

Supplementary Information

Reaction Mechanisms of Carbon Dioxide, Ethylene Oxide and Amines Catalyzed by Ionic Liquids BmimBr and BmimOAc: A DFT Study

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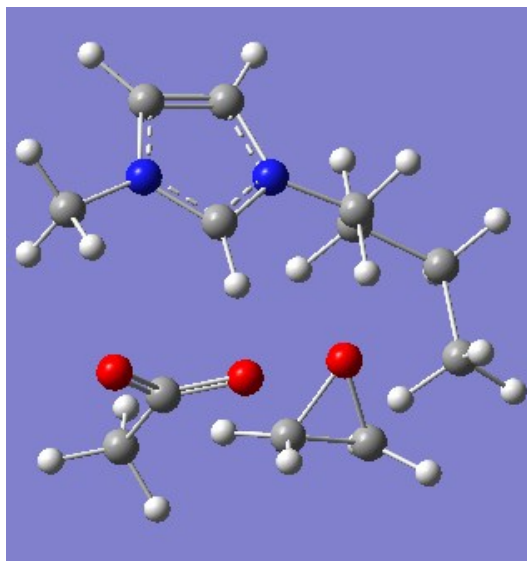
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Cartesian coordinates of structures in Figure 1

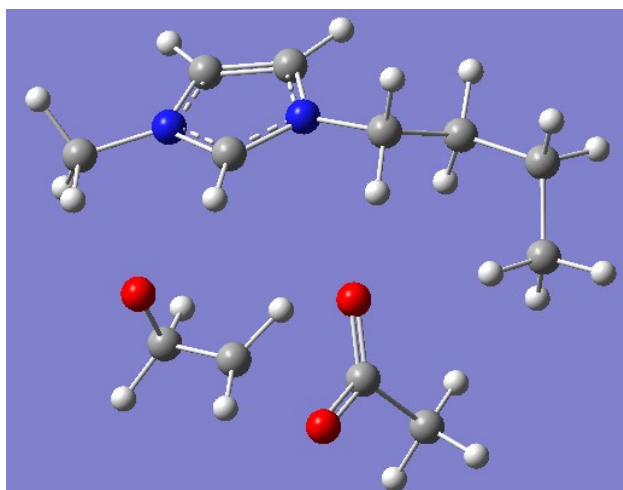
Structure and coordinates of **O1-Complex**



C	-1.55088300	-0.45411500	-0.78964500
C	0.23523200	0.68793000	-0.18524800
C	-0.86145200	1.43824400	0.10833200
N	-1.96248200	0.70585300	-0.28411000
H	-2.21150100	-1.23693200	-1.13252300
H	1.28713300	0.88117000	-0.04337800
H	-0.95216100	2.41690500	0.55252700
N	-0.21939100	-0.48482500	-0.75196800
C	-3.37706100	1.04719700	-0.08356000
C	-3.68398300	1.26219400	1.39368600
H	-3.93311500	0.19335100	-0.47595100
H	-3.60190600	1.93715500	-0.68289500
C	-5.17486000	1.51377300	1.63454900
H	-3.37342100	0.35517300	1.92414700
H	-3.10088800	2.11090300	1.77637800
H	-5.31655300	1.69460800	2.70625100
H	-5.48998400	2.43373100	1.12227100
C	-6.05345000	0.33905200	1.19779600
H	-7.07301100	0.45048200	1.57989300
H	-6.12097200	0.26792900	0.10650300
H	-5.63636700	-0.60535000	1.56537800
C	0.59099600	-1.64939400	-1.10291200
H	1.57745100	-1.30120400	-1.41263100
H	0.63493400	-2.31951400	-0.24351700
H	0.10579000	-2.17537000	-1.92429700
C	-3.89981200	-3.03786200	-1.98302900
C	-5.08384400	-2.31457500	-1.50489200

O	-4.03291600	-1.62690100	-2.18413300
H	-3.13333000	-3.32013500	-1.26114500
H	-3.96743100	-3.62305800	-2.89788400
H	-5.14397800	-2.09722200	-0.44164900
H	-6.01074600	-2.37611900	-2.07165200
C	-2.42397900	-2.63625000	1.17874500
O	-3.33418700	-1.79999200	0.91615400
O	-1.49324200	-2.96978100	0.39730300
C	-2.46775200	-3.28330500	2.56503000
H	-3.44332700	-3.75593000	2.71564300
H	-1.67471100	-4.02378600	2.68385800
H	-2.36454100	-2.50762500	3.33165400

