Amine–Thioureas and Isatylidene Malononitriles

Zheng-Hang Qi, Ye Zhang, Gui-Yu Ruan, Yi Zhang, Yong Wang,* and Xing-Wang Wang*

Key Laboratory of Organic Synthesis of Jiangsu Province, College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou 215123, P. R. China.

Email: *yowang@suda.edu.cn*; *wangxw@suda.edu.cn*

Contents

1. Computational Details……S2

2. Complete Reference 7……S3

3. B3LYP/6-31+G(d,p)–CPCM(mesitylene or dichloromethane) and B3LYP/6-311+G(d,p)–CPCM(mesitylene) optimized structures……S4

4. B3LYP/6-31G(d) optimized structures……S7

5. Coordinates and Energies of DFT-Computed Stationary Points……S10

1. Computational Details

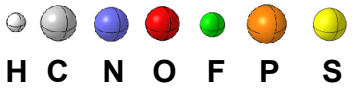
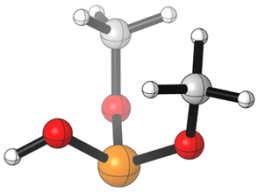
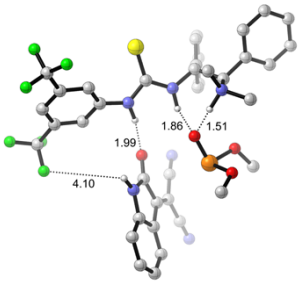
All the DFT calculations were performed with Gaussian 09 package. The geometry optimizations of all species in this study were performed using B3LYP method. The 6-31G(d) basis set was used for all atoms. Frequency calculations at the same level of theory were carried out to characterize each stationary point (minimum or transition state). In order to save computational costs, single-point energy calculations at even higher basis set level of B3LYP/6-311++G(d,p) were performed on the B3LYP/6-31G(d) optimized structures. Such a strategy is designated by the standard notation of B3LYP/6-311++G(d,p)//B3LYP/6-31G(d). In contrast, two other levels of theory are also carefully considered as M06-2X/6-311++G(d,p)–CPCM(solution)//B3LYP/6-31+G(d,p)–CPCM(solution) and M06-2X/6-311++G(d,p)–CPCM(solution)//B3LYP/6-311+G(d,p)–CPCM(solution) for comparison sake. Intrinsic reaction coordinate (IRC) was calculated to confirm the connection between the transition state and the right reactant/product. All the single point calculations were performed with B3LYP/6-311++G(d,p) and for **TSa** and **TSb**, solvent effect was considered with CPCM model and dichloromethane solvent. All the bond lengths are in angstroms (Å), and energies in kcal/mol. Optimized structures were visualized by the CYLview program.[1]

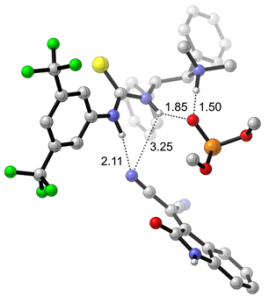
1 Legault, C. Y. *CYLview, 1.0b*, Université de Sherbrooke, 2009, http://www.cylview.org.

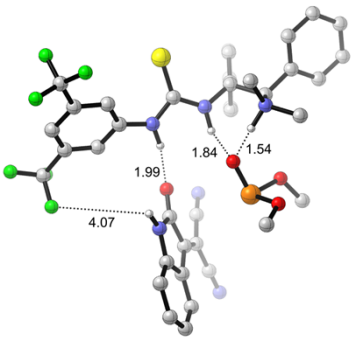
2. Complete Reference 7

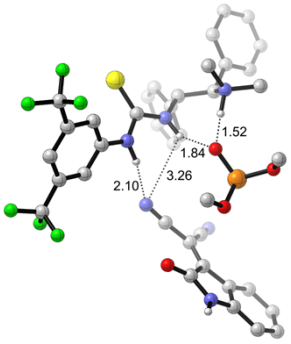
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09*, *Revision C.01*, Gaussian, Inc., Wallingford CT, 2010.

3. B3LYP/6-31+G(d,p)–CPCM(mesitylene or dichloromethane) and B3LYP/6-311+G(d,p)–CPCM(mesitylene) optimized structures and selected geometric parameters of the the most important competing stationary points. All the bond lengths are in angstroms (Å) and M06-2X/6-311++G(d,p)–CPCM(mesitylene or dichloromethane) calculated single-point energies are in kcal/mol.

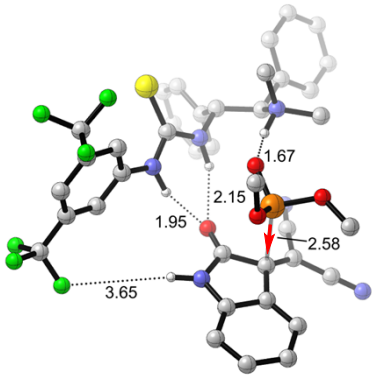
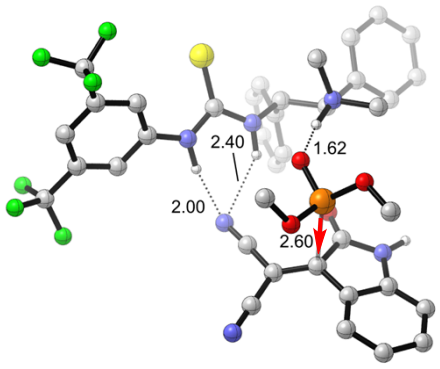
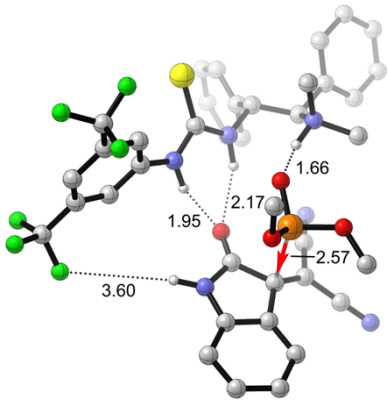
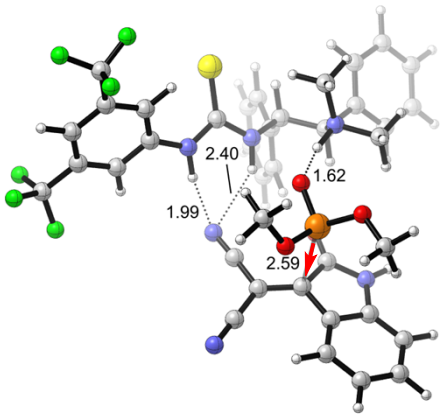
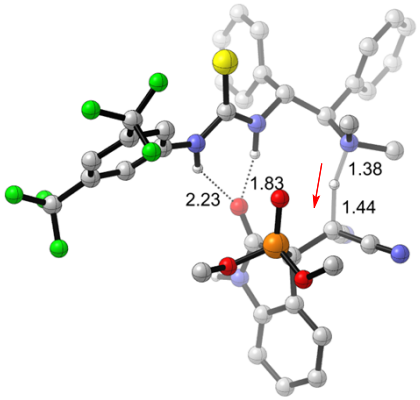
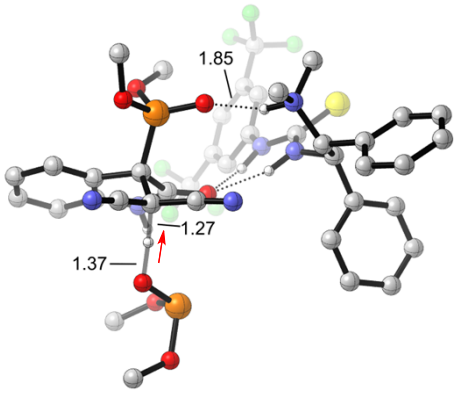
<table>
<tr>
<td> 
</td>
<td> 
B3LYP/6-31+G(d,p)–CPCM(mesitylene) optimized
Nu’</td>
</tr>
<tr>
<td> 

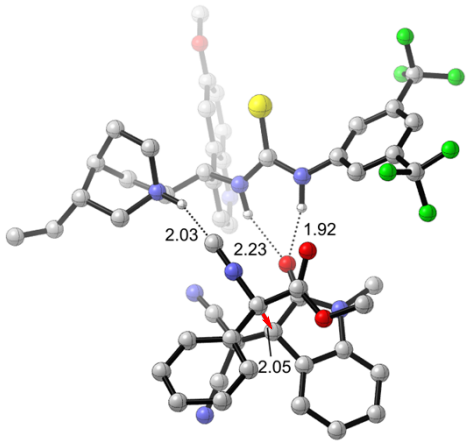
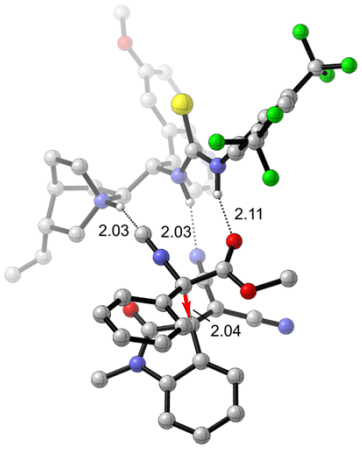
B3LYP/6-31+G(d,p)–CPCM(mesitylene) optimized
M1-O’
M06-2X/6-311++G(d,p)–CPCM(mesitylene) calculated
single-point energies: ΔE = 0.00 kcal/mol</td>
<td> 

B3LYP/6-31+G(d,p)–CPCM(mesitylene) optimized
M1-N’
M06-2X/6-311++G(d,p)–CPCM(mesitylene) calculated
single-point energies: ΔE = 3.98 kcal/mol</td>
</tr>
<tr>
<td> 

B3LYP/6-311+G(d,p)–CPCM(mesitylene) optimized
M1-O’’
M06-2X/6-311++G(d,p)–CPCM(mesitylene) calculated
single-point energies: ΔE = 0.00 kcal/mol</td>
<td> 

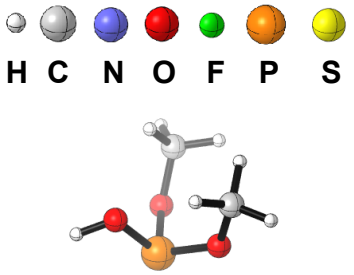
B3LYP/6-311+G(d,p)–CPCM(mesitylene) optimized
M1-N’’
M06-2X/6-311++G(d,p)–CPCM(mesitylene) calculated
single-point energies: ΔE = 3.54 kcal/mol</td>
</tr>
</table>

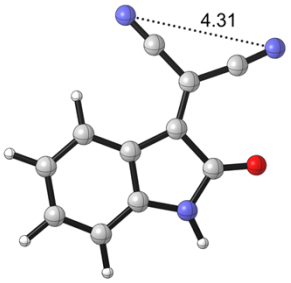
 B3LYP/6-31+G(d,p)–CPCM(mesitylene) optimized **$TS_{P\text{-}C}$'** M06-2X/6-311++G(d,p)–CPCM(mesitylene) calculated single-point energies: ΔE = **0.00** kcal/mol	 B3LYP/6-31+G(d,p)–CPCM(mesitylene) optimized **$TS_{Enantio}$'** M06-2X/6-311++G(d,p)–CPCM(mesitylene) calculated single-point energies: ΔE = **2.37** kcal/mol
 B3LYP/6-311+G(d,p)–CPCM(mesitylene) optimized **$TS_{P\text{-}C}$''** M06-2X/6-311++G(d,p)–CPCM(mesitylene) calculated single-point energies: ΔE = **0.00** kcal/mol	 B3LYP/6-311+G(d,p)–CPCM(mesitylene) optimized **$TS_{Enantio}$''** M06-2X/6-311++G(d,p)–CPCM(mesitylene) calculated single-point energies: ΔE = **2.50** kcal/mol
 B3LYP/6-31+G(d,p)–CPCM(mesitylene) optimized **$TS_{NH\text{-}CH}$'** M06-2X/6-311++G(d,p)–CPCM(mesitylene) calculated single-point energies: ΔE = **0.00** kcal/mol	 B3LYP/6-31+G(d,p)–CPCM(mesitylene) optimized **$TS_{OH\text{-}CH}$'** M06-2X/6-311++G(d,p)–CPCM(mesitylene) calculated single-point energies: ΔE = **-12.53** kcal/mol

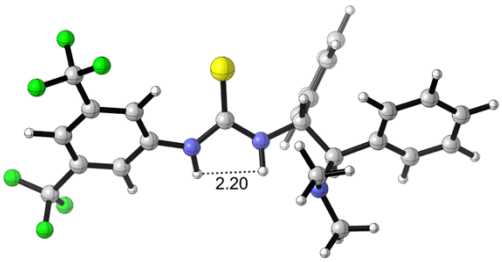
	
B3LYP/6-31+G(d,p)–CPCM(dichloromethane) optimized **TSa'** M06-2X/6-311++G(d,p)–CPCM(dichloromethane) calculated single-point energies: ΔE = **0.00** kcal/mol	B3LYP/6-31+G(d,p)–CPCM(dichloromethane) optimized **TSb'** M06-2X/6-311++G(d,p)–CPCM(dichloromethane) calculated single-point energies: ΔE = **1.73** kcal/mol

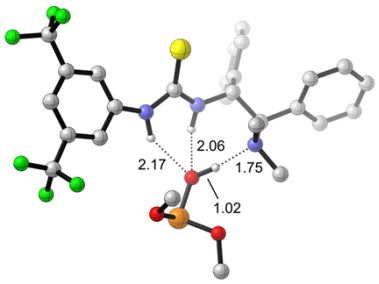
For comparison sake, the most important competing stationary points **M1-O**, **M1-N**, $\mathbf{TS_{P\text{-}C}}$, $\mathbf{TS_{Enantio}}$, $\mathbf{TS_{NH\text{-}CH}}$, $\mathbf{TS_{OH\text{-}CH}}$, **TSa** and **TSb** were re-evaluated with the M06-2X/6-311++G(d,p)–CPCM(solution)//B3LYP/6-31+G(d,p)–CPCM(solution) or M06-2X/6-311++G(d,p)–CPCM(solution)//B3LYP/6-311+G(d,p)–CPCM(solution) level of theory as shown above. Little difference was observed for the geometries of re-optimized **M1-O**, **M1-N**, $\mathbf{TS_{P\text{-}C}}$ and $\mathbf{TS_{Enantio}}$ when a larger basis set was applied. As a result, all these re-optimized geometries are validated at the level of B3LYP/6-31+G(d,p)–CPCM(solution). The single-point energies calculated at the level of M06-2X/6-311++G(d,p)–CPCM(solution) show the same trends of selectivity prediction as the results generated at the level of B3LYP/6-311++G(d,p)–CPCM(solution)// B3LYP/6-31G(d)–(gas phase).

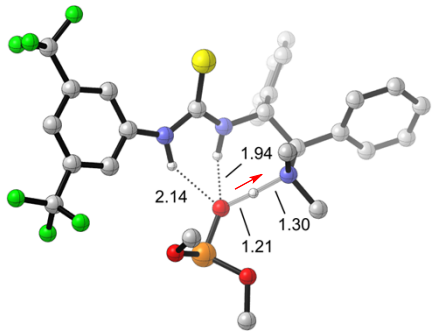
4. B3LYP/6-31G(d) optimized structures and selected geometric parameters of the stationary points of all reported species. All the bond lengths are in angstroms (Å), and B3LYP/6-311++G(d,p) calculated single-point energies in kcal/mol.

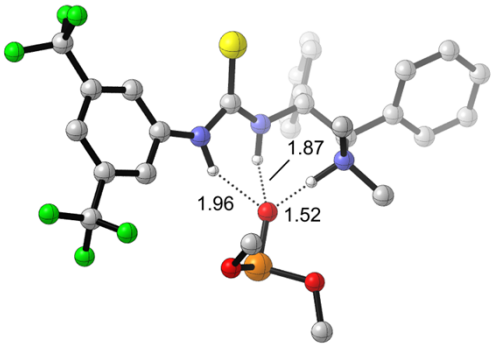
<table>
<tr>
<td> 

Nu</td>
<td> 

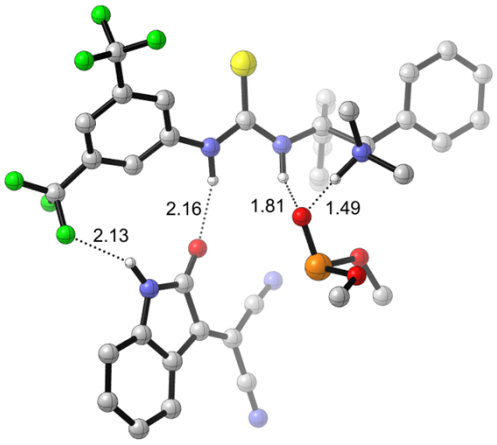
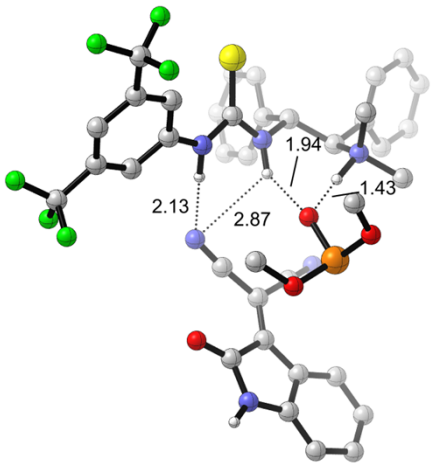
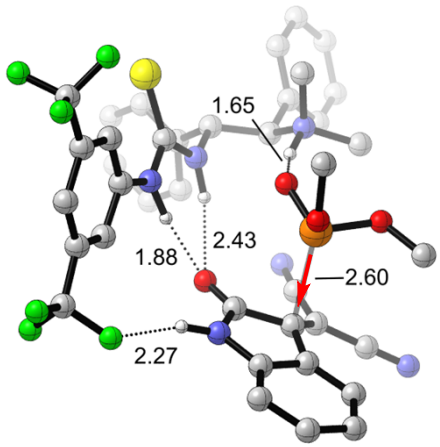
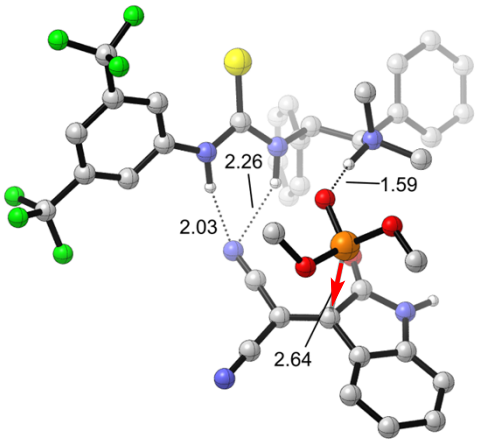
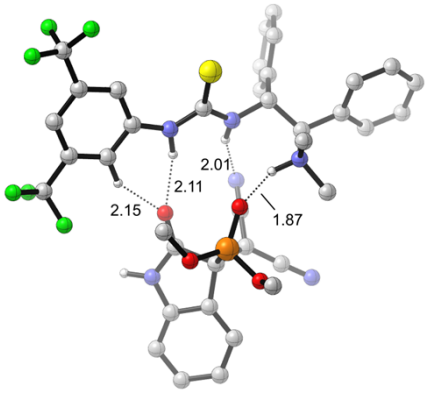
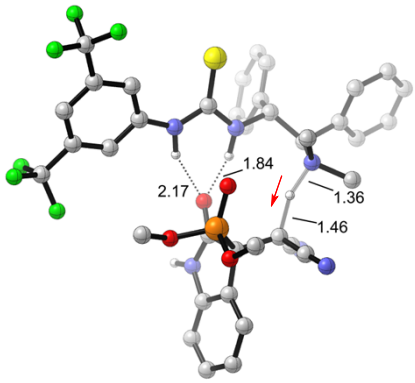
EI</td>
</tr>
<tr>
<td> 