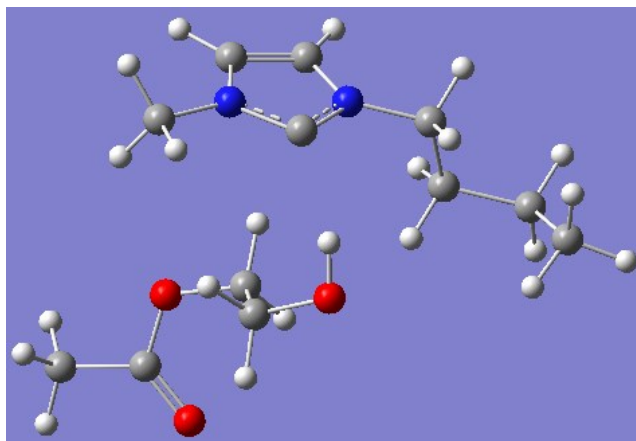
Structure and coordinates of **TS-O1**



C	-2.47743200	-0.41908700	1.64256100
C	-1.86550100	-1.73242500	1.66445400
O	-1.70137100	-0.33775200	2.80904900
H	-2.17958700	0.23502400	0.80636400
H	-3.56152100	-0.38142200	1.79945000
H	-0.83112400	-1.83179000	1.37898600
H	-2.31297100	-2.50334200	2.27527700
C	0.37624500	0.73232000	1.12012900
C	0.68536800	2.65437900	0.08190600
C	1.50438600	1.72858200	-0.48812600
N	1.29775800	0.54032400	0.17765800
H	-0.05870400	0.01938500	1.82798700
H	0.52852700	3.69839000	-0.14062700
H	2.19773700	1.81462700	-1.30885700
N	-0.00405900	2.01053500	1.08543300
C	1.94718900	-0.75137500	-0.10058500
C	2.17076300	-0.97689600	-1.59035300
H	1.26734000	-1.50790200	0.29235500

H	2.89352500	-0.77850700	0.45133800
C	2.67065400	-2.40088200	-1.86207700
H	1.21673900	-0.81020400	-2.10292800
H	2.91161000	-0.26032300	-1.96813100
H	3.03902800	-2.44345600	-2.89338900
H	3.53693800	-2.61639600	-1.22043600
C	1.59618600	-3.47291800	-1.67364200
H	2.00109700	-4.46612100	-1.89221800
H	1.19764800	-3.49243100	-0.65397800
H	0.75085300	-3.28802100	-2.34338700
C	-1.02473900	2.58805800	1.96101100
H	-1.84683000	2.96432000	1.34895500
H	-1.38158900	1.78952200	2.62084800
H	-0.58323200	3.40196300	2.53918300
C	-1.69953000	-2.15241500	-0.99358900
O	-2.33664100	-2.65811500	-0.01273000
O	-0.79725800	-1.28850600	-0.91389500
C	-2.10015600	-2.68500900	-2.36636400
H	-1.54778600	-2.17463500	-3.15848900
H	-1.90371500	-3.76108000	-2.41050200
H	-3.17510100	-2.54614900	-2.51361300

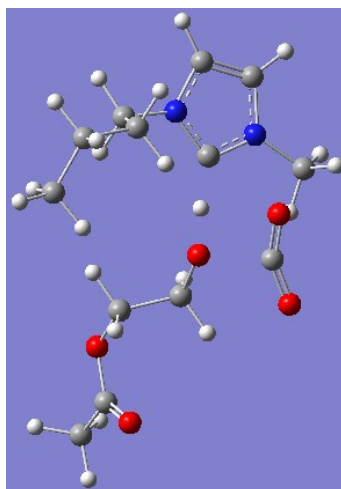
Structure and coordinates of **Int-O1**



C	-1.55088300	-0.45411500	-0.78964500
C	0.23523200	0.68793000	-0.18524800
C	-0.86145200	1.43824400	0.10833200
N	-1.96248200	0.70585300	-0.28411000
H	-2.21150100	-1.23693200	-1.13252300
H	1.28713300	0.88117000	-0.04337800
H	-0.95216100	2.41690500	0.55252700
N	-0.21939100	-0.48482500	-0.75196800
C	-3.37706100	1.04719700	-0.08356000
C	-3.68398300	1.26219400	1.39368600