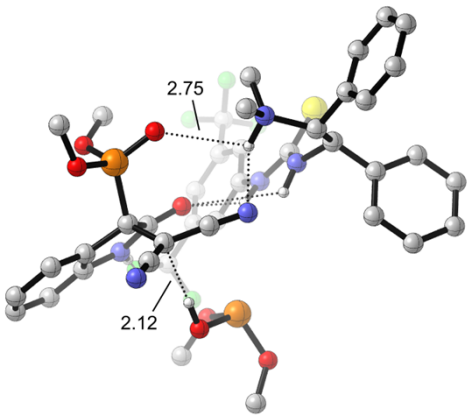
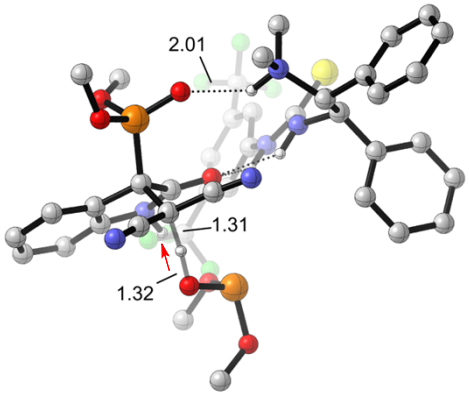
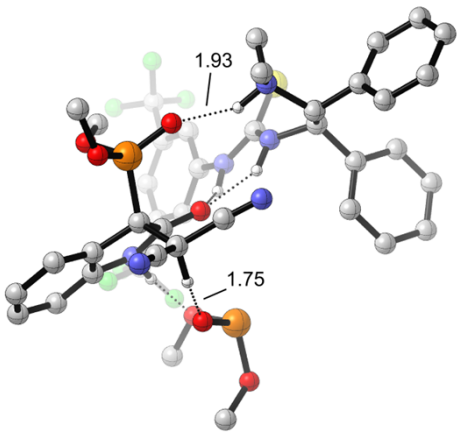
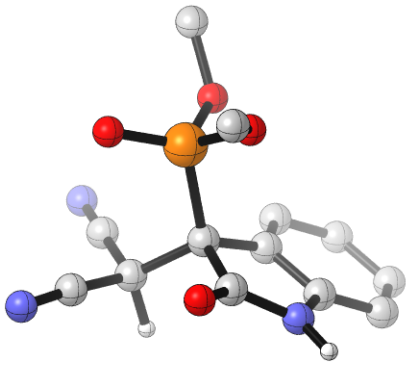
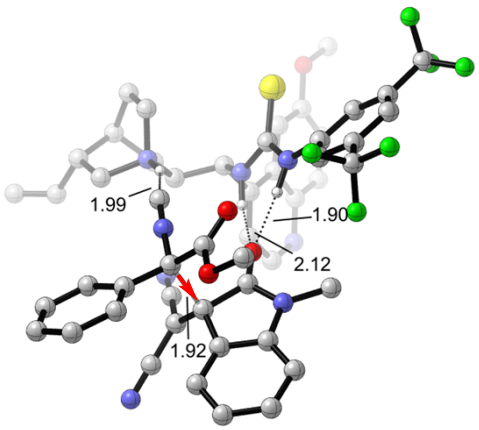
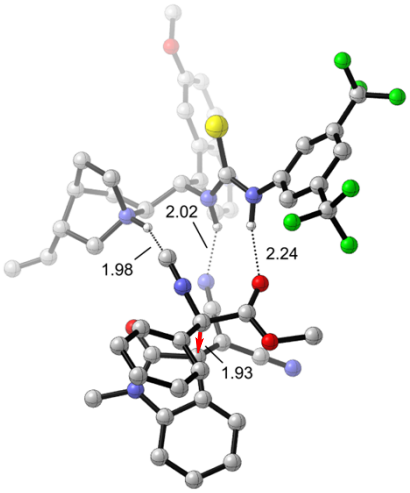
Cat</td>
<td> 

Cat-Nu
ΔE = 0.00 kcal/mol</td>
</tr>
<tr>
<td> 

Cat-TS-CatH
ΔE = 1.13 kcal/mol</td>
<td> 

CatH-Nu
ΔE = -0.17 kcal/mol</td>
</tr>
</table>

 **M1-O** ΔE = -0.68 kcal/mol	 **M1-N** ΔE = -0.35 kcal/mol
 **TS_{P-C}** ΔE = -3.90 kcal/mol	 **$TS_{Enantio}$** ΔE = -1.59 kcal/mol
 **M2** ΔE = -14.13 kcal/mol	 **TS_{NH-CH}** ΔE = 3.42 kcal/mol

 **M3** ΔE = -20.05 kcal/mol	 **TS_{OH-CH}** ΔE = -7.84 kcal/mol
 **M4** ΔE = -9.52 kcal/mol	 **Prod** ΔE = -9.57 kcal/mol
 **TSa** ΔE = 0.00 kcal/mol	 **TSb** ΔE = 2.15 kcal/mol

5. Coordinates and Energies of DFT-Computed Stationary Points

Cat

E[6-31G(d); Hartrees] = -2127.571647; G[6-31G(d); Hartrees] = -2127.641489

E[6-311++G(d,p); Hartrees] = -2128.5428226

C	-7.45190200	1.05523400	-1.07901800
C	-7.26523500	-0.32398600	-0.98442000
C	-5.97474800	-0.85135700	-0.92537400
C	-4.84664100	-0.01958000	-0.95804000
C	-5.05117800	1.36635100	-1.04840600
C	-6.33993300	1.89822800	-1.10930600
C	-3.45642700	-0.64981800	-0.94518400
C	-2.50371800	-0.00572500	0.11634800
N	-2.78588000	-0.73352000	-2.26746200
N	-1.16125500	-0.51070000	-0.16575100
C	-2.97569700	-0.34079000	1.52678700
C	-2.79211800	-1.62385800	2.05662100
C	-3.26456200	-1.94292100	3.32931500
C	-3.93191600	-0.98071200	4.08995300
C	-4.11616300	0.30130600	3.57099000
C	-3.63809100	0.61808900	2.29898300
C	-2.56285400	0.54258300	-2.94887300
C	-0.01643600	0.12522600	0.22693800
N	1.09847900	-0.56442600	-0.22938500
S	0.01334300	1.51670500	1.15419700
C	2.46914400	-0.26598400	-0.15025000
C	3.35921500	-1.34971600	-0.17110000
C	4.73555200	-1.13688300	-0.15707500
C	5.25333000	0.15626100	-0.10978800
C	4.36473100	1.23118000	-0.09134900
C	2.98411600	1.03812600	-0.12003300
C	4.90864000	2.63448500	0.00618000
F	4.09218200	3.53341300	-0.58298100
F	6.12130000	2.73857500	-0.58340800
F	5.06240300	3.01924100	1.29226300
C	5.66870400	-2.31465200	-0.25649000
F	5.94171000	-2.62218200	-1.54622200
F	6.84959000	-2.07276000	0.34942100
F	5.13946900	-3.42502800	0.30567600
H	-8.45488600	1.47086500	-1.12303100
H	-8.12269500	-0.99083100	-0.95092800
H	-5.83981800	-1.92740000	-0.84080800
H	-4.20333400	2.04475700	-1.06350600
H	-6.47352700	2.97469300	-1.17608700
H	-2.25814600	-2.37130200	1.47505000

H	-3.10786400	-2.94166200	3.72872600
H	-4.29867400	-1.22689200	5.08285700
H	-4.62470000	1.06037600	4.15935300
H	-3.77328300	1.62166700	1.90549000
H	2.97609900	-2.36606500	-0.18796000
H	6.32334200	0.32254800	-0.09147100
H	2.31426500	1.88529800	-0.11406900
H	0.90760300	-1.52477800	-0.49055900
C	-3.41116000	-1.70785500	-3.15975100
H	-4.42299700	-1.41557900	-3.48685400
H	-2.78614900	-1.82754200	-4.05131200
H	-3.48017700	-2.67920800	-2.65824100
H	-2.03680100	1.23899400	-2.28886300
H	-1.92683500	0.36549600	-3.82283700
H	-3.49277200	1.02250000	-3.29317400
H	-3.58298700	-1.69580800	-0.64147300
H	-1.14192200	-0.99264300	-1.06900400
H	-2.49442700	1.08503500	0.01104100

Nu

E[6-31G(d); Hartrees] = -647.372022; G[6-31G(d); Hartrees] = -647.405236

E[6-311++G(d,p); Hartrees] = -647.6074132

P	-0.05456600	-0.83615900	-0.53143900
O	1.14255400	0.26979600	-0.73243500
O	0.20847400	-1.14639500	1.09948900
O	-1.44399100	0.04758500	-0.47803800
H	-0.12455100	-2.03189900	1.31283800
C	1.79863800	1.02439400	0.29416300
H	2.71907700	1.41356600	-0.14803700
H	1.17880300	1.86550100	0.62482100
H	2.03866900	0.39400100	1.15382700
C	-1.64819300	1.16904700	0.38931700
H	-2.72311300	1.36509400	0.41465900
H	-1.29520600	0.95371700	1.40318600
H	-1.13414300	2.05387200	-0.00271700

EI

E[6-31G(d); Hartrees] = -661.487090; G[6-31G(d); Hartrees] = -661.525483

E[6-311++G(d,p); Hartrees] = -661.7978875

C	-2.84613100	1.53575600	0.00043400
C	-3.59993300	0.35628100	0.00083700
C	-2.98889000	-0.90343700	0.00062800
C	-1.60252300	-0.94510600	0.00003600
C	-0.81791000	0.23743300	-0.00029200

C	-1.45200700	1.48658900	-0.00009000
N	-0.76375200	-2.05966700	-0.00023600
C	0.57381900	-1.69914100	-0.00073900
C	0.57210900	-0.17615800	-0.00050600
O	1.52659000	-2.44926300	-0.00132600
C	1.73020300	0.54872700	-0.00033500
C	3.03907100	-0.03503300	-0.00007900
N	4.14404200	-0.39862300	0.00306100
C	1.70947300	1.98046900	-0.00065100
N	1.68115800	3.14402000	-0.00098600
H	-3.34888200	2.49745300	0.00055400
H	-4.68469500	0.41434000	0.00131000
H	-3.58129800	-1.81318400	0.00120300
H	-0.87245000	2.40253800	-0.00027000
H	-1.05920500	-3.02543200	-0.00051800

Cat-Nu

E[6-31G(d); Hartrees] = -2774.968355; G[6-31G(d); Hartrees] = -2775.050858

E[6-311++G(d,p); Hartrees] = -2776.1705787

N	1.17499400	-0.64923500	0.57460700
C	0.02562800	-1.13736100	0.03506400
N	-1.07787800	-0.47488800	0.54001100
S	-0.01363200	-2.35657700	-1.12668000
C	-2.44640700	-0.66755000	0.28024700
C	-3.27123100	0.46303400	0.34516600
C	-4.64274100	0.35001700	0.11941100
C	-5.21934500	-0.88534300	-0.16212200
C	-4.39581300	-2.01261100	-0.19826200
C	-3.02318900	-1.92093300	0.02552200
C	-4.99337900	-3.35364400	-0.54022100
F	-4.94424200	-3.59345400	-1.87016900
F	-6.29359900	-3.42944900	-0.17538300
F	-4.34150000	-4.36717700	0.06818400
C	-5.47243700	1.60502300	0.16336400
F	-6.78133600	1.36504400	-0.05280100
F	-5.36471500	2.23367000	1.35423200
F	-5.06816200	2.49572600	-0.77977100
H	-2.84272300	1.43672300	0.56790900
H	-6.28380000	-0.97236600	-0.33815100
H	-2.40653000	-2.80764900	0.00007100
P	-0.12898900	3.52327800	1.34909700
O	0.57032200	2.07430400	1.00778200
O	0.92424000	4.45321200	0.44031000
O	-1.48893500	3.53118800	0.40576600

C	2.52613000	-0.94275000	0.11326100
H	2.40347400	-1.49133900	-0.82144900
C	3.32331300	0.37450600	-0.14086900
H	3.54272700	0.81529300	0.83948400
C	3.26412700	-1.85070800	1.09591600
C	3.68306200	-3.12347000	0.69544500
C	3.50927600	-1.44546200	2.41502500
C	4.34264200	-3.97047300	1.58774000
H	3.48195800	-3.45694000	-0.31880200
C	4.16664100	-2.28940900	3.30937600
H	3.17780800	-0.46721700	2.75825200
C	4.58814900	-3.55526000	2.89651600
H	4.65928000	-4.95673700	1.25931500
H	4.34696700	-1.95984200	4.32921800
H	5.09972700	-4.21411500	3.59293600
C	4.66870100	0.07844100	-0.80412900
C	5.84309900	0.59543400	-0.24039200
C	4.77746900	-0.68193100	-1.97936800
C	7.08773100	0.37155800	-0.82938600
H	5.78196200	1.17545000	0.67771100
C	6.02025400	-0.90477200	-2.57391400
H	3.89304100	-1.11615000	-2.43583300
C	7.17948700	-0.37810800	-2.00237500
H	7.98377300	0.77932800	-0.36919600
H	6.08133600	-1.49741000	-3.48272300
H	8.14667700	-0.55646800	-2.46426300
N	2.51257900	1.43361100	-0.82942700
C	3.27035100	2.69300100	-0.94054900
H	2.59222600	3.47954600	-1.28008400
H	3.64811000	2.98234600	0.04461100
H	4.11754500	2.61443900	-1.63581500
H	1.08310000	0.09509000	1.25761900
H	-0.85821500	0.43739300	0.93583600
C	-1.47366400	3.33725000	-1.01727000
H	-2.51683800	3.29737100	-1.33576800
H	-0.96228900	4.16576200	-1.51735600
H	-0.98172800	2.39442400	-1.28149200
C	0.81145500	5.87394800	0.57771900
H	0.76065400	6.17300700	1.63227700
H	1.70475600	6.31179800	0.12619300
H	-0.07701400	6.25351100	0.05887200
H	1.22385500	1.95498500	0.22849700
C	1.97189400	1.05804400	-2.14674900
H	1.30345400	1.85739600	-2.48292100

H	2.75909500	0.93580600	-2.90460400
H	1.39244900	0.13451300	-2.08072700

Cat-TS-CatH

E[6-31G(d); Hartrees] = -2774.968163; G[6-31G(d); Hartrees] = -2775.048197

E[6-311++G(d,p); Hartrees] = -2776.1687881

N	1.16097800	-0.70271400	0.58519900
C	0.01778000	-1.17899200	0.01279600
N	-1.07801700	-0.46808800	0.45375900
S	0.00010800	-2.42992100	-1.11646500
C	-2.45091800	-0.65101200	0.21618800
C	-3.26455900	0.48493400	0.32433700
C	-4.63929800	0.38978800	0.10911600
C	-5.23056600	-0.83182700	-0.19801300
C	-4.41812700	-1.96627300	-0.26949100
C	-3.04241200	-1.89321800	-0.06397500
C	-5.06726700	-3.30360800	-0.51807600
F	-6.06048700	-3.20895100	-1.43213800
F	-5.62701400	-3.79793100	0.61180000
F	-4.19104000	-4.22567200	-0.96321900
C	-5.45568400	1.65262400	0.18133400
F	-6.77288100	1.42431600	0.00188900
F	-5.30828300	2.27474100	1.37066800
F	-5.07221000	2.54288100	-0.77029300
H	-2.82395000	1.44805400	0.56983300
H	-6.29589700	-0.90155300	-0.37905600
H	-2.43305500	-2.78207700	-0.13617800
P	0.00249200	3.35251400	1.34597800
O	0.67006900	1.97026300	0.86325200
O	0.98108800	4.39984500	0.44889300
O	-1.42053800	3.44172300	0.47012100
C	2.51159600	-0.97658600	0.11872800
H	2.40132300	-1.52762300	-0.81702600
C	3.28945700	0.35510800	-0.12930900
H	3.49530000	0.80086400	0.85038600
C	3.28518700	-1.86043200	1.09633900
C	3.84921700	-3.06411700	0.66317000
C	3.43263000	-1.48967000	2.43959600
C	4.55571700	-3.87850300	1.54990400
H	3.72704700	-3.37043800	-0.37204400
C	4.13676600	-2.30150200	3.32803800
H	2.98327100	-0.56834900	2.80484900
C	4.70331700	-3.49830700	2.88385600
H	4.98438200	-4.81282900	1.19774400

H	4.23857800	-2.00215200	4.36775900
H	5.25031100	-4.13275300	3.57596300
C	4.62844600	0.10411400	-0.81161700
C	5.79950700	0.62109600	-0.24122900
C	4.73648000	-0.63159200	-2.00262000
C	7.04240000	0.42286200	-0.84281300
H	5.73801600	1.17814400	0.69065800
C	5.97770600	-0.82685400	-2.60948500
H	3.85428000	-1.06955100	-2.45996600
C	7.13416900	-0.29925700	-2.03294500
H	7.93695200	0.82897000	-0.37880600
H	6.03999200	-1.39969200	-3.53060800
H	8.10027800	-0.45688000	-2.50424100
N	2.45322300	1.42315100	-0.81598400
C	3.21787900	2.68813400	-0.96242900
H	2.52066500	3.47391100	-1.25640200
H	3.64296900	2.96467700	0.00477300
H	4.01904400	2.58330600	-1.69952600
H	1.05106400	0.10076800	1.20032300
H	-0.83721900	0.45559000	0.81566900
C	-1.45670500	3.33517600	-0.95677400
H	-2.50908200	3.35052400	-1.24877900
H	-0.93105600	4.17337700	-1.42728100
H	-1.00804800	2.39378900	-1.29639600
C	0.78367100	5.79523200	0.68014700
H	0.71365400	6.02141300	1.75240500
H	1.64661100	6.32252800	0.26377200
H	-0.12792800	6.15694000	0.18782300
H	1.49015600	1.75843400	-0.00626600
C	1.86598800	1.03567000	-2.12107400
H	1.18541000	1.83268400	-2.43157900
H	2.64285900	0.92002400	-2.88373100
H	1.29968900	0.10743200	-2.02978100

CatH-Nu

E[6-31G(d); Hartrees] = -2774.965984; G[6-31G(d); Hartrees] = -2775.047068

E[6-311++G(d,p); Hartrees] = -2776.1708601

N	1.16890100	-0.71101400	0.61462300
C	0.02868600	-1.21646600	0.05222600
N	-1.06070400	-0.46901100	0.42707100
S	0.02861700	-2.53595300	-1.00165500
C	-2.43484000	-0.65674800	0.21090700
C	-3.24403300	0.48433400	0.32004000
C	-4.62286300	0.38905300	0.13842400

C	-5.22451700	-0.83621000	-0.13665400
C	-4.41627000	-1.97181900	-0.21743000
C	-3.03518000	-1.89944500	-0.04476300
C	-5.05027400	-3.29720700	-0.55283700
F	-5.16712600	-3.46816600	-1.89039100
F	-6.29740700	-3.39673100	-0.03768100
F	-4.33324500	-4.33898400	-0.08229400
C	-5.44015000	1.65047200	0.23082000
F	-6.76012200	1.41923600	0.07085700
F	-5.27674600	2.26640200	1.42073000
F	-5.07486700	2.54565100	-0.72249500
H	-2.79606600	1.44813300	0.55045400
H	-6.29608100	-0.90860300	-0.27244900
H	-2.43088700	-2.79241200	-0.10960500
P	-0.00912500	3.29467400	1.32638600
O	0.54070000	1.90348000	0.79890700
O	1.01876300	4.31002900	0.41523800
O	-1.44747100	3.52581400	0.47840400
C	2.51994800	-1.00166300	0.16899500
H	2.42089600	-1.64534000	-0.70756500
C	3.26808500	0.31803500	-0.20778600
H	3.47259900	0.85720000	0.72232000
C	3.32815500	-1.75574200	1.22394900
C	3.93916700	-2.97268400	0.90734400
C	3.46040900	-1.24894500	2.52374800
C	4.67672100	-3.66825900	1.86707500
H	3.82796200	-3.38446200	-0.09202700
C	4.19602400	-1.94200200	3.48418100
H	2.97190900	-0.31657700	2.79980700
C	4.80922700	-3.15344300	3.15673000
H	5.14104200	-4.61549100	1.60670300
H	4.28504000	-1.53918500	4.48948200
H	5.38036400	-3.69537000	3.90556400
C	4.58938900	0.06517100	-0.91257100
C	5.75547000	0.67178000	-0.42564300
C	4.68913000	-0.76927800	-2.03747000
C	6.98631000	0.46566300	-1.04866200
H	5.70146500	1.30319700	0.45789000
C	5.91827600	-0.97132200	-2.66586500
H	3.81208100	-1.28043600	-2.42320800
C	7.06965600	-0.35355500	-2.17486600
H	7.87815600	0.94132800	-0.65064000
H	5.97569300	-1.62066200	-3.53488900
H	8.02669400	-0.51719100	-2.66212400

N	2.37633800	1.31274600	-0.96626100
C	3.08012300	2.60964900	-1.20432700
H	2.33630600	3.33852000	-1.52534600
H	3.50350100	2.95935700	-0.26266000
H	3.86401600	2.47736600	-1.95112900
H	1.04496600	0.14157800	1.16496700
H	-0.80344100	0.47420400	0.74312300
C	-1.50480900	3.42651800	-0.94436100
H	-2.56120500	3.40782600	-1.22382300
H	-1.01693900	4.28542800	-1.42080500
H	-1.02843300	2.50449600	-1.30191100
C	0.86927800	5.70787000	0.64713800
H	0.81854000	5.93913600	1.72015500
H	1.74224500	6.21304500	0.22141100
H	-0.03698400	6.10165900	0.16807400
C	1.77551800	0.81025400	-2.23569400
H	1.05371300	1.55523300	-2.57686900
H	2.55543000	0.68658900	-2.98927400
H	1.26060800	-0.13637400	-2.06646400
H	1.55392600	1.57857200	-0.28132100

M1-O

E[6-31G(d); Hartrees] = -3436.467002; G[6-31G(d); Hartrees] = -3436.567990

E[6-311++G(d,p); Hartrees] = -3437.9793405

N	-1.66909200	0.95315400	0.44801200
C	-0.84433800	2.01768000	0.60302200
N	0.48212500	1.63968300	0.55311000
S	-1.37339300	3.60576900	0.84485400
C	1.63623600	2.42105100	0.41351200
C	2.82815600	1.89465500	0.92952000
C	4.04233000	2.54842400	0.71695000
C	4.09329300	3.75938400	0.03185800
C	2.89794100	4.29796800	-0.45016700
C	1.68111900	3.64101200	-0.28183900
C	2.92126400	5.63388500	-1.14889300
F	1.93673600	5.74039300	-2.06679400
F	4.09569900	5.84051400	-1.78839400
F	2.76414900	6.65409600	-0.27742900
C	5.30007500	1.87413100	1.17939100
F	5.19864000	1.39270900	2.43330700
F	5.58070900	0.78173100	0.38328500
F	6.38006100	2.66882200	1.12273800
C	5.57400100	-5.18418000	-0.83990400
C	6.28467800	-3.99956400	-1.06733800

C	5.73854500	-2.74745000	-0.75888000
C	4.46243900	-2.72470800	-0.21927500
C	3.72609000	-3.90925200	0.02810400
C	4.29237600	-5.15069700	-0.28907000
N	3.70506100	-1.61390200	0.16259100
C	2.48608400	-1.98276400	0.67922100
C	2.46336100	-3.50313000	0.61536300
O	1.61392000	-1.24334500	1.10811800
C	1.40972900	-4.23848900	1.07667300
C	0.23963400	-3.67744500	1.68339600
N	-0.74181900	-3.34716200	2.21308100
C	1.41009100	-5.66793600	0.99641000
N	1.41514300	-6.82986800	0.92980000
H	2.79136800	0.96982000	1.49550300
H	5.03551000	4.26732600	-0.13057900
H	0.77426900	4.06359900	-0.68914900
H	6.02375800	-6.13928000	-1.09134200
H	7.28334000	-4.04781600	-1.49202400
H	6.29268500	-1.82977000	-0.92852500
H	3.74926400	-6.07167000	-0.11148500
H	4.03400200	-0.65723300	0.12463300
P	-0.94206900	-2.40240700	-1.66261000
O	-0.95605000	-0.84455400	-1.47160000
O	-2.48238500	-2.77361500	-1.03526100
O	-1.43285400	-2.63164600	-3.27884000
C	-3.11871000	1.00725000	0.61107900
H	-3.38524800	2.06488800	0.57004400
C	-3.85280800	0.23298800	-0.52449200
H	-3.71518300	-0.83807400	-0.35415800
C	-3.55764000	0.45997200	1.96880600
C	-4.30335300	1.25994800	2.84064700
C	-3.20094000	-0.83573000	2.36620600
C	-4.69558400	0.77244300	4.08862200
H	-4.56981500	2.27156000	2.54622800
C	-3.58733400	-1.32039100	3.61501000
H	-2.60780300	-1.47246100	1.71524700
C	-4.33859300	-0.51895900	4.47800000
H	-5.27213700	1.40588600	4.75767100
H	-3.28797200	-2.32180700	3.91067600
H	-4.63775200	-0.89708500	5.45219700
C	-5.34123700	0.53751700	-0.55478100
C	-6.25567300	-0.52473300	-0.54396800
C	-5.84058000	1.84925000	-0.58958600
C	-7.63024400	-0.28895500	-0.57705200

H	-5.88457800	-1.54545700	-0.49940700
C	-7.21494900	2.08693700	-0.62925300
H	-5.16128000	2.69659900	-0.57100500
C	-8.11376100	1.01897600	-0.62439900
H	-8.32130100	-1.12721100	-0.56134300
H	-7.58213500	3.10921700	-0.65478300
H	-9.18379200	1.20589300	-0.64899900
N	-3.18407500	0.42078100	-1.89194900
C	-3.85564800	-0.39076000	-2.95033100
H	-3.23165200	-0.35614200	-3.84473300
H	-3.90593900	-1.42403700	-2.60888200
H	-4.84959400	0.00928300	-3.15583400
H	-1.26677200	0.09637000	0.03811000
H	0.66743900	0.64414800	0.66865200
C	-0.39662700	-2.75024900	-4.24195900
H	-0.81498300	-3.23213500	-5.13185600
H	0.00230300	-1.76719800	-4.53099000
H	0.43961600	-3.36395100	-3.87490400
C	-2.85042000	-4.15019100	-1.03083400
H	-2.04717900	-4.78245900	-0.62820700
H	-3.72895400	-4.25811900	-0.38781900
H	-3.09435500	-4.49771900	-2.04227000
C	-2.99279100	1.82455700	-2.34633400
H	-2.34020400	1.80412600	-3.22234200
H	-3.95622100	2.25971500	-2.62125600
H	-2.52320500	2.42063400	-1.56294500
H	-2.19382400	-0.06823800	-1.77553500

M1-N

E[6-31G(d); Hartrees] = -3436.455545; G[6-31G(d); Hartrees] = -3436.555535

E[6-311++G(d,p); Hartrees] = -3437.9690390

C	5.28192000	-5.66181300	-0.45577200
C	5.61105200	-4.39834000	0.03601700
C	4.65597100	-3.38141700	0.04607800
C	3.35841100	-3.60950500	-0.43294400
C	3.03451500	-4.88847100	-0.91193100
C	3.99064400	-5.90441000	-0.92717100
C	2.35823200	-2.46591600	-0.41481100
C	1.02677700	-2.84043800	0.28693100
N	2.12092400	-1.86490200	-1.80240700
N	0.06240200	-1.75006900	0.17883600
C	1.28323100	-3.24121000	1.74095700
C	1.76086100	-2.31319500	2.67505000
C	1.98482400	-2.69085100	3.99831800

C	1.72873100	-4.00171000	4.40647400
C	1.24387100	-4.92953400	3.48480400
C	1.02163700	-4.54966300	2.16018700
C	1.25499400	-2.65219000	-2.72055900
C	-1.28839500	-1.93921300	0.11713100
N	-1.96375700	-0.76886300	0.37634500
S	-1.99990700	-3.43124800	-0.21826100
C	-3.32785400	-0.44636400	0.27170700
C	-3.78616900	0.60926100	1.07738600
C	-5.11279400	1.02411000	1.00523500
C	-6.00955900	0.40083400	0.13679400
C	-5.54653200	-0.63966200	-0.66622800
C	-4.21914800	-1.06696000	-0.61331100
C	-6.47340100	-1.27616400	-1.66959900
F	-6.35293200	-0.69607200	-2.88845200
F	-7.76961400	-1.15750200	-1.30610600
F	-6.21526900	-2.58998100	-1.83595800
C	-5.57602500	2.19144000	1.83663200
F	-4.85230700	2.32836400	2.96818500
F	-5.47038300	3.35762400	1.15711900
F	-6.87324800	2.06500600	2.19498000
C	5.72949400	4.85668100	-0.15623100
C	5.32087400	6.16188900	-0.45749100
C	3.99275200	6.57222000	-0.29242100
C	3.08625700	5.63659000	0.18294700
C	3.47812000	4.30873400	0.49519900
C	4.81249400	3.92074600	0.31918900
N	1.72485900	5.79389500	0.43966700
C	1.15160700	4.62257900	0.89652700
C	2.29321600	3.61365600	0.94409800
O	-0.00697300	4.45380100	1.21479400
C	2.09226400	2.32278500	1.34064500
C	0.80869100	1.79925200	1.69922400
N	-0.17697500	1.25564600	1.99124900
C	3.14697100	1.35713300	1.34774400
N	3.99576400	0.55991900	1.35937200
H	6.02353300	-6.45579400	-0.46389300
H	6.60945200	-4.20278400	0.41717400
H	4.91378700	-2.40222400	0.44244600
H	2.02940700	-5.10781600	-1.25995300
H	3.72187200	-6.88890000	-1.29999000
H	1.95109400	-1.28646500	2.37552900
H	2.35625500	-1.95966800	4.71122500
H	1.90011000	-4.29508100	5.43872400

H	1.03042800	-5.94862900	3.79587600
H	0.62947700	-5.27105800	1.44883900
H	-3.10349900	1.09515200	1.76747800
H	-7.04621900	0.71162400	0.09610100
H	-3.88559500	-1.88369200	-1.23682600
H	6.76634000	4.56983100	-0.29834100
H	6.04874500	6.87688100	-0.83051900
H	3.68590100	7.58557100	-0.53184100
H	5.12885700	2.90849100	0.54330100
H	1.17892600	6.62392600	0.25839200
H	-1.41696300	-0.06839600	0.87681200
C	3.39803100	-1.48832000	-2.47472900
H	3.94211300	-2.38038100	-2.78900200
H	3.14707600	-0.85900300	-3.33080500
H	4.00391000	-0.90752000	-1.77704800
H	0.29774400	-2.86801200	-2.24413500
H	1.08160700	-2.04637300	-3.61206200
H	1.75502200	-3.58047500	-3.00635100
H	2.80925400	-1.63000000	0.12856000
H	0.41002200	-0.79447600	0.06438700
H	0.57662100	-3.70076100	-0.21405100
P	1.77101400	1.67429500	-2.03148400
O	0.63113300	2.88114200	-1.75850000
O	1.19956900	0.44000000	-1.20088500
O	1.48684600	1.20802000	-3.63687000
C	-0.76606900	2.64013400	-1.55133700
H	-1.11138000	3.31910000	-0.76677600
H	-1.32384800	2.84448900	-2.47322300
H	-0.94888600	1.60881000	-1.23686900
C	0.20143800	0.80492100	-4.10315400
H	0.34221700	0.21234400	-5.01442900
H	-0.33013500	0.19792900	-3.36008200
H	-0.41428700	1.67748300	-4.35339100
H	1.63940000	-0.86430900	-1.60400000

TS_{P-C}

E[6-31G(d); Hartrees] = -3436.461064; G[6-31G(d); Hartrees] = -3436.558031

E[6-311++G(d,p); Hartrees] = -3437.9746870

C	7.96542700	-0.61044500	-1.11324000
C	7.47946700	0.49146000	-0.40883400
C	6.11263200	0.61159600	-0.15686000
C	5.20949200	-0.36285700	-0.60551000
C	5.71261300	-1.47459000	-1.29937800
C	7.07887200	-1.59420700	-1.55470200

C	3.73184100	-0.18495100	-0.30660300
C	3.05650900	-1.44519000	0.29192400
N	2.94992400	0.33500600	-1.52523000
N	1.62094200	-1.21812300	0.42294500
C	3.69821700	-1.84302300	1.62019300
C	3.76851700	-0.94975100	2.69925300
C	4.33031900	-1.35519300	3.91025100
C	4.82601000	-2.65191700	4.06009300
C	4.75392900	-3.54628600	2.99188300
C	4.19211100	-3.14304700	1.77972500
C	2.86751900	-0.58973300	-2.69598400
C	0.65149000	-2.11241200	0.06284800
N	-0.57793500	-1.71346200	0.50735100
S	0.97636500	-3.52601300	-0.80503100
C	-1.86975500	-2.22177900	0.32416000
C	-2.83998900	-1.69997400	1.19445200
C	-4.18386600	-2.02849000	1.04693500
C	-4.59278000	-2.92550900	0.06235700
C	-3.62029300	-3.47617300	-0.77419400
C	-2.27238100	-3.13082000	-0.66645700
C	-4.02619400	-4.49572300	-1.80921500
F	-3.27449500	-4.40395000	-2.92678400
F	-5.31938300	-4.34834300	-2.17630700
F	-3.88993800	-5.75696000	-1.34292400
C	-5.17197900	-1.35463800	1.95582300
F	-4.89558800	-1.56791800	3.25798500
F	-5.13506600	0.00794000	1.78443100
F	-6.43895200	-1.73926700	1.73235900
C	-3.54904100	5.84970400	0.20680000
C	-4.62007600	4.98044900	0.43872200
C	-4.40305100	3.64422300	0.79063500
C	-3.08687500	3.21787200	0.89418700
C	-1.98968700	4.07044500	0.64630600
C	-2.22773600	5.40416100	0.30727700
N	-2.61387100	1.95553800	1.25913300
C	-1.24101700	1.90483100	1.28369500
C	-0.76604700	3.27227900	0.84047600
O	-0.56284800	0.94280000	1.65063500
C	0.52152400	3.74805500	1.13030300
C	1.59989100	2.88394300	1.44954900
N	2.54125700	2.22830000	1.67112200
C	0.87956400	5.10366100	0.90034100
N	1.16913800	6.21522600	0.69011200
H	9.02960100	-0.70791500	-1.30921800

H	8.16258200	1.25561600	-0.04888800
H	5.74150700	1.46414300	0.40632200
H	5.04472600	-2.26281500	-1.63384000
H	7.45058700	-2.46233300	-2.09183200
H	3.38581200	0.06376400	2.60677800
H	4.37927100	-0.65347000	4.73859400
H	5.26260800	-2.96362300	5.00522400
H	5.13069800	-4.55979300	3.10034800
H	4.12456500	-3.84679500	0.95446000
H	-2.52686000	-1.02852800	1.98851900
H	-5.63743300	-3.18296000	-0.05605600
H	-1.54138300	-3.54795300	-1.34406100
H	-3.74314200	6.88551800	-0.05444600
H	-5.63912700	5.34670500	0.35216500
H	-5.22838800	2.96554300	0.98374700
H	-1.40669400	6.08853000	0.12966300
H	-3.20676500	1.15785400	1.44806300
H	-0.58666100	-0.81876500	1.00431200
C	3.42781700	1.68885700	-1.94811900
H	4.41622900	1.60286900	-2.40060100
H	2.69924400	2.09771700	-2.64873200
H	3.46814700	2.33165600	-1.06785400
H	2.46155700	-1.55114100	-2.37627600
H	2.17965900	-0.13791000	-3.41175800
H	3.85680100	-0.71002800	-3.13884900
H	3.61750100	0.63105400	0.41074300
H	1.33286600	-0.40728600	0.96619200
H	3.15363600	-2.28847200	-0.39311300
P	-0.51082500	2.13145500	-1.48153300
O	-1.81409100	1.93556000	-2.47738300
O	0.33712800	0.86121400	-1.44644700
O	0.44844600	3.21060800	-2.32561700
H	1.93617600	0.48805400	-1.24874500
C	-1.68506600	1.14025200	-3.67000200
H	-1.30510100	0.14332700	-3.42942900
H	-2.68430100	1.06348800	-4.10440000
H	-1.01149700	1.62407200	-4.38698200
C	-0.06084600	4.50326300	-2.68289700
H	-1.14608900	4.48131100	-2.82696200
H	0.19780400	5.24215800	-1.91752100
H	0.41545900	4.78836800	-3.62560300

$TS_{Enantio}$

E[6-31G(d); Hartrees] = -3436.454852; G[6-31G(d); Hartrees] = -3436.553954

E[6-311++G(d,p); Hartrees] = -3437.9710113

C	-5.01700800	5.72409600	-1.00020200
C	-5.44245500	4.57932700	-0.32562500
C	-4.55860600	3.51882500	-0.12536500
C	-3.23849200	3.58149600	-0.59244900
C	-2.81790800	4.74537500	-1.25576300
C	-3.70232900	5.80448600	-1.46243900
C	-2.31089700	2.40276300	-0.35004900
C	-0.97602500	2.82164200	0.32432800
N	-2.07935200	1.57104100	-1.61593200
N	-0.01061200	1.72813300	0.30845000
C	-1.23912800	3.33277200	1.73980300
C	-1.77616700	2.49205600	2.72580100
C	-1.98376500	2.96960200	4.01969700
C	-1.66057200	4.28881800	4.34468700
C	-1.12291200	5.12867500	3.36923400
C	-0.91239100	4.65153800	2.07459400
C	-1.27037300	2.20086400	-2.70269500
C	1.31148500	1.87825100	-0.01784000
N	2.06309500	0.82214800	0.41768300
S	1.90429100	3.22457200	-0.85357700
C	3.41286000	0.48950800	0.20218700
C	4.00762300	-0.34733300	1.15960000
C	5.32561300	-0.76872600	1.00568800
C	6.07669800	-0.36830800	-0.09903700
C	5.47749300	0.45446800	-1.05192300
C	4.15726200	0.88375700	-0.91796900
C	6.25116000	0.82085700	-2.29241500
F	6.15985800	-0.14794900	-3.23530500
F	7.56721800	0.98426000	-2.02929400
F	5.80329300	1.96131100	-2.85554400
C	5.97269900	-1.60689300	2.07734200
F	6.64334900	-0.84051800	2.96847500
F	5.06680100	-2.32383800	2.77514200
F	6.86821900	-2.47484200	1.55644900
C	-4.06035800	-6.24417900	0.23291200
C	-5.33991300	-5.71724200	0.03428700
C	-5.58019100	-4.34100000	0.13368300
C	-4.50178100	-3.52319700	0.43882600
C	-3.19972400	-4.03471900	0.63750700
C	-2.97974400	-5.40900700	0.53323200
N	-4.47189700	-2.13521600	0.59489000
C	-3.20633000	-1.66760600	0.89679600
C	-2.32120100	-2.89389300	0.93150800

O	-2.92287500	-0.49655700	1.12515200
C	-1.10090700	-2.91906300	1.60809900
C	-0.39528300	-1.73765100	1.95040800
N	0.25560100	-0.80869800	2.22811200
C	-0.39964200	-4.13329000	1.85269400
N	0.17156400	-5.12741600	2.06558300
H	-5.70202900	6.55263800	-1.15686300
H	-6.45954700	4.51262600	0.05049800
H	-4.89093700	2.63468500	0.41309600
H	-1.79402200	4.83986400	-1.60543300
H	-3.35891200	6.69717000	-1.97763900
H	-2.02326700	1.45850100	2.49543000
H	-2.39414700	2.30651500	4.77650900
H	-1.82166900	4.65732100	5.35423900
H	-0.86069000	6.15432100	3.61450700
H	-0.48185300	5.30550600	1.32102200
H	3.43577200	-0.66918400	2.02424400
H	7.10400400	-0.69258600	-0.21542200
H	3.71424100	1.52507100	-1.66536900
H	-3.89995800	-7.31475400	0.15133400
H	-6.16649100	-6.38282300	-0.19806800
H	-6.57581700	-3.93293000	-0.01511900
H	-1.98929300	-5.82402300	0.67654200
H	-5.26803100	-1.51815300	0.52633600
H	1.58821900	0.20129300	1.07624100
C	-3.36424900	1.04029900	-2.16295000
H	-3.95187000	1.85472400	-2.58794400
H	-3.12561600	0.28876200	-2.91678000
H	-3.91344700	0.56680200	-1.34799700
H	-0.33135500	2.58275600	-2.29762100
H	-1.05222300	1.41698400	-3.43022200
H	-1.84353200	3.00205100	-3.17193100
H	-2.81431300	1.68839100	0.30560400
H	-0.26419700	0.89146200	0.83000600
H	-0.50946800	3.62415100	-0.24790300
P	-1.57375700	-2.13818500	-1.48954800
O	-0.42137100	-3.31013300	-1.59949700
O	-0.89503800	-0.76700300	-1.39180900
O	-2.25249600	-2.14333900	-3.03233800
H	-1.54106800	0.68469400	-1.34253800
C	0.84523000	-3.02502900	-2.22097000
H	1.48652300	-3.88778500	-2.02900700
H	0.72353700	-2.89006100	-3.30180300
H	1.29139900	-2.12309900	-1.79397800

C	-2.82377300	-3.36350600	-3.51229400
H	-3.23006500	-3.15719500	-4.50608800
H	-2.06631300	-4.15137300	-3.58617100
H	-3.63508700	-3.71520500	-2.86173000

M2

E[6-31G(d); Hartrees] = -3436.477240; G[6-31G(d); Hartrees] = -3436.574199

E[6-311++G(d,p); Hartrees] = -3437.9909863

C	7.75901300	-1.33970700	-0.99264200
C	7.38078000	-0.34180200	-0.09415500
C	6.02927300	-0.10621500	0.15878700
C	5.03467400	-0.85965100	-0.48084100
C	5.42869300	-1.87124100	-1.37102400
C	6.77962600	-2.10518500	-1.62791700
C	3.57889900	-0.56491100	-0.17298500
C	2.71969500	-1.82121400	0.12581700
N	2.91940200	0.28641800	-1.28127400
N	1.32931700	-1.41518100	0.32524100
C	3.28067000	-2.60907700	1.30919600
C	3.34179300	-2.05811400	2.59750700
C	3.85298700	-2.80942200	3.65632600
C	4.30523000	-4.11354000	3.44571800
C	4.23809700	-4.66935200	2.16792500
C	3.72698700	-3.92049600	1.10717700
C	2.74783200	-0.39332800	-2.60479400
C	0.25664900	-2.08969100	-0.18524500
N	-0.93312800	-1.60969800	0.30577000
S	0.41692800	-3.32048600	-1.33564300
C	-2.25620400	-2.06358400	0.13948000
C	-3.27005400	-1.15220800	0.47731900
C	-4.61060200	-1.50187400	0.34701500
C	-4.98158000	-2.76982600	-0.09822300
C	-3.97204600	-3.68261800	-0.40035300
C	-2.62119200	-3.34982600	-0.28621000
C	-4.34053200	-5.08721900	-0.80627200
F	-3.45637500	-5.61023500	-1.68062800
F	-5.56230500	-5.13718400	-1.38419100
F	-4.37718300	-5.91756000	0.26193400
C	-5.65601300	-0.49121000	0.73156300
F	-5.28092400	0.77145600	0.38745100
F	-6.84176200	-0.73125300	0.13588400
F	-5.87740300	-0.46983400	2.06522700
C	-0.95335500	7.13160900	0.51607800
C	-2.13482500	7.08634400	1.25843700