H	-3.93311500	0.19335100	-0.47595100
H	-3.60190600	1.93715500	-0.68289500
C	-5.17486000	1.51377300	1.63454900
H	-3.37342100	0.35517300	1.92414700
H	-3.10088800	2.11090300	1.77637800
H	-5.31655300	1.69460800	2.70625100
H	-5.48998400	2.43373100	1.12227100
C	-6.05345000	0.33905200	1.19779600
H	-7.07301100	0.45048200	1.57989300
H	-6.12097200	0.26792900	0.10650300
H	-5.63636700	-0.60535000	1.56537800
C	0.59099600	-1.64939400	-1.10291200
H	1.57745100	-1.30120400	-1.41263100
H	0.63493400	-2.31951400	-0.24351700
H	0.10579000	-2.17537000	-1.92429700
C	-3.89981200	-3.03786200	-1.98302900
C	-5.08384400	-2.31457500	-1.50489200
O	-4.03291600	-1.62690100	-2.18413300
H	-3.13333000	-3.32013500	-1.26114500
H	-3.96743100	-3.62305800	-2.89788400
H	-5.14397800	-2.09722200	-0.44164900
H	-6.01074600	-2.37611900	-2.07165200
C	-2.42397900	-2.63625000	1.17874500
O	-3.33418700	-1.79999200	0.91615400
O	-1.49324200	-2.96978100	0.39730300
C	-2.46775200	-3.28330500	2.56503000
H	-3.44332700	-3.75593000	2.71564300
H	-1.67471100	-4.02378600	2.68385800
H	-2.36454100	-2.50762500	3.33165400

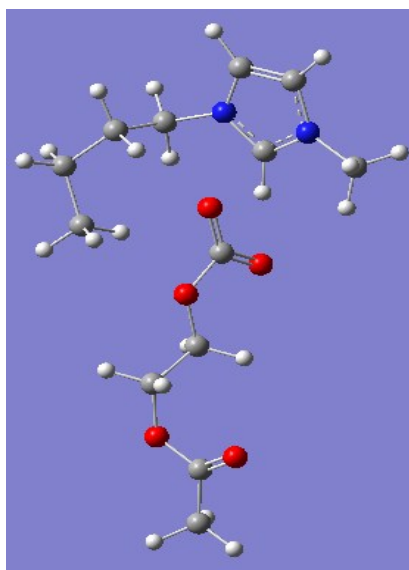
Structure and coordinates of **TS-O2**



C	3.69932500	-0.68869300	3.54091200
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O	4.83906700	-0.33297300	3.51329600
O	2.87249800	-1.52618700	3.70309200
C	4.41314300	1.37947200	1.07102600
C	6.12129300	1.06630400	-0.34843200
C	6.13367500	2.37245000	0.02806200
N	5.07113900	2.53784800	0.89366200
H	3.51632800	1.13673300	2.03963300
H	6.76384800	0.51314100	-1.01648400
H	6.78738600	3.18560100	-0.24902200
N	5.05403500	0.48144700	0.30484300
C	4.76265900	3.73017200	1.68518100
C	5.29298700	3.58806200	3.11070400
H	3.67579800	3.84631100	1.67598100
H	5.20080600	4.59499400	1.17597600
C	4.89911500	4.76547300	4.00515500
H	4.90093400	2.65342700	3.53318600
H	6.38497800	3.48855000	3.06887900
H	5.40349900	4.64167500	4.96980700
H	5.27708300	5.70498200	3.57860100
C	3.39038900	4.86531300	4.23968500
H	3.16128100	5.61921300	4.99890900
H	2.84853100	5.14813400	3.33050300
H	2.99084300	3.90418500	4.58291500
C	4.73032400	-0.93948200	0.29551200
H	4.78075600	-1.32087600	-0.72619800
H	5.42526600	-1.48035000	0.94186900
H	3.71739200	-1.06306700	0.68185400
O	2.80542600	0.83926000	3.00099500
C	1.47092500	0.69677300	2.59683700
H	1.40185000	0.60867200	1.49656000
H	1.04451300	-0.21078400	3.04115400
C	0.69076700	1.92681600	3.04188200
H	1.14645300	2.83321000	2.63449100
H	0.66073900	1.98676800	4.13263500
O	-0.64267400	1.90626300	2.51248900
C	-2.91092500	1.28272900	2.54037800
H	-3.23408000	2.32182900	2.43311100
H	-2.83001400	0.85507900	1.53745400
H	-3.63666800	0.72326800	3.12945800
C	-1.56970200	1.23415400	3.22392300
O	-1.33871400	0.67938200	4.26957600