C	-2.66568500	5.86635500	1.69357400
C	-1.97381100	4.71316600	1.35141700
C	-0.78922600	4.73657000	0.60029900
C	-0.27000600	5.95489400	0.18072800
N	-2.28613700	3.38169300	1.67272500
C	-1.38084200	2.49323100	1.17321800
C	-0.27753000	3.31029400	0.44758700
O	-1.45763700	1.27290800	1.26388500
C	1.09451900	3.05769400	1.07220900
C	1.37764400	1.85970100	1.71755000
N	1.62280500	0.83608900	2.24933200
C	2.16560400	3.92551000	0.80206800
N	3.07787800	4.61998400	0.54931300
H	8.81073400	-1.52696600	-1.19029300
H	8.13474800	0.25163000	0.41496200
H	5.74335200	0.66631900	0.86819700
H	4.68590500	-2.49636900	-1.85759300
H	7.06583900	-2.89389400	-2.31801400
H	2.96897400	-1.05408500	2.78198700
H	3.89217000	-2.37288300	4.65077500
H	4.70083700	-4.69513700	4.27419700
H	4.57694300	-5.68731900	1.99498400
H	3.66446700	-4.36259800	0.11640700
H	-2.99918900	-0.16638400	0.83732700
H	-6.02454000	-3.03677700	-0.21417700
H	-1.86268200	-4.07356200	-0.54408400
H	-0.55494100	8.08937200	0.19500300
H	-2.65157400	8.00852800	1.50890700
H	-3.58028700	5.82639900	2.27798000
H	0.65080100	5.99340900	-0.38880900
H	-3.10453600	3.07423800	2.18163100
H	-0.87843000	-0.69835800	0.76250400
C	3.60480000	1.60832200	-1.45414600
H	4.59834700	1.44404600	-1.87083500
H	2.99685500	2.21329000	-2.12576700
H	3.67375200	2.11852400	-0.49365200
H	2.18538500	-1.31911000	-2.47324900
H	2.17253400	0.28175300	-3.23805500
H	3.72908900	-0.58653800	-3.03826200
H	3.52310800	0.09454000	0.69658800
H	1.18973900	-0.75731500	1.10157700
H	2.71394000	-2.48582200	-0.73892300
P	-0.29339400	2.70011700	-1.31619400
O	-1.82160000	2.72480900	-1.84089400

O	0.38347100	1.37760300	-1.53673800
O	0.37353700	3.93912600	-2.10004100
H	1.94974800	0.51240400	-0.97749100
C	-2.58028000	1.52606100	-2.12016500
H	-3.03959500	1.65764500	-3.10272800
H	-1.93152400	0.64825100	-2.12448100
H	-3.35782100	1.41775100	-1.36107600
C	0.32336200	4.01061700	-3.53599300
H	0.92502000	4.87511300	-3.81929200
H	0.74375900	3.10567700	-3.98724600
H	-0.70868400	4.14670600	-3.87051700

$TS_{NH–CH}$

E[6-31G(d); Hartrees] = -3436.459170; G[6-31G(d); Hartrees] = -3436.554922

E[6-311++G(d,p); Hartrees] = -3437.9630304

C	7.08282800	-3.26743600	-0.72924600
C	6.96453400	-2.22747900	0.19308100
C	5.75311000	-1.54894000	0.33064700
C	4.63962400	-1.89965500	-0.44382900
C	4.76768400	-2.95362600	-1.36209400
C	5.98060700	-3.62778200	-1.50669800
C	3.33499000	-1.12747400	-0.26606000
C	2.19029900	-2.11730700	0.09339500
N	3.02422100	-0.18142000	-1.43061600
N	0.89606300	-1.45571700	0.13561400
C	2.50536000	-2.80922200	1.42308200
C	2.51118500	-2.08294700	2.62217800
C	2.79036700	-2.71640200	3.83269600
C	3.06191100	-4.08609700	3.86171500
C	3.04697400	-4.81754400	2.67408500
C	2.76903600	-4.18183700	1.46288500
C	2.24634400	-0.76619800	-2.55293600
C	-0.28863200	-2.08355000	-0.10807800
N	-1.34917400	-1.32029900	0.33021200
S	-0.39433300	-3.59726900	-0.83996000
C	-2.73628800	-1.44371600	0.20118100
C	-3.50165900	-0.51305300	0.92810300
C	-4.89092700	-0.52084200	0.85651800
C	-5.55925000	-1.45852900	0.06800900
C	-4.79879900	-2.37896300	-0.65043100
C	-3.40399400	-2.38379100	-0.59903200
C	-5.49192900	-3.43209200	-1.47857700
F	-4.81852200	-3.70014500	-2.61707300
F	-6.74294500	-3.05305800	-1.82691700

F	-5.60651100	-4.59744400	-0.80318400
C	-5.67701000	0.45950300	1.68395600
F	-5.02508300	1.64761800	1.81233600
F	-6.88449100	0.72481000	1.14429200
F	-5.89268200	0.00713400	2.93831900
C	0.87732300	6.69577300	0.28915600
C	0.56861600	6.77637700	1.64795400
C	0.35381800	5.61957900	2.40573700
C	0.46254200	4.40218300	1.75052400
C	0.77255000	4.29594200	0.38730700
C	0.97815100	5.45467600	-0.35357400
N	0.30101200	3.11170700	2.28211600
C	0.48849800	2.13193700	1.36345300
C	0.83121200	2.81691600	0.00834500
O	0.39580300	0.92746200	1.59846800
C	2.23110300	2.32691600	-0.51918600
C	3.24683900	2.42696600	0.51269600
N	4.05248300	2.39608500	1.35441800
C	2.60679200	3.05506000	-1.71476400
N	2.87160600	3.57737800	-2.72274000
H	8.02503800	-3.79723300	-0.83921300
H	7.81371300	-1.94228000	0.80792100
H	5.66869100	-0.73819400	1.05021500
H	3.91963800	-3.26311600	-1.96649100
H	6.06097200	-4.44038100	-2.22363900
H	2.27881900	-1.02014700	2.61878500
H	2.79221500	-2.14030500	4.75431900
H	3.27698700	-4.58003200	4.80553800
H	3.24569300	-5.88584000	2.68788800
H	2.74818100	-4.75720800	0.54196100
H	-3.00017600	0.22887800	1.54254100
H	-6.63999700	-1.46082600	0.00420600
H	-2.83472300	-3.10029500	-1.17343700
H	1.04073000	7.60485600	-0.28146400
H	0.49367000	7.74727800	2.12901200
H	0.11451100	5.67492400	3.46355300
H	1.21405700	5.40470500	-1.40933000
H	0.07916600	2.89510200	3.24496800
H	-1.06998200	-0.46523000	0.80295700
C	4.27994300	0.41170600	-1.97506200
H	4.90067100	-0.35284300	-2.44729400
H	4.01119200	1.16756000	-2.71281100
H	4.84637700	0.88102900	-1.16826600
H	1.31373900	-1.18780600	-2.18921100

H	2.00768300	0.04101900	-3.24825100
H	2.83582300	-1.52619200	-3.07817700
H	3.47603500	-0.44639100	0.57934300
H	0.85647600	-0.54359500	0.58832600
H	2.11593500	-2.88402900	-0.67982000
P	-0.49730400	2.33528200	-1.21087900
O	-1.78543000	2.63903400	-0.29234100
O	-0.35651000	0.96196900	-1.76263600
O	-0.55488900	3.50449100	-2.31656600
H	2.41781200	0.93964700	-0.95141100
C	-3.10035800	2.69850800	-0.89210500
H	-3.20076900	3.62511000	-1.46300300
H	-3.26901000	1.83240700	-1.53828800
H	-3.81095100	2.67807600	-0.06718400
C	-0.32258600	3.25552000	-3.72446800
H	0.67476700	3.61706100	-3.98028800
H	-0.40670500	2.18924800	-3.94402700
H	-1.08540000	3.81564400	-4.26913700

M3

E[6-31G(d); Hartrees] = -4083.862481; G[6-31G(d); Hartrees] = -4083.973433

E[6-311++G(d,p); Hartrees] = -4085.6078337

C	-8.33893700	-0.72012300	-1.31868800
C	-7.82137800	-1.66407000	-0.43124000
C	-6.47357000	-1.62027100	-0.07447500
C	-5.62184500	-0.63542400	-0.59436900
C	-6.15744800	0.31713800	-1.47620200
C	-7.50386000	0.27039400	-1.83860200
C	-4.16425800	-0.62441600	-0.17423000
C	-3.69785900	0.76795400	0.35068600
N	-3.23175100	-1.17182700	-1.26616200
N	-2.24432700	0.91798400	0.31012700
C	-4.26952100	1.00179400	1.74756600
C	-3.86445400	0.21096600	2.83303300
C	-4.38182600	0.44575300	4.10652500
C	-5.31052700	1.46908900	4.31027100
C	-5.71542500	2.26028400	3.23513200
C	-5.19559300	2.02836600	1.96048100
C	-3.04894300	-0.32574900	-2.48680300
C	-1.61772100	2.07086400	-0.09931000
N	-0.27490200	2.03495500	0.15036900
S	-2.45021500	3.33713600	-0.84935500
C	0.78449300	2.90885200	-0.16460900
C	2.01346400	2.59861300	0.44194300

C	3.15562100	3.33237600	0.13399600
C	3.10128800	4.41044000	-0.74906800
C	1.87192400	4.73373600	-1.32050200
C	0.71839100	3.99564900	-1.04787800
C	1.76718800	5.93284600	-2.22785800
F	0.84803200	5.75024100	-3.20044600
F	2.94572100	6.20956900	-2.83184300
F	1.40474300	7.04285900	-1.54621400
C	4.45537800	2.92114500	0.76729300
F	4.78756200	1.63084100	0.43443300
F	5.48932800	3.69069000	0.37962800
F	4.40380000	2.95275000	2.11383600
C	4.77527200	-5.03984400	-0.54816000
C	5.68927400	-4.03155700	-0.23795500
C	5.27440400	-2.70283000	-0.09159700
C	3.92433400	-2.43336800	-0.26736600
C	2.99010900	-3.43254500	-0.58448800
C	3.41621400	-4.74726500	-0.72555000
N	3.26734700	-1.19693900	-0.16992300
C	1.92863900	-1.30387100	-0.38971400
C	1.60961100	-2.79656200	-0.67636500
O	1.11569700	-0.38610400	-0.36990200
C	0.60066700	-3.31338000	0.36708200
C	0.53966600	-4.70209900	0.64219600
N	0.50414500	-5.84736800	0.87706700
C	-0.55170700	-2.56980200	0.61735400
N	-1.50158300	-1.91828500	0.86822600
H	-9.38856500	-0.75006400	-1.59727600
H	-8.46513900	-2.43175100	-0.01139900
H	-6.07959400	-2.35232600	0.62608000
H	-5.53275400	1.11011800	-1.87701600
H	-7.90131000	1.01598800	-2.52145900
H	-3.13275000	-0.58170800	2.69026600
H	-4.05470900	-0.16881400	4.94073400
H	-5.71131600	1.65148400	5.30373200
H	-6.43156400	3.06340800	3.38662000
H	-5.50369500	2.65407200	1.12744500
H	2.07758600	1.77949300	1.15181100
H	3.99081900	4.97902500	-0.98796500
H	-0.21815100	4.25124900	-1.52107000
H	5.11724500	-6.06524400	-0.65108200
H	6.73933600	-4.27656500	-0.10471400
H	5.98007300	-1.91403100	0.15156200
H	2.70913900	-5.53315100	-0.96038000

H	3.69223000	-0.32083300	0.11193400
H	0.07889900	1.13821100	0.47882300
C	-3.57616600	-2.57997900	-1.64554300
H	-4.53824200	-2.59054100	-2.15788200
H	-2.77097800	-2.94406700	-2.28327100
H	-3.61904000	-3.17905400	-0.73541900
H	-2.84503800	0.70542100	-2.19826500
H	-2.19776000	-0.74072800	-3.02773300
H	-3.95554700	-0.37795900	-3.09120800
H	-4.02019100	-1.35279100	0.62512800
H	-1.71457700	0.24164200	0.85993400
H	-4.07907900	1.54872200	-0.30750500
P	0.88273900	-2.86343500	-2.39259800
O	1.92671800	-2.07814500	-3.35581400
O	-0.52790300	-2.38339400	-2.53720400
O	1.12718100	-4.40616200	-2.77186000
C	1.61319100	-0.76869200	-3.87323600
H	2.45293000	-0.49192900	-4.51275700
H	0.69086000	-0.79745000	-4.45883300
H	1.50834500	-0.04447500	-3.06093200
C	0.60851600	-4.93684000	-4.00489300
H	0.77380400	-6.01409300	-3.96630300
H	-0.46108900	-4.72679300	-4.09398200
H	1.14774000	-4.50763100	-4.85502200
H	-2.31814000	-1.25801900	-0.77580200
P	1.28140300	-0.58296900	3.21207700
O	2.69228700	0.22156700	2.83805100
O	1.74619000	-2.15560200	3.01550900
O	1.23967000	-0.53473400	4.85833600
H	1.35801900	-2.56564700	2.20593700
C	3.95692700	-0.11606100	3.42447100
H	4.72154100	0.43957700	2.87872400
H	3.98200200	0.18759300	4.47665900
H	4.14879300	-1.19101500	3.34356100
C	1.78944200	-1.51880600	5.74314300
H	1.29219000	-1.38239800	6.70704500
H	1.60925400	-2.52963500	5.36997600
H	2.86797300	-1.37320700	5.87458400

$TS_{OH–CH}$

E[6-31G(d); Hartrees] = -4083.849460; G[6-31G(d); Hartrees] = -4083.958909

E[6-311++G(d,p); Hartrees] = -4085.5883800

C	-8.22562200	1.51643900	-0.20716500
C	-7.74977800	0.34212400	0.37724900

C	-6.38597200	0.05087000	0.34873800
C	-5.47658100	0.92733000	-0.26080400
C	-5.96497800	2.11346400	-0.83140300
C	-7.32998400	2.40159400	-0.80963600
C	-4.00241400	0.56718500	-0.25604400
C	-3.10225700	1.71164700	0.27434900
N	-3.52537800	0.04938900	-1.63524800
N	-1.69081700	1.43568700	-0.00003700
C	-3.36751100	1.93674900	1.76202600
C	-3.05728100	0.94880700	2.70802000
C	-3.27262500	1.18199000	4.06599000
C	-3.80312900	2.40090700	4.49386500
C	-4.11283600	3.38819200	3.55813700
C	-3.89339600	3.15741000	2.19926100
C	-3.38154300	1.08049300	-2.71056700
C	-0.78165100	2.44299700	-0.26527400
N	0.49021000	2.06586100	0.04830900
S	-1.24575600	3.92536400	-0.92619700
C	1.74941100	2.66489400	-0.13927200
C	2.80348700	2.06638300	0.57040000
C	4.11157900	2.51017100	0.39189800
C	4.39594100	3.57206100	-0.46430500
C	3.33936800	4.18158500	-1.14200500
C	2.02413200	3.73927500	-0.99804200
C	3.62048000	5.37322000	-2.02169600
F	2.72169900	5.48700700	-3.02298800
F	4.84780300	5.29750500	-2.58582200
F	3.58171400	6.52853100	-1.32096400
C	5.21047400	1.78761800	1.12477100
F	5.27879800	0.48320700	0.73816600
F	6.42367100	2.33027000	0.90116200
F	5.00553700	1.77805600	2.45837700
C	3.28624700	-5.61384800	-1.27307500
C	4.32169200	-4.81883000	-0.77733000
C	4.08189500	-3.51149000	-0.33966100
C	2.77702600	-3.04459900	-0.40506100
C	1.72371700	-3.83245400	-0.89300000
C	1.97527900	-5.12445000	-1.33838200
N	2.30652400	-1.76192300	-0.05892600
C	0.96061300	-1.68104600	-0.22709100
C	0.43931200	-3.02354800	-0.79842200
O	0.24952600	-0.72230600	0.06408800
C	-0.55759600	-3.58761700	0.28634700
C	-0.79697500	-5.01403500	0.19467100

N	-0.97582000	-6.16327300	0.16153600
C	-1.80843800	-2.87148400	0.41529600
N	-2.81315400	-2.31365900	0.60415200
H	-9.28721500	1.74623900	-0.18531000
H	-8.43733500	-0.34627700	0.86030200
H	-6.01828600	-0.86008600	0.81405400
H	-5.28445700	2.83002200	-1.28212900
H	-7.69098500	3.32441900	-1.25492100
H	-2.63441400	-0.00518200	2.40014500
H	-3.01734400	0.41160700	4.78783500
H	-3.96740600	2.58166400	5.55267400
H	-4.51803700	4.34247700	3.88366000
H	-4.12300200	3.93373100	1.47445500
H	2.59801100	1.25851000	1.27042700
H	5.41384600	3.91352400	-0.60349800
H	1.22301600	4.21401000	-1.54548200
H	3.49491200	-6.62546400	-1.60774200
H	5.33180300	-5.21620000	-0.73218100
H	4.88336200	-2.88267900	0.03582000
H	1.17217600	-5.74738300	-1.71384300
H	2.69212400	-1.22430900	0.72739200
H	0.57112100	1.11226300	0.40660700
C	-4.36764700	-1.09805500	-2.10946900
H	-5.36774300	-0.73354400	-2.34117000
H	-3.88244500	-1.51650200	-2.98983500
H	-4.39627500	-1.84799200	-1.31953800
H	-2.76169000	1.90498600	-2.35560700
H	-2.89771400	0.59521700	-3.55955700
H	-4.37163500	1.43738700	-2.99487300
H	-3.85804800	-0.31406600	0.37095700
H	-1.31159900	0.60464200	0.44892400
H	-3.32485700	2.63734800	-0.25736700
P	-0.31974900	-2.68578300	-2.45152900
O	0.89327700	-2.31533800	-3.44957900
O	-1.42341200	-1.67226600	-2.47372600
O	-0.70530300	-4.16969100	-2.91182700
C	1.26777700	-0.94913100	-3.72257900
H	1.78326000	-0.95944600	-4.68413400
H	0.38446200	-0.30847000	-3.77549000
H	1.94753000	-0.58822600	-2.94562300
C	-1.25776600	-4.42945700	-4.21724000
H	-1.52457200	-5.48638200	-4.22590100
H	-2.15069700	-3.82007100	-4.38424000
H	-0.51040800	-4.22301300	-4.98816700

H	-2.58230800	-0.35604700	-1.49995200
P	0.84645900	-1.56776500	3.09254800
O	2.40112200	-0.89024100	2.65419100
O	0.89266600	-2.98224300	2.38684300
O	1.14001400	-1.92086200	4.70130700
H	0.08087300	-3.32737600	1.40084400
C	3.59226200	-1.42485400	3.24192600
H	4.44427200	-0.90185100	2.79909800
H	3.59610200	-1.25525100	4.32384100
H	3.68417600	-2.50150900	3.04733600
C	1.51089200	-3.22009100	5.16544400
H	1.01459800	-3.38016400	6.12837400
H	1.20679800	-3.99510800	4.45664600
H	2.59680900	-3.28072400	5.31559600

M4

E[6-31G(d); Hartrees] = -4083.848729; G[6-31G(d); Hartrees] = -4083.959415

E[6-311++G(d,p); Hartrees] = -4085.5910607

C	8.10614100	-2.05683400	0.16452800
C	7.69986200	-0.80157000	0.61871200
C	6.36585700	-0.41262800	0.49623200
C	5.41759800	-1.27042700	-0.07956500
C	5.83500100	-2.53668700	-0.51992100
C	7.17044200	-2.92345500	-0.40309000
C	3.97814800	-0.80272100	-0.18456700
C	2.95736400	-1.82838100	0.37180000
N	3.61271200	-0.36547800	-1.62446700
N	1.59663200	-1.46614500	-0.02681000
C	3.10542400	-1.94418800	1.88817700
C	2.71766700	-0.89396000	2.73249100
C	2.82495000	-1.02454000	4.11654500
C	3.32890400	-2.20206900	4.67276000
C	3.71739600	-3.25121800	3.83907900
C	3.60181000	-3.12375300	2.45406700
C	3.47143000	-1.46805100	-2.62720400
C	0.62686600	-2.41886700	-0.27642800
N	-0.62710100	-1.93558200	-0.03970700
S	1.00896300	-3.96379900	-0.83949700
C	-1.90758500	-2.50248500	-0.19675700
C	-2.93361100	-1.91464700	0.56083100
C	-4.24632200	-2.36520600	0.42466400
C	-4.55995700	-3.40557700	-0.44737400
C	-3.53273700	-3.98845700	-1.18976000
C	-2.21494700	-3.54667100	-1.08101900