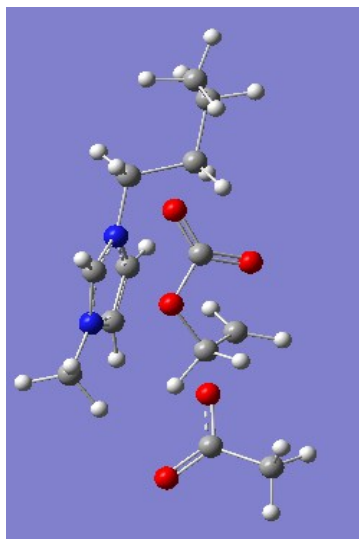
Structure and coordinates of **Int-O2**



C	2.92978500	1.10142700	2.34623100
O	4.11724700	1.06268600	2.72723500
O	2.48373500	1.04757900	1.17256500
C	5.18667900	1.54127900	0.43880200
C	7.09304700	0.44940300	0.60124200
C	7.32863000	1.75187100	0.91247300
N	6.12501600	2.41911400	0.78494300
H	4.11429600	1.71495300	0.35600000
H	7.75322400	-0.40331700	0.56813700
H	8.23433300	2.25959800	1.20617600
N	5.75034700	0.34547600	0.29868600
C	5.81353300	3.76329000	1.28202900
C	5.80622800	3.80278300	2.81457300
H	4.82725700	4.00857400	0.87946300
H	6.53490900	4.46432600	0.85123800
C	4.87842500	4.90401600	3.34114800
H	5.44900800	2.83215700	3.17943900
H	6.83112700	3.95217200	3.17587100
H	5.11934300	5.08987700	4.39357700
H	5.07085100	5.84858600	2.81153400
C	3.40265900	4.51440100	3.22798400
H	2.75530200	5.31404300	3.60204400
H	3.10496300	4.31239100	2.19169800
H	3.20048800	3.60295800	3.80022300
C	4.98106400	-0.88149100	0.10731600
H	5.25741800	-1.35463300	-0.83687100
H	5.18062400	-1.54907300	0.94714700
H	3.92321700	-0.60893600	0.11900000
O	2.00825000	1.24542400	3.36972400
C	0.64974800	1.31922300	2.98010800

H	0.47665900	2.18968400	2.33584300
H	0.35133200	0.42054100	2.43099700
C	-0.13661200	1.45335900	4.27229800
H	0.18073200	2.33992700	4.82448400
H	-0.01664600	0.56417900	4.89543600
O	-1.52760200	1.66153100	3.98321800
C	-3.70355300	0.93662800	3.46676100
H	-4.11968000	1.51008100	4.29951700
H	-3.73902600	1.57058200	2.57665600
H	-4.28669500	0.03074700	3.30498500
C	-2.27522900	0.56374300	3.76694500
O	-1.84493200	-0.56302500	3.81551700

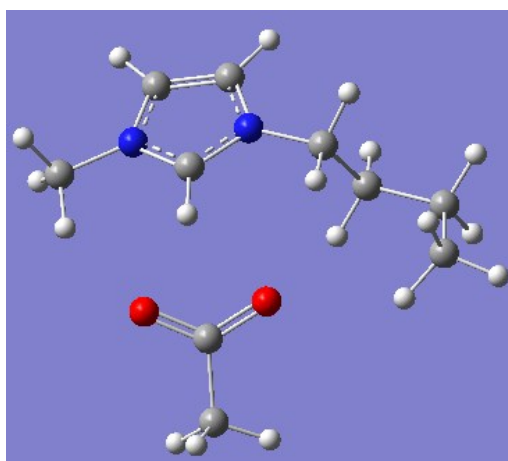
Structure and coordinates of **TS-O3**



O	0.15553500	0.05605000	-1.25772100
C	0.80876400	0.95926500	-1.75741400
O	1.39218600	1.02219600	-2.89574200
O	1.06281300	2.07751500	-0.97378700
C	1.91520700	2.96639900	-1.68131800
H	2.41864800	3.58660100	-0.94019000
C	2.87317300	2.12611900	-2.49986200
H	3.07038100	2.35570100	-3.53717900
H	3.35398700	1.25370100	-2.08628900
H	1.31675000	3.59788100	-2.34772800
C	2.76520100	0.27946000	0.43185600
C	4.88200200	0.66125500	-0.04384600
C	4.55373200	-0.56659200	-0.53327900
N	3.22423000	-0.78340600	-0.22804300
H	1.74164200	0.41492300	0.75448400
H	5.78468900	1.24751100	-0.11893300
H	5.13760400	-1.28664900	-1.08410200