C	-3.84714100	-5.15080500	-2.09630500
F	-2.97979100	-5.23644100	-3.12851600
F	-5.09064300	-5.05200200	-2.61978500
F	-3.79293700	-6.32787900	-1.43450800
C	-5.32810700	-1.68097300	1.21934800
F	-5.51848400	-0.40581500	0.79289500
F	-6.51559500	-2.31326100	1.11736100
F	-5.01616800	-1.60691900	2.52986800
C	-2.87451900	5.74201900	-1.56637700
C	-3.92515000	5.07522200	-0.93214700
C	-3.73887900	3.81405200	-0.35627100
C	-2.46966300	3.25546500	-0.42485300
C	-1.40114400	3.91994200	-1.04871600
C	-1.59974200	5.16590300	-1.63271600
N	-2.06678400	1.99305800	0.04696100
C	-0.74138800	1.81355100	-0.15609700
C	-0.16294400	3.04963600	-0.90638000
O	-0.07570700	0.83650400	0.18732900
C	0.90336800	3.69377600	0.06962400
C	1.29287600	5.05676200	-0.30742400
N	1.60886800	6.13881400	-0.58313800
C	2.12271800	2.89758900	0.26525900
N	3.11146100	2.32589800	0.46901300
H	9.14411000	-2.36276300	0.26061600
H	8.41795700	-0.12565100	1.07413300
H	6.05180900	0.56153600	0.86209800
H	5.12048100	-3.23762600	-0.94187100
H	7.47623400	-3.90742600	-0.74722300
H	2.30887800	0.02907500	2.32799000
H	2.49987500	-0.20827100	4.75482500
H	3.40874500	-2.30402700	5.75160600
H	4.10064100	-4.17481800	4.26442600
H	3.89036900	-3.94976900	1.80952100
H	-2.70475500	-1.11322000	1.26194900
H	-5.58083400	-3.75149400	-0.54873500
H	-1.43503500	-4.00560900	-1.67047400
H	-3.04288300	6.71856800	-2.01007500
H	-4.90677600	5.53860600	-0.88686200
H	-4.55458000	3.28736400	0.12885600
H	-0.78547900	5.68816500	-2.12137100
H	-2.42885700	1.57932900	0.94971300
H	-0.65427100	-0.98805500	0.34464800
C	4.54162200	0.69634900	-2.13122500
H	5.53073300	0.26439200	-2.27993900

H	4.13096800	1.07264600	-3.06750000
H	4.57515500	1.50187700	-1.39833700
H	2.78096100	-2.22647400	-2.25421500
H	3.07163300	-1.02577600	-3.54136200
H	4.45342100	-1.90068100	-2.81954700
H	3.87328900	0.13317000	0.36784200
H	1.25329100	-0.58140400	0.34223900
H	3.13973200	-2.80972900	-0.06718600
P	0.50699500	2.45305300	-2.52243000
O	-0.76635600	1.96623600	-3.37619600
O	1.59583000	1.42726000	-2.44307900
O	0.89565400	3.83810500	-3.22232400
C	-1.19948300	0.58737100	-3.40311000
H	-1.67049000	0.43199500	-4.37480000
H	-0.34932900	-0.08773000	-3.28364300
H	-1.92919800	0.42121500	-2.60685600
C	1.41138800	3.87758100	-4.56880000
H	1.66756700	4.91933700	-4.76154600
H	2.30497600	3.25274700	-4.65384300
H	0.64556000	3.54121100	-5.27270300
H	2.68589600	0.09587300	-1.57153900
P	-0.81950800	1.81773100	3.22491000
O	-2.41918700	1.17982000	2.58424500
O	-0.61859500	3.09940700	2.38830700
O	-1.36418300	2.32742700	4.73730900
H	0.38169800	3.69360000	1.07451400
C	-3.64380300	1.59796700	3.18248100
H	-4.46032500	1.03027100	2.72501400
H	-3.63514700	1.40130000	4.25987500
H	-3.82891000	2.67178200	3.02823200
C	-1.74726300	3.67893400	4.98414400
H	-1.32847300	3.98067400	5.95105900
H	-1.37529700	4.34261900	4.19756900
H	-2.84133400	3.76329200	5.03632200

Prod

E[6-31G(d); Hartrees] = -1308.882333; G[6-31G(d); Hartrees] = -1308.932678

E[6-311++G(d,p); Hartrees] = -1309.4202756

C	-3.48547300	1.34555600	0.03288900
C	-4.20037500	0.19674700	-0.31045400
C	-3.56315100	-1.04439800	-0.41713100
C	-2.19716000	-1.08764700	-0.17036600
C	-1.45826400	0.05869200	0.16854100
C	-2.10656700	1.28467900	0.27206400

N	-1.34682400	-2.20013800	-0.19148600
C	-0.04142700	-1.88269500	0.09713500
C	-0.00896000	-0.34774200	0.39609700
O	0.89936800	-2.65017700	0.11669700
C	0.41922500	-0.13485600	1.90218800
C	0.48587700	1.29548400	2.25708600
N	0.49986700	2.41972900	2.54081300
C	1.66284500	-0.80954800	2.32310200
N	2.58916400	-1.34324700	2.77045900
H	-3.99891700	2.29886700	0.11089000
H	-5.26847100	0.26125600	-0.49763400
H	-4.11773300	-1.94023600	-0.68033700
H	-1.55373200	2.18147300	0.52380400
H	-1.61320300	-3.13978400	-0.45264300
P	1.24670700	0.43288400	-0.75402700
O	1.08888600	-0.38330700	-2.13719200
O	2.61900600	0.51301600	-0.19989500
O	0.51878800	1.83021300	-1.07380200
C	2.12579200	-1.29686700	-2.57804900
H	2.00634000	-1.38411200	-3.65920700
H	3.11238800	-0.89970800	-2.33251700
H	1.98707300	-2.26557500	-2.09414100
C	1.29055200	2.89732900	-1.66739200
H	0.66837300	3.79057000	-1.60354300
H	2.22237700	3.04521800	-1.11651300
H	1.50235600	2.66642900	-2.71579500
H	-0.38878100	-0.56842400	2.50881500

TSa

E[6-31G(d); Hartrees] = -3705.101319; G[6-31G(d); Hartrees] = -3705.206889

E[6-311++G(d,p), CPCM, solvent = CH_2Cl_2; Hartrees] = -3706.9494476

C	6.58934200	-1.00545200	3.37245500
C	5.25285300	-1.32659300	3.02870200
C	4.81521600	-1.12435000	1.67289000
C	5.73719000	-0.59475300	0.73823000
C	7.03741300	-0.29272600	1.10901600
C	7.47145400	-0.50460100	2.44284200
C	3.46032100	-1.48832400	1.36908000
C	2.67371000	-1.97978800	2.39188200
C	3.20965300	-2.11548700	3.69567400
N	4.44915200	-1.81384100	4.01704900
C	2.87548800	-1.35349800	-0.04180100
C	2.41112400	-2.74308700	-0.53058800
N	1.60018300	-2.65287500	-1.81704600

C	2.39732300	-2.13376500	-2.98564600
C	3.63014900	-3.04658800	-3.18791600
C	3.53533400	-4.25009800	-2.22751100
C	3.58658200	-3.72626300	-0.77952300
C	2.19624100	-4.99064700	-2.50361000
C	1.04186000	-4.02106300	-2.12705200
C	2.06363800	-6.30863400	-1.78366000
C	2.01525400	-7.49453900	-2.39077300
O	7.83702200	0.20793000	0.12399800
C	9.16043800	0.60462000	0.45112900
N	1.78549200	-0.38055100	-0.09608800
C	1.91932500	0.88572000	-0.61241400
S	3.21659500	1.35840800	-1.58840600
N	0.85983000	1.68402000	-0.28840400
C	0.63657300	3.05275800	-0.54602500
C	-0.69528100	3.45377500	-0.69822700
C	-1.01024800	4.80788300	-0.81830000
C	-0.01019700	5.77602100	-0.82786200
C	1.31912200	5.36466600	-0.70199300
C	1.65237000	4.02035900	-0.54670000
C	-2.46116800	5.19027700	-0.92007400
F	-3.06646100	4.62011800	-1.98420300
C	2.41419700	6.39828600	-0.76547500
F	2.01660200	7.57671000	-0.23224100
F	-3.15867100	4.77543400	0.17927700
F	-2.64128100	6.52192400	-1.01597800
F	3.52212100	6.00627600	-0.10208600
F	2.78349300	6.65199500	-2.04128900
H	2.57743500	-2.50197000	4.49392600
H	1.64368900	-2.28429800	2.21979400
H	0.07498800	1.21045800	0.16656300
H	6.89090200	-1.17019200	4.40196800
H	0.99560200	-0.54362600	0.52772200
H	3.63548000	-0.96820300	-0.71915200
H	-1.48234400	2.70787000	-0.73853300
H	2.66163300	-1.09478700	-2.77526300
H	2.68428600	3.72657600	-0.41786100
H	4.54366000	-3.22001200	-0.61290100
H	-0.25587800	6.82636700	-0.92130300
H	1.71843500	-2.14266100	-3.84211200
H	8.48749200	-0.26897500	2.73768900
H	5.44652900	-0.36312100	-0.27988800
H	1.69626200	-3.15143100	0.18451200
H	3.54076800	-4.55003300	-0.06193700

H	3.67752900	-3.38899900	-4.22703600
H	4.36930400	-4.93610900	-2.40428500
H	0.31963200	-3.89173900	-2.93639300
H	0.49951800	-4.33335300	-1.23125600
H	2.15392600	-5.19216500	-3.58124800
H	4.54965800	-2.48477600	-2.99194300
H	9.58840700	0.99722700	-0.47290300
H	9.16992300	1.39171400	1.21606800
H	9.76579400	-0.24394700	0.79633800
H	1.99725800	-6.26380100	-0.69603700
H	1.92494200	-8.41930800	-1.82828100
H	2.06152800	-7.58744900	-3.47424800
C	-6.65086100	-0.58137900	2.73133300
C	-6.38005800	0.68978200	3.23677200
C	-5.11788700	1.27603000	3.07207600
C	-4.16052000	0.54494200	2.38269000
C	-4.41754900	-0.72966500	1.84981500
C	-5.67098800	-1.30325400	2.03463500
N	-2.82434000	0.90544200	2.12217500
C	-2.16794900	-0.08738300	1.44490300
C	-3.17440400	-1.20998200	1.15878000
O	-0.97263600	-0.04569300	1.13895100
C	-2.69088200	-2.55553900	1.47589800
C	-1.36519600	-2.96440300	1.25747700
N	-0.27710900	-3.37169400	1.08623800
C	-3.55440800	-3.55384100	1.98938200
N	-4.25366700	-4.38439600	2.42473500
H	-7.62995600	-1.02561500	2.88359900
H	-7.15095500	1.23395000	3.77542400
H	-4.90109000	2.25980700	3.47621900
H	-5.88801900	-2.29657500	1.66375300
H	0.77023900	-2.03383200	-1.67146700
C	-5.86732900	-1.90013000	-1.19373500
C	-4.47680800	-2.10002200	-1.11824800
C	-3.98352000	-3.39448800	-1.36714200
C	-4.84308500	-4.44666500	-1.67680400
C	-6.21789000	-4.23362000	-1.75410700
C	-6.72082500	-2.95492900	-1.51449100
H	-6.28559400	-0.92348100	-1.00204200
H	-2.91863200	-3.58482200	-1.31950600
H	-4.43120300	-5.43638400	-1.85293400
H	-6.88915800	-5.05278200	-1.99651500
H	-7.79018000	-2.76964200	-1.57283700
C	-3.49601000	-1.02025100	-0.72224100

C	-3.78853200	0.44553100	-0.99008700
N	-2.22207800	-1.27550300	-1.27796600
C	-1.14126900	-1.46707000	-1.68204600
O	-2.92281700	1.23950800	-1.31116400
O	-5.05739900	0.80874800	-0.75759800
C	-5.34303100	2.21288200	-0.93017100
H	-6.41406400	2.30638000	-0.75340100
H	-4.77827400	2.80876300	-0.21164000
H	-5.08071600	2.53415800	-1.94012600
C	-2.18905800	2.12469900	2.58827300
H	-2.54231700	2.99484200	2.02469300
H	-2.40026600	2.27102600	3.65238500
H	-1.11283900	2.01802700	2.44897700

TSb

E[6-31G(d); Hartrees] = -3705.097819; G[6-31G(d); Hartrees] = -3705.205044

E[6-311++G(d,p), CPCM, solvent = CH_2Cl_2; Hartrees] = -3706.9460178

C	7.29925300	-2.08098400	2.40713900
C	5.88334900	-2.03945400	2.44336600
C	5.16443100	-1.73057700	1.23599400
C	5.90745800	-1.46256700	0.06050000
C	7.29172200	-1.51185900	0.06097100
C	7.99830900	-1.83041900	1.24887700
C	3.73099600	-1.72614600	1.31815700
C	3.14980300	-1.98415600	2.54285300
C	3.96302800	-2.25467300	3.67012900
N	5.27757100	-2.29665100	3.63793100
C	2.84991600	-1.48115100	0.08664000
C	2.07579100	-2.77352900	-0.26083900
N	1.12789300	-2.55059600	-1.43334600
C	1.84744000	-2.21127800	-2.71442600
C	2.84841400	-3.34500900	-3.03640200
C	2.64852700	-4.49661300	-2.03039700
C	2.98999900	-3.97634600	-0.62097800
C	1.16711600	-4.96376900	-2.10682800
C	0.27861500	-3.78434300	-1.62355500
C	0.88435800	-6.22383900	-1.32954000
C	0.53862500	-7.38714100	-1.88125500
O	7.89843000	-1.23886200	-1.13034600
C	9.31633300	-1.18521300	-1.17956100
N	1.91400700	-0.37412200	0.25797000
C	2.08760300	0.86336400	-0.28980900
S	3.33343100	1.23165900	-1.37407700
N	1.11949400	1.75974400	0.08856600

C	1.10069100	3.15207100	-0.16294200
C	-0.11020700	3.74573500	-0.52366800
C	-0.19500900	5.13093100	-0.67602800
C	0.92639000	5.93640000	-0.50405200
C	2.13932000	5.33372800	-0.15882400
C	2.23282400	3.95679300	0.02665100
C	-1.53892600	5.73602200	-0.97387900
F	-2.22129600	5.01644800	-1.89223700
C	3.36921400	6.19213100	-0.01584600
F	4.29930300	5.61899900	0.77644300
F	-2.32173600	5.77732900	0.13829900
F	-1.44455100	7.00042200	-1.43204300
F	3.95505100	6.42567700	-1.21240500
F	3.07167100	7.40090500	0.51437800
H	3.49161900	-2.45373800	4.63172400
H	2.06967400	-1.98581300	2.65787800
H	0.24588600	1.38900600	0.46182300
H	7.81267400	-2.31742400	3.33367600
H	1.18322300	-0.52649500	0.96172000
H	3.48462300	-1.19723400	-0.75056600
H	-0.98620700	3.12661300	-0.66590100
H	2.32078300	-1.23557100	-2.58365600
H	3.17224400	3.51189600	0.32433100
H	4.04064700	-3.67079000	-0.59537000
H	0.85998900	7.01053600	-0.62728600
H	1.06865200	-2.10341300	-3.47312800
H	9.08149100	-1.86922500	1.25501100
H	5.42514200	-1.15770300	-0.86087000
H	1.40988000	-3.00747500	0.57178800
H	2.87781700	-4.76628400	0.12685900
H	2.69662800	-3.69962000	-4.06132500
H	3.30480000	-5.33432300	-2.28485200
H	-0.50404200	-3.52156800	-2.33754500
H	-0.21489200	-3.97311700	-0.66885200
H	0.94531100	-5.16608300	-3.16219900
H	3.87585300	-2.97113900	-2.97378200
H	9.56686600	-0.91573700	-2.20709400
H	9.71633800	-0.42284300	-0.49882400
H	9.76877400	-2.15704700	-0.94164900
H	0.97109700	-6.15522000	-0.24447900
H	0.35368300	-8.27158900	-1.27843500
H	0.42616800	-7.50080300	-2.95783200
C	-7.21082500	-0.74781000	2.50415000
C	-7.81166200	-1.82261200	1.84854900

C	-7.06161800	-2.67190300	1.02698100
C	-5.70744600	-2.39745100	0.88419400
C	-5.08380700	-1.30700400	1.51833200
C	-5.84407500	-0.48281800	2.34327700
N	-4.76002700	-3.13530700	0.16227000
C	-3.49406300	-2.61529300	0.32166100
C	-3.63075600	-1.31429300	1.13596700
O	-2.47323100	-3.12565400	-0.11999300
C	-2.62242200	-1.13324600	2.18393500
C	-1.27900300	-1.48447000	2.00771600
N	-0.13462900	-1.73158400	1.90964400
C	-2.89715200	-0.34874200	3.32761500
N	-3.13476300	0.31841800	4.26040000
H	-7.80380700	-0.10915200	3.15203900
H	-8.87310400	-2.01328400	1.98162900
H	-7.52316100	-3.51753200	0.52707000
H	-5.38933700	0.34615800	2.86841200
H	0.46730100	-1.76709600	-1.23006100
C	-5.80573800	0.63990400	-0.97196000
C	-4.58256300	-0.00267400	-1.23441500
C	-4.46620900	-0.72697200	-2.43567100
C	-5.52278200	-0.79784200	-3.34165000
C	-6.72711100	-0.14767100	-3.07313800
C	-6.85834300	0.56773500	-1.88344000
H	-5.93859200	1.19813400	-0.05743500
H	-3.53886200	-1.23681700	-2.67029900
H	-5.39630400	-1.35842900	-4.26429800
H	-7.55001400	-0.19665900	-3.78097300
H	-7.78920300	1.07956800	-1.65460700
C	-3.42529500	0.00970000	-0.25795700
C	-3.10094600	1.25496000	0.55143800
N	-2.22001200	-0.35380800	-0.89258400
C	-1.19617900	-0.70165500	-1.33956500
O	-1.95565500	1.60208900	0.78493900
O	-4.16745600	1.87028900	1.06041600
C	-3.89000200	2.98163900	1.95096000
H	-4.87105300	3.37143600	2.22127500
H	-3.36089400	2.61510700	2.83333200
H	-3.30230300	3.74106500	1.43246400
C	-5.03401300	-4.35103500	-0.57371300
H	-5.48217000	-5.10837300	0.07991200
H	-5.71492100	-4.15114200	-1.40899900
H	-4.08286700	-4.72224800	-0.95768000

Nu'

B3LYP/6-31+G(d,p)–CPCM(mesitylene): E = -647.410886 Hartrees; G = -647.444401 Hartrees

M06-2X/6-311++G(d,p)–CPCM(mesitylene): single-point energy = -647.4467159 Hartrees

P	-0.03993200	-0.84459300	-0.52984100
O	1.18418000	0.23951600	-0.71311900
O	0.18562000	-1.14854000	1.11032300
O	-1.42208100	0.05890300	-0.50859600
H	-0.16877400	-2.01493700	1.35550400
C	1.79398000	1.06026400	0.30343500
H	2.72301600	1.43774000	-0.12716400
H	1.14656600	1.90283800	0.56294500
H	2.01009000	0.47196400	1.19764100
C	-1.68937500	1.16394000	0.37606600
H	-2.77030300	1.31644300	0.37430400
H	-1.35327200	0.94196500	1.39274800
H	-1.19772300	2.06863900	0.00576400

M1-O'

B3LYP/6-31+G(d,p)–CPCM(mesitylene): E = -3436.665663 Hartrees; G = -3436.769538 Hartrees

M06-2X/6-311++G(d,p)–CPCM(mesitylene): single-point energy = -3436.9229871 Hartrees

N	1.32126100	-1.27708200	0.11334400
C	0.29940400	-2.15892900	0.24339300
N	-0.92719900	-1.53247100	0.25507800
S	0.51487300	-3.83140600	0.39652900
C	-2.20830700	-2.10636700	0.18959000
C	-3.23405000	-1.50151300	0.92778100
C	-4.54255700	-1.98518600	0.84033400
C	-4.85111100	-3.08008700	0.03604300
C	-3.81997600	-3.67703100	-0.69762800
C	-2.51169500	-3.20117500	-0.63647300
C	-4.13333400	-4.88121200	-1.54773200
F	-3.23837900	-5.05890800	-2.54936500
F	-5.36060400	-4.79423800	-2.12381100
F	-4.13447100	-6.03103400	-0.81904200
C	-5.62389000	-1.27388700	1.60990800
F	-5.26195600	-1.02580100	2.89429300
F	-5.91712800	-0.05984100	1.05848400
F	-6.78344200	-1.96998500	1.64956300
C	-3.30326500	6.30038600	-1.37182400
C	-3.87245500	5.35220200	-2.23284200
C	-3.66034000	3.97730000	-2.05357700
C	-2.86164100	3.58910400	-0.98951600
C	-2.27426600	4.52826800	-0.10538100