N	3.75317000	1.16733200	0.55718100
C	2.41902000	-1.95578100	-0.61497000
C	2.42879400	-2.16893400	-2.12490100
H	1.40412000	-1.74993700	-0.26909900
H	2.82040500	-2.82447300	-0.08059600
C	1.58178500	-3.38028100	-2.52740900
H	2.03762300	-1.26490000	-2.60716600
H	3.46053500	-2.31609400	-2.47048200
H	1.66536300	-3.49664100	-3.61367900
H	2.00495800	-4.29388900	-2.08647700
C	0.10701900	-3.24298000	-2.14461800
H	-0.48545900	-4.04178000	-2.60102600
H	-0.04242900	-3.30654800	-1.06127500
H	-0.29009600	-2.27667600	-2.47039300
C	3.66062200	2.47751600	1.20571100
H	4.21769700	3.20423000	0.60256300
H	2.60639700	2.75449300	1.25907300
H	4.07917300	2.41042000	2.21217300
C	4.67739200	4.21482700	-1.77515400
O	5.05134100	4.76470600	-0.73817000
O	4.51579800	2.93163200	-1.87685800
C	4.34631400	5.04015200	-3.01176700
H	4.79763800	4.59093100	-3.90106400
H	3.26001700	5.05586100	-3.16530500
H	4.69320400	6.06669300	-2.88881300

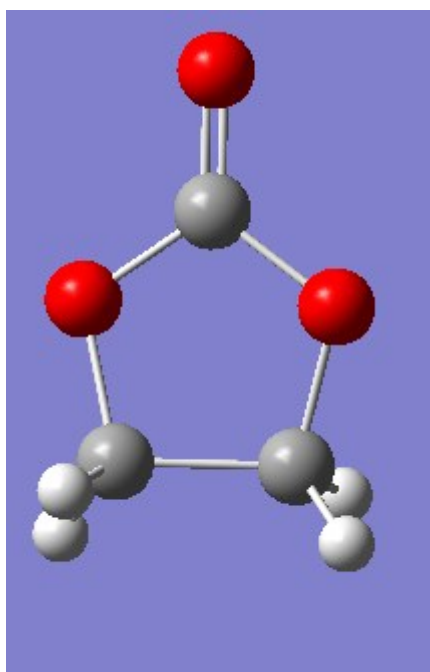
Structure and coordinates of **BmimOAc**



C	-1.99114100	-0.56443000	0.23554100
C	-0.32372600	0.47183700	-0.77648400
C	-1.45556600	1.20527000	-0.96772700
N	-2.48043300	0.53734400	-0.32999300
H	-2.51605100	-1.25205900	0.89998300
H	0.69096200	0.63212400	-1.10672800

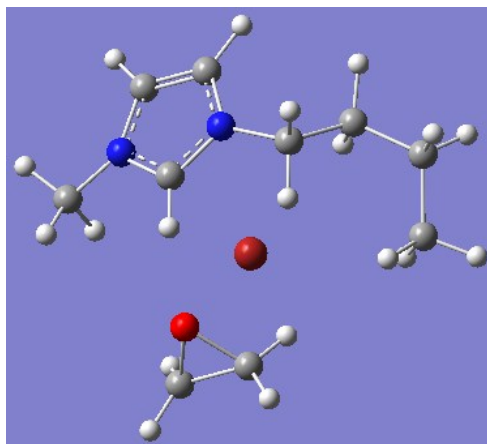
H	-1.61839000	2.13413800	-1.49252500
N	-0.68384000	-0.62312200	-0.01857100
C	-3.85963800	1.01026000	-0.13597900
C	-3.90798600	2.14952100	0.87585500
H	-4.41728800	0.15272700	0.24376100
H	-4.25119500	1.30769700	-1.11531700
C	-5.33841200	2.64384600	1.10818500
H	-3.49791600	1.76128200	1.81519800
H	-3.27489600	2.97838000	0.53056400
H	-5.29515300	3.45753900	1.84129100
H	-5.73898700	3.08304100	0.18345300
C	-6.27140800	1.54359200	1.62103200
H	-7.20941400	1.96979400	1.99019900
H	-6.52901000	0.83008400	0.83034900
H	-5.79185700	0.97541200	2.42534600
C	0.18436600	-1.68152500	0.49940100
H	1.09812400	-1.22769300	0.88602800
H	-0.35964800	-2.17459600	1.31080300
H	0.42556000	-2.38640600	-0.29877400
C	-3.08252700	-1.39279800	3.11249400
O	-3.77316000	-0.54231800	2.48697400
O	-2.17431600	-2.10909900	2.60004000
C	-3.36290800	-1.59747300	4.60020100
H	-3.80123200	-2.59077500	4.74316400
H	-2.42509600	-1.57361400	5.16264500
H	-4.05263000	-0.84148200	4.98032000