C	-2.50115100	5.89785900	-0.30189900
N	-2.50778000	2.29316700	-0.59552500
C	-1.69430300	2.30475400	0.50499300
C	-1.51890000	3.77189300	0.87315100
O	-1.23124800	1.33311900	1.08946100
C	-0.78707900	4.17314200	1.95599600
C	-0.09042500	3.27510500	2.82900000
N	0.51718800	2.64233200	3.59362600
C	-0.64622600	5.55666700	2.29451600
N	-0.52731700	6.68063700	2.57302600
H	-3.00239800	-0.65838800	1.56999900
H	-5.86472500	-3.45574200	-0.02443600
H	-1.73259700	-3.66574600	-1.22339000
H	-3.48695300	7.35662600	-1.53635400
H	-4.49422800	5.68511000	-3.05818500
H	-4.10660000	3.24863100	-2.72191900
H	-2.06416300	6.63692800	0.35854700
H	-2.76125500	1.44422700	-1.08183500
P	1.26444300	2.48326200	-1.47862700
O	1.09409600	0.92416200	-1.58857300
O	2.80583200	2.55693800	-0.77054900
O	1.80751000	2.97726500	-3.01861200
C	2.72566500	-1.62462500	0.32458900
H	2.82371500	-2.68400300	0.07769600
C	3.65913200	-0.78318300	-0.59227200
H	3.63617100	0.25497800	-0.24895800
C	3.13894900	-1.44782600	1.78714200
C	3.75303000	-2.49832700	2.47946200
C	2.89447400	-0.24173500	2.45964300
C	4.12901100	-2.34478600	3.81726300
H	3.93077500	-3.44386100	1.97539300
C	3.26401700	-0.08736100	3.79733300
H	2.39811400	0.57925400	1.94959800
C	3.88664500	-1.13825500	4.47888500
H	4.60100700	-3.17043900	4.34196100
H	3.05340400	0.84893000	4.30494100
H	4.17144100	-1.01979300	5.52031500
C	5.09847400	-1.27094900	-0.54809500
C	6.11443700	-0.35800300	-0.22878800
C	5.45304400	-2.60537500	-0.80474100
C	7.45088000	-0.76039200	-0.17349500
H	5.85590500	0.67486400	-0.01249100
C	6.78974100	-3.00879000	-0.75832400
H	4.69253400	-3.34694200	-1.02760100

C	7.79288300	-2.08788300	-0.44316900
H	8.22066500	-0.03861000	0.08254700
H	7.04405000	-4.04522500	-0.95918700
H	8.83066700	-2.40471300	-0.40090300
N	3.11515000	-0.65926000	-2.02203800
C	4.02690200	0.14576000	-2.89179100
H	3.50215100	0.35205400	-3.82529100
H	4.24104300	1.08849700	-2.38969900
H	4.94487000	-0.40869900	-3.08649200
H	1.09686900	-0.32488800	-0.20521400
H	-0.92392800	-0.53947300	0.49568200
C	0.81453700	3.33366000	-3.98117400
H	1.31409200	3.88726600	-4.78063700
H	0.33828900	2.44329200	-4.41197500
H	0.03602600	3.97332100	-3.54349300
C	3.34911100	3.85312200	-0.49444400
H	2.61304800	4.50017600	0.00006200
H	4.20092400	3.71390600	0.17580600
H	3.68688100	4.33994400	-1.41618700
C	2.72824200	-1.92963200	-2.70052900
H	2.20827900	-1.66732100	-3.62339300
H	3.61928000	-2.51070100	-2.94126800
H	2.05885800	-2.50819700	-2.06564900
H	2.22671800	-0.02683600	-1.91252000

M1-N'

B3LYP/6-31+G(d,p)–CPCM(mesitylene): E = -3436.658416 Hartrees; G = -3436.762030 Hartrees

M06-2X/6-311++G(d,p)–CPCM(mesitylene): single-point energy = -3436.9166489 Hartrees

C	-1.67286800	7.88579700	-0.15777200
C	-2.71102700	6.95148700	-0.12307100
C	-2.42794900	5.58808500	-0.23257700
C	-1.10801000	5.13471900	-0.37528600
C	-0.07149800	6.08218100	-0.39494800
C	-0.35282500	7.44667200	-0.29255700
C	-0.84767500	3.64120200	-0.49296700
C	0.19281700	3.14516800	0.55405100
N	-0.50023100	3.20348800	-1.92058300
N	0.65407000	1.78681300	0.27229900
C	-0.40154600	3.26147500	1.95890500
C	-1.48981000	2.46613700	2.34792100
C	-2.02318400	2.57119700	3.63386100
C	-1.47191000	3.47381800	4.54972500
C	-0.38409600	4.26478100	4.17242500

C	0.14806300	4.15735700	2.88353100
C	0.87568200	3.53127400	-2.39601100
C	1.93465200	1.37364300	0.45489700
N	2.04897600	0.00332300	0.38884800
S	3.23221100	2.42296700	0.74824700
C	3.21275900	-0.78094300	0.29888500
C	3.21806200	-2.02042200	0.95820200
C	4.32514300	-2.86124900	0.85477600
C	5.44423800	-2.49114500	0.10444700
C	5.42501500	-1.26043600	-0.55208100
C	4.32182700	-0.40780300	-0.47041400
C	6.58568900	-0.84897500	-1.42020700
F	6.30624200	-1.00913000	-2.74581900
F	7.70500000	-1.57077800	-1.17273500
F	6.91080700	0.45826300	-1.25834000
C	4.30994900	-4.20803600	1.52926600
F	3.42059600	-4.27181600	2.54820600
F	3.97777500	-5.20538000	0.66142200
F	5.52455500	-4.53820300	2.03900600
C	-7.16807400	-3.83393700	0.39835900
C	-7.10133400	-4.95024000	-0.44788500
C	-5.87473200	-5.47179500	-0.88249300
C	-4.71991300	-4.84201000	-0.44221600
C	-4.76201300	-3.71170600	0.41522000
C	-6.00123600	-3.20532400	0.83507400
N	-3.39060500	-5.16321000	-0.72778800
C	-2.51511700	-4.30716500	-0.09959500
C	-3.39357700	-3.31123200	0.65282500
O	-1.29874300	-4.36042200	-0.12053300
C	-2.86554200	-2.27242500	1.36684800
C	-1.46419100	-1.98187100	1.40834600
N	-0.35529100	-1.64015100	1.48209300
C	-3.68579000	-1.35906300	2.10127900
N	-4.34429800	-0.62052000	2.71457500
H	-1.88887700	8.94650300	-0.07217800
H	-3.73933700	7.28028500	-0.00710700
H	-3.24130800	4.86825600	-0.19683200
H	0.96422100	5.76804600	-0.47535100
H	0.46199800	8.16422600	-0.30919400
H	-1.92335300	1.75098800	1.65343900
H	-2.86493700	1.94646400	3.91756900
H	-1.88506900	3.55495100	5.55087000
H	0.05539400	4.96225400	4.87957200
H	1.00007800	4.76795800	2.59887600

H	2.35949800	-2.31425200	1.55115400
H	6.30740000	-3.14140800	0.03714700
H	4.32305800	0.53852400	-0.99345400
H	-8.13352400	-3.45459500	0.71518100
H	-8.02033800	-5.42496900	-0.77788800
H	-5.83354900	-6.33415700	-1.53928900
H	-6.05807900	-2.34180500	1.48685100
H	-3.08020000	-5.93839500	-1.29664400
H	1.20435600	-0.51952000	0.62026500
C	-1.51947300	3.67393100	-2.90751300
H	-1.49501700	4.76074100	-2.98492000
H	-1.28348200	3.22331600	-3.87191400
H	-2.50562700	3.33585700	-2.58967200
H	1.61651400	3.20673900	-1.66694600
H	1.03863500	2.99869900	-3.33441000
H	0.96241800	4.60481100	-2.56953000
H	-1.79097300	3.11835100	-0.31303500
H	-0.00647000	1.13277500	-0.17224600
H	1.08123300	3.77822700	0.51303200
P	-2.40460200	-0.03512600	-1.64930600
O	-2.05221000	-1.63904500	-2.05820000
O	-0.98500400	0.67304100	-1.67870800
O	-3.17259600	0.51268000	-3.05912400
C	-0.84732500	-2.05965700	-2.71653200
H	-0.52924400	-2.99876400	-2.25605500
H	-1.03954900	-2.22556300	-3.78323700
H	-0.05823700	-1.31104400	-2.60309800
C	-2.60197000	0.33689800	-4.35992300
H	-3.13285400	1.00216700	-5.04698500
H	-1.53436000	0.58679400	-4.37057500
H	-2.72937300	-0.69706300	-4.70027400
H	-0.63936900	2.11685700	-1.89348000

M1-O''

B3LYP/6-311+G(d,p)–CPCM(mesitylene): E = -3437.317891 Hartrees; G = -3437.422436 Hartrees

M06-2X/6-311++G(d,p)–CPCM(mesitylene): single-point energy = -3436.9253898 Hartrees

N	1.35066600	-1.24420300	0.13644400
C	0.34658100	-2.14288100	0.26672500
N	-0.89133900	-1.54010100	0.26088300
S	0.59004200	-3.80678800	0.43860100
C	-2.15848000	-2.14075200	0.19550200
C	-3.19808800	-1.55541000	0.92401400
C	-4.49238600	-2.06620300	0.83456700

C	-4.77329300	-3.17057000	0.03904000
C	-3.72893800	-3.74894300	-0.68419000
C	-2.43484700	-3.24513900	-0.62163300
C	-4.00779600	-4.96698300	-1.52432000
F	-3.13538400	-5.10036800	-2.54758900
F	-5.24934800	-4.94040100	-2.06421500
F	-3.93058900	-6.11104300	-0.79792600
C	-5.59118200	-1.37215200	1.59248600
F	-5.23866300	-1.10147500	2.87064300
F	-5.91028200	-0.17514200	1.02648000
F	-6.73035800	-2.09273000	1.63761800
C	-3.45220600	6.25151100	-1.34682000
C	-4.00431000	5.29946100	-2.20882500
C	-3.76563700	3.93135600	-2.03811600
C	-2.95835900	3.55290600	-0.98095400
C	-2.38807100	4.49688300	-0.09504600
C	-2.64076100	5.85978400	-0.28448700
N	-2.57762600	2.26358800	-0.59590200
C	-1.76083600	2.28303600	0.50124200
C	-1.61356000	3.75258400	0.87513800
O	-1.27911300	1.32348800	1.07436900
C	-0.88755500	4.16269800	1.95321800
C	-0.17059500	3.27719000	2.81601100
N	0.44814500	2.65516000	3.56765900
C	-0.77328100	5.54307100	2.29814000
N	-0.67484300	6.65879800	2.58269900
H	-2.98698500	-0.70579900	1.56164300
H	-5.77664300	-3.56750500	-0.02302800
H	-1.64527900	-3.69483200	-1.20291800
H	-3.65666000	7.30288000	-1.50526800
H	-4.63403400	5.62441400	-3.02886000
H	-4.19921400	3.19947300	-2.70826300
H	-2.21698000	6.60290500	0.37699200
H	-2.81760800	1.41351000	-1.08467200
P	1.22310700	2.49522700	-1.49288100
O	1.08566300	0.93685500	-1.55849000
O	2.78816400	2.61647400	-0.85174400
O	1.69539100	2.95955500	-3.06336500
C	2.76018200	-1.56759600	0.34459400
H	2.87130600	-2.62747700	0.11448200
C	3.67552900	-0.72797400	-0.59019900
H	3.63657800	0.31380000	-0.26532000
C	3.18043700	-1.36284300	1.80037400
C	3.82947900	-2.38491800	2.49661400

C	2.90758300	-0.15990400	2.46036800
C	4.21170300	-2.20596700	3.82578300
H	4.03009100	-3.32908200	2.00294000
C	3.28381500	0.01942600	3.78947600
H	2.38251700	0.63892900	1.94802600
C	3.94107300	-1.00274500	4.47467200
H	4.71082400	-3.01015300	4.35475200
H	3.05061500	0.95259900	4.28877400
H	4.23074600	-0.86497900	5.51035300
C	5.12130500	-1.19112200	-0.54544800
C	6.12165800	-0.25899300	-0.24791900
C	5.49415300	-2.52130600	-0.77902700
C	7.46096100	-0.63901400	-0.19133900
H	5.84888000	0.77173300	-0.04979200
C	6.83388000	-2.90194600	-0.73137800
H	4.74596700	-3.27708400	-0.98577300
C	7.82109400	-1.96238300	-0.43778900
H	8.21968700	0.09723400	0.04777200
H	7.10393800	-3.93568600	-0.91432500
H	8.86200100	-2.26177600	-0.39441300
N	3.12200400	-0.63703500	-2.01867100
C	4.00961100	0.17891900	-2.90171300
H	3.48472900	0.34508500	-3.84121700
H	4.18721800	1.13791800	-2.42000900
H	4.94507100	-0.34796700	-3.07901600
H	1.11101700	-0.30279400	-0.20147700
H	-0.90850900	-0.54763000	0.49558900
C	0.66968100	3.25355000	-4.00998000
H	1.12836800	3.79969900	-4.83585500
H	0.21526500	2.33674800	-4.40283600
H	-0.11929400	3.87755700	-3.57231900
C	3.32458800	3.92227900	-0.61910000
H	2.60329100	4.56592600	-0.10251600
H	4.20590300	3.80638700	0.01323700
H	3.61387900	4.39950500	-1.56013100
C	2.76330700	-1.92451000	-2.67754600
H	2.23396500	-1.68851000	-3.60020900
H	3.66611200	-2.48524300	-2.91427200
H	2.11263600	-2.51037600	-2.03281200
H	2.22643300	-0.02961500	-1.90950600

M1-N’’

B3LYP/6-311+G(d,p)–CPCM(mesitylene): E = -3437.311008 Hartrees; G = -3437.413843 Hartrees

M06-2X/6-311++G(d,p)–CPCM(mesitylene): single-point energy = -3436.9197406 Hartrees

C	-1.66961600	7.89276500	-0.24229100
C	-2.71075500	6.96762600	-0.19934800
C	-2.43581900	5.60447700	-0.28615000
C	-1.12073600	5.14292600	-0.41360500
C	-0.08096000	6.08160400	-0.44166400
C	-0.35464400	7.44570000	-0.36248400
C	-0.86819700	3.64785300	-0.50476000
C	0.16390200	3.16362400	0.55398300
N	-0.51748700	3.18308700	-1.92287800
N	0.61896000	1.79925100	0.29715300
C	-0.43569700	3.30680600	1.95270900
C	-1.52210200	2.51977100	2.35166500
C	-2.05908800	2.64894000	3.63010300
C	-1.51380000	3.56743100	4.52809200
C	-0.42788500	4.34982300	4.14118000
C	0.10845900	4.21834900	2.86000400
C	0.85715200	3.50550400	-2.40162200
C	1.89909200	1.38946800	0.47483900
N	2.01495300	0.01943200	0.41903200
S	3.19600700	2.43939300	0.75216300
C	3.17866300	-0.76162400	0.32351800
C	3.19664200	-1.99413400	0.98640600
C	4.30367300	-2.83084200	0.87506700
C	5.40917500	-2.46250200	0.11293200
C	5.37871300	-1.23604100	-0.54700100
C	4.27739300	-0.38968600	-0.45764000
C	6.52674100	-0.83433500	-1.43400600
F	6.27703100	-1.12055400	-2.74086300
F	7.67527500	-1.47063000	-1.11593300
F	6.77840200	0.49287900	-1.37885900
C	4.28112000	-4.17236000	1.55710300
F	3.60262800	-4.14406600	2.72617400
F	3.68139700	-5.11935300	0.78830600
F	5.52313800	-4.63138700	1.82977300
C	-7.10983700	-3.85833900	0.30606100
C	-7.01339100	-4.96687900	-0.54157300
C	-5.77525700	-5.48123400	-0.93916000
C	-4.63850100	-4.85331800	-0.46022500
C	-4.71099000	-3.72959000	0.39942500
C	-5.96192900	-3.23055100	0.78132500
N	-3.30180600	-5.16836700	-0.70628800
C	-2.44765500	-4.31569900	-0.04583200
C	-3.35434100	-3.32215400	0.67747800

O	-1.23948100	-4.37008200	-0.02120100
C	-2.85538100	-2.28011800	1.39963400
C	-1.46234400	-1.97543700	1.47056600
N	-0.36663200	-1.62260200	1.55918500
C	-3.69801500	-1.37388500	2.10931700
N	-4.37023400	-0.64214700	2.69957100
H	-1.87974100	8.95396300	-0.17432300
H	-3.73576600	7.30401500	-0.09455000
H	-3.25219500	4.89138000	-0.24431100
H	0.95151300	5.76106300	-0.51076200
H	0.46220600	8.15782500	-0.38537900
H	-1.95115000	1.79152300	1.67113700
H	-2.89932500	2.02995100	3.92350200
H	-1.93013000	3.66713200	5.52414000
H	0.00744500	5.05929700	4.83590200
H	0.96005300	4.82279400	2.56841400
H	2.34746800	-2.28668200	1.59103600
H	6.27267000	-3.10831500	0.04055100
H	4.27083900	0.55309300	-0.98292200
H	-8.08440100	-3.48453400	0.59360300
H	-7.91871600	-5.44107200	-0.90258200
H	-5.71138800	-6.33795400	-1.59844900
H	-6.04226600	-2.37236600	1.43461800
H	-2.97299600	-5.94420700	-1.26157100
H	1.17564700	-0.50171500	0.66712700
C	-1.53752000	3.62941700	-2.91817400
H	-1.52446000	4.71365900	-3.00892000
H	-1.29507000	3.17034500	-3.87507000
H	-2.51954300	3.28592100	-2.59884900
H	1.59645400	3.19935500	-1.66539600
H	1.02439000	2.95616000	-3.32759900
H	0.94012700	4.57389700	-2.59605200
H	-1.81282300	3.13406000	-0.31933300
H	-0.04190800	1.14280700	-0.14182700
H	1.05417300	3.79017500	0.50704500
P	-2.40929700	-0.10581600	-1.66085100
O	-1.95907900	-1.70642800	-1.96377600
O	-1.02556500	0.65802500	-1.61450400
O	-3.07961700	0.35305300	-3.14636800
C	-0.71859800	-2.10568500	-2.56548100
H	-0.38756400	-3.01789800	-2.06704200
H	-0.86313500	-2.30849000	-3.63126800
H	0.04029700	-1.32985000	-2.44493900
C	-2.40644300	0.19638600	-4.39810400

H	-2.89112500	0.85573600	-5.12123500
H	-1.34746600	0.46372400	-4.32412400
H	-2.48919200	-0.83528400	-4.75352600
H	-0.65210300	2.10397800	-1.87363300

$TS_{P\text{-}C}$'

B3LYP/6-31+G(d,p)–CPCM(mesitylene): E = -3436.656272 Hartrees; G = -3436.754720 Hartrees

M06-2X/6-311++G(d,p)–CPCM(mesitylene): single-point energy = -3436.9227280 Hartrees

C	7.75591900	-1.69925000	-1.05733400
C	7.41434300	-0.51669700	-0.39642000
C	6.07101000	-0.18939600	-0.19802800
C	5.04872200	-1.03464400	-0.65623500
C	5.40439900	-2.22808500	-1.30561400
C	6.74714600	-2.55493700	-1.50869600
C	3.60307700	-0.63641400	-0.41156700
C	2.74572700	-1.77422500	0.20282600
N	2.93518100	-0.05569200	-1.67050900
N	1.35723400	-1.33235600	0.32946100
C	3.31241400	-2.25028400	1.54049600
C	3.49525900	-1.36839200	2.61665800
C	3.97458900	-1.83963200	3.84120100
C	4.27535900	-3.19520800	4.00772400
C	4.09222300	-4.07907100	2.94146100
C	3.61198400	-3.60791500	1.71609700
C	2.71565500	-1.01379400	-2.79868900
C	0.27186500	-2.09897800	0.03728400
N	-0.89375800	-1.54724200	0.49573200
S	0.36577900	-3.57977000	-0.78143200
C	-2.22165500	-1.95370700	0.25902100
C	-3.13809100	-1.81998200	1.30659700
C	-4.48865900	-2.12623000	1.10462600
C	-4.93796000	-2.59075700	-0.12764900
C	-4.01125300	-2.72647700	-1.16908000
C	-2.66811300	-2.40639300	-0.99379800
C	-4.51135800	-3.20522200	-2.50795400
F	-3.53062800	-3.30223300	-3.43317700
F	-5.45650300	-2.36862400	-3.01987700
F	-5.09845700	-4.42849300	-2.41989400
C	-5.43986100	-1.97207000	2.26196600
F	-5.18271000	-2.86372300	3.25577000
F	-5.34589400	-0.73677600	2.82954800
F	-6.73241300	-2.14371600	1.90386400
C	-2.64768500	6.28262500	0.60608600

C	-3.78736700	5.52817800	0.91041300
C	-3.69132300	4.16440800	1.21537200
C	-2.42531700	3.59455600	1.20036400
C	-1.26400600	4.32993800	0.88165000
C	-1.37944100	5.69091800	0.58820300
N	-2.06453100	2.27317000	1.48686800
C	-0.71183400	2.07607700	1.40179400
C	-0.11865900	3.40057600	0.96176700
O	-0.12551800	1.02375300	1.67491900
C	1.21852000	3.74483900	1.24190100
C	2.22172900	2.77956600	1.51150400
N	3.10226300	2.03513400	1.70357200
C	1.69132500	5.07585300	1.10400500
N	2.09105100	6.16765400	0.98536600
H	8.79934800	-1.95765900	-1.21104000
H	8.19000700	0.14873500	-0.02970700
H	5.81373900	0.72536100	0.32855100
H	4.64208800	-2.92151100	-1.64616900
H	7.00286900	-3.48282800	-2.01138000
H	3.27029200	-0.31089800	2.51027200
H	4.11321000	-1.14500400	4.66458900
H	4.64735700	-3.55865300	4.96123200
H	4.31866200	-5.13456000	3.06107300
H	3.46145600	-4.30219700	0.89446700
H	-2.79274400	-1.48512500	2.27979700
H	-5.98196700	-2.83661900	-0.27905400
H	-1.97059800	-2.49758400	-1.81346300
H	-2.74560700	7.33946400	0.38021800
H	-4.76260200	6.00516100	0.91634500
H	-4.57131300	3.57872300	1.46078400
H	-0.50820300	6.28865400	0.35048300
H	-2.70884100	1.53960000	1.74781700
H	-0.79200900	-0.70568000	1.06820500
C	3.64974700	1.17030500	-2.15383800
H	4.61079000	0.88942200	-2.58359100
H	3.01586200	1.65417300	-2.89634900
H	3.79544100	1.84705700	-1.31199600
H	2.13537000	-1.86763400	-2.44895700
H	2.14710700	-0.48745400	-3.56562400
H	3.67606200	-1.33427900	-3.20084000
H	3.59439000	0.21163100	0.27846900
H	1.18706500	-0.46525800	0.83700900
H	2.71973300	-2.63191300	-0.47049000
P	-0.14288200	2.40857400	-1.42385200

O	-1.59674600	2.49816100	-2.20060800
O	0.47750100	1.01984700	-1.58547700
O	0.85017400	3.38897500	-2.33624900
H	1.96913500	0.29214800	-1.41687500
C	-1.78649400	1.87290800	-3.49153200
H	-1.56096600	0.80501700	-3.43523400
H	-2.83576100	2.01947000	-3.75207600
H	-1.14982800	2.34564800	-4.24593500
C	0.53194200	4.77244800	-2.57846000
H	-0.53389600	4.90437700	-2.78752600
H	0.82334800	5.39115600	-1.72516800
H	1.11257500	5.07566100	-3.45208000

$TS_{Enantio}$'

B3LYP/6-31+G(d,p)–CPCM(mesitylene): E = -3436.655206 Hartrees; G = -3436.756075 Hartrees

M06-2X/6-311++G(d,p)–CPCM(mesitylene): single-point energy = -3436.9189517 Hartrees

C	-4.76522900	5.89544400	-0.85323500
C	-5.19461500	4.73185000	-0.21008700
C	-4.33200500	3.63959900	-0.09333700
C	-3.03018500	3.68855700	-0.61399300
C	-2.60500100	4.86905800	-1.24496300
C	-3.46760600	5.96094900	-1.36820600
C	-2.12830000	2.47420600	-0.45855400
C	-0.75544600	2.83153800	0.17026700
N	-1.97131400	1.68802300	-1.77105400
N	0.13492700	1.66957700	0.17656600
C	-0.93008200	3.41428100	1.57269600
C	-1.53870700	2.67717100	2.60049600
C	-1.65362300	3.21798600	3.88321500
C	-1.16384500	4.49923500	4.15582100
C	-0.55335500	5.23638200	3.13826100
C	-0.43659300	4.69474600	1.85481800
C	-1.11006000	2.31172900	-2.82335900
C	1.47325500	1.73478100	-0.09159000
N	2.15502300	0.64687600	0.37991000
S	2.18927200	3.03215900	-0.91281100
C	3.49692600	0.27436100	0.17038700
C	4.16175800	-0.36149900	1.22778600
C	5.47324000	-0.80912300	1.06219000
C	6.14731700	-0.62279400	-0.14501500
C	5.47286600	0.00623000	-1.19433200
C	4.15648500	0.44625000	-1.05449500
C	6.15790900	0.14537200	-2.52955500

F	5.98461000	-0.96354900	-3.30470900
F	7.49768200	0.31670300	-2.40431400
F	5.68739600	1.19240100	-3.24817900
C	6.19133600	-1.43841400	2.22776200
F	6.82254300	-0.50637700	2.99616800
F	5.34876200	-2.10765400	3.05144700
F	7.14487800	-2.31675900	1.83096700
C	-4.57196000	-5.91439200	0.46846400
C	-5.81260900	-5.26755500	0.41463300
C	-5.91218500	-3.87617200	0.55606800
C	-4.73469400	-3.16671800	0.75340800
C	-3.47237600	-3.79898200	0.80460500
C	-3.39223600	-5.18560900	0.66165100
N	-4.56380000	-1.78824600	0.91876300
C	-3.24320400	-1.44729200	1.10575600
C	-2.46381600	-2.74676400	1.01672800
O	-2.82356300	-0.31571900	1.33345200
C	-1.21065600	-2.89671900	1.63036500
C	-0.38553200	-1.79053100	1.95202300
N	0.35328300	-0.92160900	2.20626400
C	-0.61275700	-4.17086400	1.82997400
N	-0.11306300	-5.21004500	2.01266600
H	-5.43214100	6.74742800	-0.94479400
H	-6.19643600	4.67445500	0.20483300
H	-4.66937500	2.74225800	0.41815400
H	-1.59543100	4.95653900	-1.63367200
H	-3.12022800	6.86540500	-1.85840000
H	-1.91921400	1.67719600	2.41175300
H	-2.12345600	2.63516600	4.67017500
H	-1.25351800	4.91658300	5.15448000
H	-0.16415800	6.22985300	3.34100200
H	0.04904200	5.26820100	1.07048600
H	3.65222400	-0.50253400	2.17492500
H	7.16876100	-0.96156300	-0.26730100
H	3.64670400	0.91910200	-1.88160400
H	-4.52103500	-6.99263600	0.35793000
H	-6.71643600	-5.85004100	0.26400400
H	-6.87441400	-3.37544800	0.51927100
H	-2.43657400	-5.69463300	0.69088300
H	-5.30687500	-1.10412500	0.94191000
H	1.65403900	0.06912000	1.06028100
C	-3.30289200	1.31704500	-2.34713600
H	-3.79543600	2.20679500	-2.73794000
H	-3.13491200	0.58498300	-3.13660900

H	-3.91297800	0.86600300	-1.56472600
H	-0.13426300	2.56318400	-2.40865100
H	-0.98360100	1.57617800	-3.61867300
H	-1.59997400	3.20068100	-3.22053900
H	-2.62877200	1.75085100	0.19069700
H	-0.18930000	0.85753600	0.69715800
H	-0.25273100	3.58007200	-0.44284300
P	-1.87800200	-2.12056900	-1.43419800
O	-0.86830500	-3.40810400	-1.63333400
O	-1.08144900	-0.81385300	-1.54646500
O	-2.80911700	-2.14501000	-2.83071900
H	-1.52727100	0.74851400	-1.53721300
C	0.22976000	-3.36045600	-2.57116300
H	0.83149900	-4.25132100	-2.38537200
H	-0.14344800	-3.37521200	-3.60035200
H	0.83131400	-2.46248100	-2.41102300
C	-3.57992700	-3.31574300	-3.15475200
H	-4.09082400	-3.10075700	-4.09535300
H	-2.93150200	-4.18803100	-3.28352600
H	-4.32449000	-3.52960800	-2.38073000

$TS_{P\text{-}C}$''

B3LYP/6-311+G(d,p)–CPCM(mesitylene): E = -3437.308612 Hartrees; G = -3437.407013 Hartrees

M06-2X/6-311++G(d,p)–CPCM(mesitylene): single-point energy = -3436.9258074 Hartrees

C	7.76758800	-1.60543900	-1.05668500
C	7.41415600	-0.42801500	-0.40059700
C	6.07070400	-0.11576500	-0.20298800
C	5.06037100	-0.97202500	-0.65674200
C	5.42812700	-2.16033500	-1.30154700
C	6.77106100	-2.47155300	-1.50411000
C	3.61104100	-0.59201600	-0.41086900
C	2.77174100	-1.74062400	0.20487900
N	2.93429900	-0.02021800	-1.66755400
N	1.37795400	-1.32054700	0.33948200
C	3.35115700	-2.21191100	1.53733700
C	3.53005000	-1.33148500	2.61093800
C	4.02090600	-1.79788300	3.82890200
C	4.33709200	-3.14678100	3.99090700
C	4.15784200	-4.02909600	2.92746700
C	3.66547900	-3.56322000	1.70887500
C	2.73202300	-0.97914200	-2.79607400
C	0.30517700	-2.09994200	0.04245100
N	-0.86740700	-1.56766200	0.50333700

S	0.42080400	-3.57212100	-0.78287800
C	-2.18941900	-1.98689100	0.26657300
C	-3.10918600	-1.84506800	1.30733800
C	-4.45246000	-2.16452400	1.10738200
C	-4.89488700	-2.65022900	-0.11636600
C	-3.96691400	-2.79352100	-1.14979900
C	-2.62931400	-2.46021400	-0.97631100
C	-4.45185100	-3.24833700	-2.50129800
F	-3.45985500	-3.73786500	-3.27235100
F	-5.01873200	-2.22743200	-3.19926800
F	-5.39646400	-4.21202300	-2.40425900
C	-5.40653800	-2.01109000	2.26095000
F	-5.18237500	-2.93075100	3.23204800
F	-5.28324600	-0.79567300	2.85524400
F	-6.69642000	-2.13924000	1.89030200
C	-2.73663000	6.23872300	0.58896900
C	-3.86594600	5.47264000	0.88580600
C	-3.75552500	4.11355300	1.19088400
C	-2.48590200	3.55907900	1.18384300
C	-1.33443600	4.30708800	0.87152400
C	-1.46428600	5.66370200	0.57917700
N	-2.11126800	2.24385800	1.47210400
C	-0.75655700	2.06149700	1.39445900
C	-0.17868100	3.39354300	0.95853500
O	-0.16140700	1.02264400	1.66856300
C	1.14988800	3.75350100	1.24298300
C	2.15896500	2.80239000	1.52086100
N	3.03730500	2.06952100	1.71711500
C	1.60688200	5.08580700	1.10622900
N	1.99374600	6.17355300	0.98939900
H	8.81196600	-1.85203000	-1.20980800
H	8.18157900	0.24552000	-0.03704500
H	5.80429500	0.79598000	0.32018000
H	4.67506400	-2.86203700	-1.63927700
H	7.03744700	-3.39591700	-2.00357600
H	3.29312100	-0.27815200	2.50801400
H	4.15653100	-1.10493800	4.65166300
H	4.71845300	-3.50680500	4.93980800
H	4.39653600	-5.08016900	3.04467900
H	3.51749800	-4.25711400	0.88904000
H	-2.76943800	-1.49455500	2.27493500
H	-5.93382400	-2.90964400	-0.26489100
H	-1.92914100	-2.56168600	-1.79049100
H	-2.84628400	7.29244100	0.36310600

H	-4.84505600	5.93726200	0.88587900
H	-4.62868000	3.51909100	1.43125300
H	-0.60050600	6.27071300	0.34639200
H	-2.74803600	1.50358400	1.72786800
H	-0.77633800	-0.73050000	1.08113100
C	3.62784700	1.21771900	-2.14641700
H	4.59453200	0.95615400	-2.57139000
H	2.98985400	1.68980700	-2.89053700
H	3.75587700	1.89587900	-1.30501600
H	2.16613300	-1.84164400	-2.44897200
H	2.15631700	-0.46231200	-3.56185400
H	3.69598400	-1.28328100	-3.19769200
H	3.59318300	0.25320100	0.27961900
H	1.19576700	-0.45840000	0.84797300
H	2.75450800	-2.59555800	-0.46907900
P	-0.18103800	2.39953800	-1.41357600
O	-1.62540900	2.44127000	-2.20166200
O	0.47934400	1.03364000	-1.56327200
O	0.78988200	3.40230900	-2.31763900
H	1.96427300	0.31140100	-1.41241100
C	-1.81091800	1.79387000	-3.48155100
H	-1.57751000	0.73059000	-3.40747000
H	-2.85936600	1.92686600	-3.74390900
H	-1.17911300	2.25838800	-4.24255800
C	0.45105400	4.77707700	-2.57754200
H	-0.62261600	4.89759400	-2.73844400
H	0.77851900	5.41536900	-1.75462700
H	0.98510700	5.06369100	-3.48356200

$TS_{Enantio}$''

B3LYP/6-311+G(d,p)–CPCM(mesitylene): E = -3437.307550 Hartrees; G = -3437.408685 Hartrees

M06-2X/6-311++G(d,p)–CPCM(mesitylene): single-point energy = -3436.9218161 Hartrees

C	-4.77169600	5.89237600	-0.83269500
C	-5.20128900	4.72612100	-0.20260500
C	-4.34156400	3.63503900	-0.09528100
C	-3.04201000	3.68888000	-0.61177800
C	-2.61644100	4.87215300	-1.22984300
C	-3.47676900	5.96241700	-1.34402600
C	-2.13953200	2.47555000	-0.46418600
C	-0.77301600	2.83053700	0.17647700
N	-1.97326600	1.70232100	-1.78187200
N	0.12048600	1.67207100	0.18194800
C	-0.95966700	3.40258000	1.58044500

C	-1.56115600	2.65254600	2.59840600
C	-1.68775100	3.18196100	3.88115000
C	-1.21704400	4.46447400	4.16300400
C	-0.61363200	5.21429800	3.15553800
C	-0.48465100	4.68412100	1.87223300
C	-1.10931400	2.33796300	-2.82265000
C	1.45731900	1.74234100	-0.08332500
N	2.14051700	0.65402700	0.38278800
S	2.17023700	3.04446700	-0.89353600
C	3.48244500	0.28712500	0.17356600
C	4.14583400	-0.35590000	1.22359600
C	5.45572500	-0.79692700	1.05743900
C	6.13059300	-0.59800900	-0.14338000
C	5.45808700	0.03696600	-1.18574600
C	4.14387400	0.47194900	-1.04477300
C	6.14391500	0.18990200	-2.51761500
F	5.96642700	-0.90563600	-3.30429500
F	7.48012100	0.35394900	-2.38959600
F	5.67849800	1.24462900	-3.22049200
C	6.17274500	-1.43284600	2.21843200
F	6.80062100	-0.50718700	2.99060200
F	5.33211000	-2.10586900	3.03416000
F	7.12421200	-2.30503300	1.81720600
C	-4.52746900	-5.93623800	0.44510900
C	-5.76680000	-5.29660800	0.37288300
C	-5.87393100	-3.90875600	0.50904300
C	-4.70539000	-3.19412800	0.71978300
C	-3.44381800	-3.81991300	0.78853200
C	-3.35647200	-5.20351700	0.65136900
N	-4.54265800	-1.81648600	0.88339200
C	-3.22658200	-1.46799300	1.08695200
C	-2.44272700	-2.76504800	1.01075200
O	-2.81714300	-0.34103900	1.31825400
C	-1.19635100	-2.90944200	1.63070700
C	-0.37884900	-1.80224800	1.95086600
N	0.34981600	-0.93331600	2.19618900
C	-0.59910400	-4.17737400	1.84268700
N	-0.10190600	-5.20664200	2.03489700
H	-5.43714400	6.74381400	-0.91693000
H	-6.20207100	4.66587500	0.20937000
H	-4.67967700	2.73486700	0.40640000
H	-1.60817500	4.96310200	-1.61557000
H	-3.13009500	6.87003200	-1.82452000
H	-1.92662800	1.65030300	2.40250100

H	-2.15151300	2.58951600	4.66181600
H	-1.31562300	4.87345100	5.16219600
H	-0.23860500	6.20936300	3.36669700
H	-0.00384300	5.26833700	1.09561200
H	3.63511600	-0.50865000	2.16625100
H	7.15160800	-0.93204000	-0.26612700
H	3.63629400	0.95171800	-1.86684700
H	-4.47104100	-7.01273300	0.33902500
H	-6.66432000	-5.88265100	0.21227300
H	-6.83639000	-3.41380300	0.45803000
H	-2.40105100	-5.70784400	0.69542500
H	-5.28834000	-1.13683700	0.89542700
H	1.64302200	0.07773900	1.06509500
C	-3.29958400	1.33150400	-2.36650900
H	-3.79432000	2.22114400	-2.75004600
H	-3.12522900	0.60987200	-3.16194000
H	-3.91014800	0.86985800	-1.59306000
H	-0.13762800	2.58755300	-2.40129600
H	-0.97700200	1.61217700	-3.62376800
H	-1.59845400	3.22812800	-3.21322700
H	-2.64045300	1.74724000	0.17609700
H	-0.20264800	0.85681200	0.69494700
H	-0.26873300	3.58328300	-0.42667600
P	-1.85878800	-2.12788900	-1.43398000
O	-0.80504400	-3.37600300	-1.61740600
O	-1.10983600	-0.80009100	-1.55338400
O	-2.78075300	-2.19667700	-2.83039000
H	-1.52946400	0.76434500	-1.55143200
C	0.32330300	-3.30288100	-2.51531000
H	0.91597300	-4.19900300	-2.33776300
H	-0.01328900	-3.28374000	-3.55512500
H	0.92023500	-2.41384400	-2.30683500
C	-3.50199000	-3.39279000	-3.17153400
H	-4.01203900	-3.19030600	-4.11303800
H	-2.81945800	-4.23603900	-3.30192500
H	-4.24289600	-3.64237700	-2.40729500

$TS_{NH\text{-}CH}$'

B3LYP/6-31+G(d,p)–CPCM(mesitylene): E = -3436.650829 Hartrees; G = -3436.748309 Hartrees

M06-2X/6-311++G(d,p)–CPCM(mesitylene): single-point energy = -3436.9375866 Hartrees

C	7.16968600	-3.12239200	-0.74888300
C	7.00611500	-2.16260800	0.25286500
C	5.78151300	-1.50572700	0.39987400

C	4.69978100	-1.79734200	-0.44271200
C	4.87280400	-2.77233500	-1.43848900
C	6.09797600	-3.42461200	-1.59418200
C	3.37934300	-1.05305100	-0.24961200
C	2.23650600	-2.08137400	-0.01152700
N	3.09222600	-0.02564600	-1.34946200
N	0.94332500	-1.42251900	0.11654100
C	2.54108800	-2.93277000	1.22667700
C	2.51298800	-2.36619100	2.50968700
C	2.78225500	-3.14436600	3.63773700
C	3.07916600	-4.50398000	3.49834600
C	3.09966600	-5.07817000	2.22489500
C	2.83017100	-4.29630200	1.09774100
C	2.35342200	-0.53964400	-2.53301500
C	-0.24466400	-2.02167000	-0.14294200
N	-1.29959300	-1.33657900	0.41863200
S	-0.39792800	-3.45699300	-1.02128500
C	-2.68251200	-1.48945800	0.23888000
C	-3.51162300	-1.13747400	1.31454600
C	-4.89915100	-1.21034800	1.18833600
C	-5.48918800	-1.64460400	0.00088200
C	-4.65577000	-1.99144700	-1.06553800
C	-3.26625800	-1.91024300	-0.96581100
C	-5.27476400	-2.39279900	-2.38045400
F	-4.49052400	-3.23666400	-3.08948600
F	-5.50036900	-1.30998300	-3.18024600
F	-6.47544500	-3.00259100	-2.21819000
C	-5.76569300	-0.77002900	2.33835000
F	-6.00135700	0.57436900	2.30499800
F	-6.97884100	-1.37101000	2.33470600
F	-5.19575100	-1.02461700	3.54278100
C	0.67522700	6.72602000	0.53124900
C	0.38137500	6.75029700	1.89809500
C	0.22503600	5.56121700	2.62237300
C	0.37482900	4.36919300	1.92621800
C	0.66633900	4.32017900	0.55560800
C	0.81653100	5.50924300	-0.15180000
N	0.27988700	3.05758700	2.42231300
C	0.50414300	2.11807800	1.47349900
C	0.77765500	2.85667700	0.12790700
O	0.49839000	0.90147800	1.67008600
C	2.19085200	2.44716200	-0.44082300
C	3.21841300	2.64746600	0.56696300
N	4.03213900	2.71957500	1.39795700

C	2.50004200	3.19035800	-1.64808600
N	2.72756100	3.72738900	-2.65701300
H	8.12012600	-3.63416500	-0.86715400
H	7.82821000	-1.92394100	0.92108400
H	5.66519400	-0.76110500	1.18294600
H	4.05337200	-3.03916300	-2.09836200
H	6.21108000	-4.17418000	-2.37192800
H	2.27030200	-1.31429200	2.63792000
H	2.75763700	-2.68948600	4.62388000
H	3.28678600	-5.11033700	4.37517000
H	3.31957900	-6.13516900	2.10615100
H	2.83904600	-4.75130600	0.11198000
H	-3.06691600	-0.82018700	2.25200100
H	-6.56581800	-1.71684500	-0.08958700
H	-2.63836700	-2.17204500	-1.80521100
H	0.79334800	7.65812700	-0.01174900
H	0.27379400	7.70158200	2.40991600
H	0.00002400	5.57260600	3.68388700
H	1.03496500	5.50338500	-1.21240600
H	0.09501300	2.80845500	3.38557800
H	-1.03829100	-0.60356400	1.07119200
C	4.36041200	0.60888500	-1.81554500
H	4.99355700	-0.11274700	-2.33542800
H	4.11049700	1.41762600	-2.50095900
H	4.90926800	1.01387700	-0.96428200
H	1.39223300	-0.94814300	-2.23332900
H	2.17081000	0.30133800	-3.20384600
H	2.94302200	-1.29094200	-3.06792600
H	3.48411000	-0.44322500	0.65387500
H	0.91493900	-0.53842300	0.62597500
H	2.16475000	-2.75030300	-0.87129600
P	-0.57649800	2.37616400	-1.07733300
O	-1.83499100	2.57212000	-0.09376800
O	-0.40056300	1.04337400	-1.71711300
O	-0.71789800	3.59793100	-2.11519800
H	2.44644900	1.09045300	-0.84547800
C	-3.19308700	2.50808300	-0.59954400
H	-3.35499400	3.30149200	-1.33292300
H	-3.38640600	1.52928000	-1.04402700
H	-3.83968000	2.65972400	0.26382400
C	-0.57439000	3.43459900	-3.55295600
H	0.42154400	3.77157400	-3.84334200
H	-0.71987700	2.39123600	-3.83629300
H	-1.34011900	4.06371800	-4.00805600

$TS_{OH\text{-}CH}$'

B3LYP/6-31+G(d,p)–CPCM(mesitylene): E = -4084.077793 Hartrees; G = -4084.190884 Hartrees

M06-2X/6-311++G(d,p)–CPCM(mesitylene): single-point energy = -4084.4042665 Hartrees

C	7.97717300	-2.35252700	-0.06293700
C	7.61495900	-1.00692300	0.03787900
C	6.27237700	-0.63547800	-0.06194200
C	5.27219400	-1.59940500	-0.26429400
C	5.64658000	-2.95037300	-0.34939900
C	6.98950100	-3.32265200	-0.25456500
C	3.82760500	-1.14198200	-0.35875100
C	2.87104700	-1.94550300	0.55898600
N	3.31475100	-1.11110400	-1.81616400
N	1.47132400	-1.60792300	0.27689200
C	3.22002700	-1.72474400	2.02997600
C	3.20006900	-0.44326900	2.60220100
C	3.49048600	-0.26981500	3.95717100
C	3.80547500	-1.37340100	4.75613900
C	3.82322500	-2.65246900	4.19444700
C	3.52990700	-2.82606900	2.83886400
C	3.11327100	-2.44423800	-2.46829900
C	0.46025000	-2.53120300	0.28858800
N	-0.77178100	-1.94993900	0.42916000
S	0.72710900	-4.19517400	0.14132400
C	-2.05927300	-2.52028000	0.40477800
C	-3.04511300	-1.88639000	1.17859300
C	-4.35986400	-2.34727000	1.15561800
C	-4.71987000	-3.45306200	0.38109900
C	-3.73486500	-4.07298400	-0.38707900
C	-2.41387100	-3.61725100	-0.39083500
C	-4.07836700	-5.28136400	-1.22098300
F	-3.47065400	-5.25250200	-2.43589800
F	-5.40896000	-5.39477500	-1.44684500
F	-3.68344800	-6.43713000	-0.62279100
C	-5.39966600	-1.68024500	2.01929700
F	-5.09730300	-0.38533300	2.28299300
F	-6.62623100	-1.69335500	1.44041300
F	-5.53448900	-2.30061500	3.22252200
C	-2.95831400	5.17878700	-2.56083100
C	-3.91622400	4.91097800	-1.57804100
C	-3.69447900	3.93177200	-0.60105500
C	-2.48475800	3.25112300	-0.64219600
C	-1.50862900	3.51204400	-1.61452400

C	-1.74464200	4.47707100	-2.58787300
N	-2.05141300	2.21106700	0.20065200
C	-0.81446100	1.77004500	-0.13363200
C	-0.31095800	2.60877500	-1.34747600
O	-0.18304000	0.88435700	0.44538000
C	0.93599800	3.43005800	-0.83165400
C	1.28318500	4.58120500	-1.64836700
N	1.57114200	5.53504800	-2.24903500
C	2.13182000	2.65768300	-0.54540800
N	3.11376100	2.10249900	-0.26043700
H	9.01988100	-2.64497500	0.01638100
H	8.37302600	-0.24674400	0.19974900
H	5.99701800	0.41157000	0.02858800
H	4.89842000	-3.72670800	-0.47417000
H	7.26077700	-4.37194700	-0.32062300
H	2.95453900	0.42993700	2.00329900
H	3.46676800	0.72730600	4.38605600
H	4.03105900	-1.23618800	5.80952300
H	4.06124200	-3.51598000	4.80862100
H	3.53565800	-3.82374700	2.40948600
H	-2.77749000	-1.03586300	1.79652100
H	-5.74133700	-3.81194200	0.36766300
H	-1.66898600	-4.10432200	-1.00342900
H	-3.15153500	5.93904100	-3.31065500
H	-4.84951500	5.46558900	-1.57036200
H	-4.43769500	3.71492900	0.15876800
H	-1.00570200	4.68906900	-3.35076800
H	-2.39192600	2.08119300	1.15157600
H	-0.76023600	-0.95289100	0.65154700
C	4.16570100	-0.22546100	-2.67840500
H	5.14308000	-0.68668000	-2.81229900
H	3.66145200	-0.11173400	-3.63734200
H	4.26056700	0.74538000	-2.19389200
H	2.46158300	-3.06543100	-1.85398100
H	2.64255200	-2.27003700	-3.43635000
H	4.08124000	-2.92324000	-2.61024900
H	3.78163000	-0.08803200	-0.07909500
H	1.19626300	-0.63706600	0.42528200
H	2.96065700	-3.01136000	0.34865400
P	0.04545100	1.47385800	-2.77764100
O	-1.38428000	0.92900600	-3.27668200
O	1.03747000	0.37743500	-2.52828900
O	0.45555300	2.55095900	-3.88621500
C	-1.81185100	-0.44802300	-3.11788300

H	-2.56113100	-0.61857300	-3.89061900
H	-0.96931400	-1.12848400	-3.24732400
H	-2.25832600	-0.58230600	-2.13071900
C	0.72929900	2.17207700	-5.25851800
H	1.07299100	3.07991800	-5.75238500
H	1.50958900	1.40845400	-5.29374800
H	-0.18537200	1.80799700	-5.73193500
H	2.38545900	-0.64865900	-1.79596600
P	-0.03337100	3.54140300	2.82891000
O	-1.72422600	3.27831700	3.01824900
O	0.06588000	4.35989400	1.47575600
O	0.22475800	4.71873100	4.01174500
H	0.56690900	3.87995000	0.29328900
C	-2.63442100	4.38047800	3.12518100
H	-3.65096200	3.97647700	3.09099300
H	-2.49637000	4.90143400	4.07907100
H	-2.50158400	5.09088600	2.30101300
C	0.23774000	6.12913100	3.75597300
H	1.01217400	6.57105500	4.39017600
H	0.45738700	6.33538500	2.70482100
H	-0.73059800	6.57437000	4.01495900

TSa'

B3LYP/6-31+G(d,p)–CPCM(dichloromethane): E = -3705.338474 Hartrees; G = -3705.446470 Hartrees

M06-2X/6-311++G(d,p)–CPCM(dichloromethane): single-point energy = -3705.7122954 Hartrees

C	6.72557800	-1.04421500	3.16683400
C	5.35938500	-1.32642600	2.90967500
C	4.86403600	-1.20418300	1.56323200
C	5.76720800	-0.80448900	0.54688000
C	7.09776900	-0.54089600	0.83247000
C	7.58548100	-0.66214700	2.16056800
C	3.47766300	-1.51009000	1.34889600
C	2.72295400	-1.90036600	2.43755600
C	3.31149300	-1.97819600	3.72249100
N	4.57873700	-1.70540500	3.96520600
C	2.81728700	-1.40650100	-0.03246100
C	2.31404700	-2.79929000	-0.47635400
N	1.53013200	-2.73346500	-1.78029400
C	2.35784400	-2.25238200	-2.94924900
C	3.60812300	-3.15331100	-3.07487900
C	3.46046400	-4.35554400	-2.11994500
C	3.45902200	-3.83283500	-0.66940600
C	2.12451400	-5.07635500	-2.45405400

C	0.97026000	-4.10882000	-2.07436500
C	1.96241000	-6.41570000	-1.78178700
C	1.85410600	-7.57674100	-2.43529200
O	7.87618300	-0.16501900	-0.22383800
C	9.26041700	0.12562000	-0.00165200
N	1.73146000	-0.42127300	-0.03155900
C	1.85534700	0.85100300	-0.51445300
S	3.14096000	1.34475800	-1.50776500
N	0.81737200	1.66376300	-0.16426500
C	0.67700800	3.04535600	-0.44353500
C	-0.55482000	3.51223200	-0.90869800
C	-0.73920700	4.88462000	-1.12054200
C	0.28935500	5.79349400	-0.88804300
C	1.51536700	5.31142900	-0.41540300
C	1.71491500	3.95256500	-0.18368400
C	-2.08441600	5.36423300	-1.59758100
F	-2.49311000	4.71336400	-2.71870100
C	2.64166100	6.28414900	-0.18401500
F	2.20319800	7.46568000	0.32225600
F	-3.05606400	5.15641900	-0.66389500
F	-2.09924800	6.68737200	-1.88339100
F	3.57606400	5.80811400	0.67353300
F	3.29686100	6.58668400	-1.34117600
H	2.70251700	-2.28215600	4.57140200
H	1.67385800	-2.16260200	2.33438600
H	0.02663600	1.22313200	0.31500000
H	7.07939100	-1.14074400	4.18832900
H	0.94740500	-0.59845400	0.59393600
H	3.54034300	-1.03274900	-0.75418300
H	-1.35894300	2.80974200	-1.10645600
H	2.59839100	-1.20210200	-2.77886000
H	2.65842700	3.59529400	0.20476400
H	4.42738200	-3.37028300	-0.45909200
H	0.14066300	6.85201100	-1.06066900
H	1.70705700	-2.31266400	-3.82324100
H	8.62313700	-0.45589500	2.39197300
H	5.44270500	-0.67347300	-0.47798300
H	1.58142000	-3.15701700	0.24969400
H	3.34208400	-4.65125200	0.04493200
H	3.71411700	-3.49529800	-4.10815600
H	4.29454700	-5.04802200	-2.26002700
H	0.24238100	-3.99368400	-2.87880700
H	0.44076500	-4.42397700	-1.17315900
H	2.10421300	-5.24166600	-3.53693700

H	4.51190000	-2.58897800	-2.82535100
H	9.66201400	0.39814200	-0.97753800
H	9.38322700	0.96594400	0.69040700
H	9.79339900	-0.75227100	0.37951400
H	1.93152100	-6.41697300	-0.69192200
H	1.74655700	-8.51752500	-1.90360700
H	1.86919300	-7.62352300	-3.52211500
C	-6.81430000	-0.48618800	2.75103700
C	-6.54536400	0.79430600	3.24160800
C	-5.27624400	1.37369400	3.09111100
C	-4.30710800	0.62740100	2.43320200
C	-4.55755500	-0.66106100	1.92483600
C	-5.82050200	-1.22451000	2.08989100
N	-2.96909900	0.98488000	2.18303000
C	-2.30117500	-0.02715600	1.55126300
C	-3.30055100	-1.15467100	1.29519800
O	-1.10001400	-0.00873200	1.25643000
C	-2.83440300	-2.50107300	1.57006700
C	-1.48205700	-2.89810600	1.50222700
N	-0.38491100	-3.31183600	1.49192900
C	-3.71241400	-3.52706900	1.98714400
N	-4.40576000	-4.39516300	2.36150700
H	-7.80089500	-0.91886700	2.88283300
H	-7.32491400	1.35177500	3.75189600
H	-5.06630800	2.36484100	3.47805300
H	-6.04335200	-2.21632500	1.71886900
H	0.70762400	-2.10604100	-1.66355500
C	-5.98546000	-1.75997300	-1.15274500
C	-4.59639700	-1.99609500	-1.09685700
C	-4.14069700	-3.30272200	-1.36982900
C	-5.03289300	-4.32891500	-1.68462400
C	-6.40568500	-4.07965400	-1.73862100
C	-6.87203400	-2.78885300	-1.47429700
H	-6.37670300	-0.77450000	-0.94929100
H	-3.08099700	-3.52386900	-1.34659600
H	-4.64819300	-5.32387000	-1.88852100
H	-7.10089700	-4.87588500	-1.98743600
H	-7.93605800	-2.57436500	-1.51608300
C	-3.59119600	-0.94090800	-0.72663000
C	-3.84802300	0.52115700	-1.00645800
N	-2.31384300	-1.25027600	-1.21444700
C	-1.23197800	-1.50443200	-1.58151900
O	-2.99707400	1.27854000	-1.45121000
O	-5.07851500	0.92180500	-0.66820400

C	-5.39653800	2.31353500	-0.91166100
H	-6.42531300	2.43071500	-0.57584700
H	-4.72689300	2.96024000	-0.34307100
H	-5.30974700	2.53514300	-1.97704700
C	-2.35067300	2.22106400	2.63754900
H	-2.76622000	3.08017200	2.10337000
H	-2.51732400	2.34720900	3.71100200
H	-1.28019500	2.15861500	2.44804700

TSb'

B3LYP/6-31+G(d,p)–CPCM(dichloromethane): E = -3705.335746 Hartrees; G = -3705.446079 Hartrees

M06-2X/6-311++G(d,p)–CPCM(dichloromethane): single-point energy = -3705.7095358 Hartrees

C	7.44455600	-1.72233600	2.26592000
C	6.02769300	-1.74697900	2.33040100
C	5.27135000	-1.53493000	1.12413100
C	5.97915600	-1.30613900	-0.08220700
C	7.36469100	-1.29096800	-0.11036500
C	8.10964900	-1.50319200	1.07978400
C	3.84044400	-1.57828400	1.23562900
C	3.29315000	-1.80939800	2.48179000
C	4.13342200	-1.99738200	3.60522000
N	5.45084000	-1.97361700	3.54802200
C	2.91960300	-1.39070400	0.02197600
C	2.21774000	-2.72666800	-0.32389100
N	1.29686900	-2.57971400	-1.53129300
C	2.04288300	-2.28847200	-2.81352100
C	3.05379100	-3.42956000	-3.07276400
C	2.87583000	-4.51828200	-1.99640700
C	3.18917200	-3.90212900	-0.61911600
C	1.41190700	-5.03487700	-2.06107500
C	0.48148500	-3.84672600	-1.68764100
C	1.14904900	-6.24070200	-1.19458000
C	0.82090300	-7.44773300	-1.66581600
O	7.93883600	-1.06055400	-1.32716000
C	9.36614900	-1.01973200	-1.42808400
N	1.91342700	-0.34940100	0.23774400
C	2.02784100	0.92671400	-0.21564900
S	3.33616800	1.46806800	-1.15495300
N	0.97473100	1.73469700	0.11568500
C	0.90277600	3.12810500	-0.14787700
C	-0.15171200	3.62791800	-0.91207500
C	-0.26358600	5.00709200	-1.12448700
C	0.67120800	5.89151200	-0.59208400

C	1.72313100	5.37708800	0.17470600
C	1.84121100	4.00820200	0.40603800
C	-1.43325000	5.52026500	-1.92128400
F	-1.60984400	4.82491700	-3.07594800
C	2.75902400	6.32038200	0.72708700
F	3.37594900	5.82820900	1.82848400
F	-2.60409400	5.40937800	-1.23166600
F	-1.30500300	6.82418800	-2.26029700
F	3.74211400	6.58336900	-0.18039200
F	2.22897000	7.52151100	1.07118700
H	3.68745800	-2.17741200	4.58125600
H	2.21778500	-1.84710300	2.62228900
H	0.09625700	1.31222700	0.41769100
H	7.99620100	-1.88335400	3.18663000
H	1.18084200	-0.56875600	0.92141900
H	3.51636800	-1.05426000	-0.82348500
H	-0.87653100	2.94327300	-1.33622600
H	2.51282300	-1.31003900	-2.71201500
H	2.64605800	3.61939000	1.01664400
H	4.22372700	-3.55006300	-0.61914300
H	0.58203000	6.95715400	-0.76223700
H	1.28255500	-2.21326500	-3.59252300
H	9.19248400	-1.49112200	1.06757200
H	5.46092300	-1.11394100	-1.01337400
H	1.54227600	-2.97646000	0.49774900
H	3.11260300	-4.64847600	0.17479900
H	2.89187100	-3.84976000	-4.06929500
H	3.56199500	-5.34672500	-2.19007100
H	-0.26317300	-3.64654600	-2.45919500
H	-0.04740500	-3.99681700	-0.74503700
H	1.21406000	-5.32081100	-3.09989200
H	4.07662100	-3.04351600	-3.04470300
H	9.57901900	-0.82213500	-2.47852300
H	9.78429500	-0.21490200	-0.81400400
H	9.81153000	-1.97806200	-1.13987800
H	1.23545400	-6.10004500	-0.11677500
H	0.65059300	-8.28836400	-0.99965800
H	0.71197900	-7.63397400	-2.73220400
C	-7.25107100	-0.76638600	2.51603000
C	-7.82469900	-1.87261700	1.88174800
C	-7.04452600	-2.75047200	1.11654100
C	-5.68508700	-2.47638200	1.00918600
C	-5.08649000	-1.36319800	1.63329300
C	-5.87869200	-0.50470300	2.39349500

N	-4.71247700	-3.23192200	0.34019500
C	-3.45808400	-2.70649500	0.54111400
C	-3.63081300	-1.38747400	1.30883000
O	-2.40692500	-3.22616600	0.18015000
C	-2.63807200	-1.11723000	2.34185700
C	-1.27123400	-1.40196000	2.18170500
N	-0.11432300	-1.58623100	2.10390200
C	-2.95243600	-0.40137900	3.51646400
N	-3.19084800	0.18513200	4.50389000
H	-7.87038800	-0.10162300	3.10971300
H	-8.88897000	-2.06196800	1.98487100
H	-7.48810900	-3.61431800	0.63365800
H	-5.45078300	0.35805000	2.88668900
H	0.60894100	-1.81506400	-1.37051300
C	-5.79732600	0.46383300	-0.96993300
C	-4.55561800	-0.15701900	-1.21150200
C	-4.41758900	-0.90691500	-2.39749600
C	-5.46944000	-1.02292900	-3.30741100
C	-6.69163200	-0.39321400	-3.05973600
C	-6.84505600	0.34761000	-1.88539100
H	-5.95033600	1.04086600	-0.07075200
H	-3.48096400	-1.40335200	-2.62117200
H	-5.32606500	-1.60489200	-4.21314900
H	-7.50957900	-0.47856800	-3.76878300
H	-7.78794200	0.84294400	-1.67232500
C	-3.40264600	-0.08047800	-0.24117800
C	-3.10747600	1.18108100	0.53665400
N	-2.19548700	-0.48663800	-0.82905400
C	-1.17572800	-0.85288100	-1.27238700
O	-1.96938900	1.55212400	0.78688500
O	-4.19233100	1.80058100	0.99984600
C	-3.97154600	2.98036100	1.81517400
H	-4.96795900	3.35658100	2.03952000
H	-3.44633000	2.70397900	2.73118200
H	-3.39519100	3.71813300	1.25571700
C	-4.96615600	-4.48575200	-0.34915200
H	-5.36715500	-5.23235000	0.34403600
H	-5.67847700	-4.33327100	-1.16517900
H	-4.02063700	-4.84344700	-0.75577100