Structure and coordinates of **Pro-C1**



C	-1.30604900	0.75391100	0.12709700
C	-1.30605800	-0.75390100	-0.12707900
H	-1.93987000	1.31860500	-0.55647600
H	-1.55425800	1.00415600	1.16296900
H	-1.55428200	-1.00414700	-1.16294700
H	-1.93987500	-1.31858500	0.55650500
O	0.05528500	-1.10453400	0.11624900
O	0.05529400	1.10453700	-0.11624800
C	0.83239600	-0.00000700	-0.00004500
O	2.02199000	-0.00000500	0.00002100

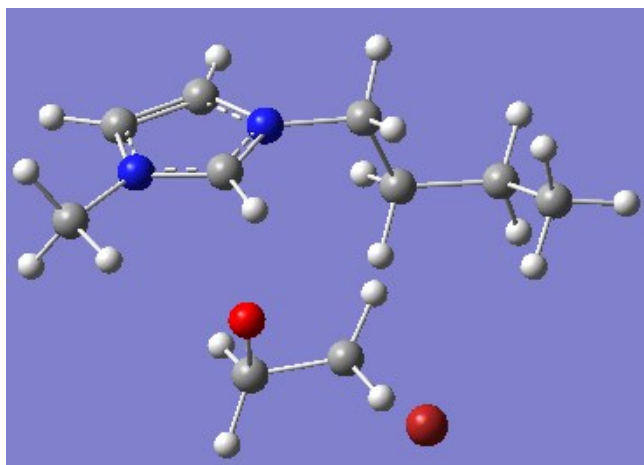
Structure and coordinates of **B1-Complex**



C	-1.75945200	-0.13774800	-1.04325400
C	-0.00053700	0.28627700	0.20667200
C	-0.98937700	1.14470900	0.56873300
N	-2.07148300	0.88211000	-0.24658200
H	-2.44181400	-0.62632600	-1.73358400
H	0.99574500	0.14938300	0.59655400
H	-1.01609600	1.90391000	1.33372600
N	-0.48951800	-0.47980900	-0.83190000
C	-3.45566300	1.33776300	-0.05654400
C	-3.83316000	1.37853700	1.42245700
H	-4.06846700	0.60273600	-0.58623600
H	-3.58222700	2.31512000	-0.53466400
C	-5.34696700	1.50407000	1.62174000
H	-3.48028800	0.44843300	1.88399700
H	-3.32717900	2.22171200	1.90991000
H	-5.53122700	1.62592600	2.69498400
H	-5.71972300	2.41912500	1.14018500
C	-6.12272100	0.28542300	1.11470600
H	-7.16246700	0.31966100	1.45462100
H	-6.14388400	0.23965600	0.02021100
H	-5.66464500	-0.64180600	1.47717900

C	0.07844900	-1.73706000	-1.30175000
H	1.16647100	-1.66387700	-1.28443500
H	-0.28189000	-2.53013100	-0.63815000
H	-0.25912900	-1.91866500	-2.32308300
Br	-2.77671000	-2.13157000	0.87293400
C	-3.93062100	-3.07906600	-2.38048700
C	-4.98907900	-2.17288900	-1.92636800
O	-3.85854200	-1.67521100	-2.64759400
H	-3.21977900	-3.43365900	-1.63725100
H	-4.09213500	-3.68965000	-3.26593100
H	-5.00227100	-1.90828700	-0.87116200
H	-5.92454000	-2.12063600	-2.47878100

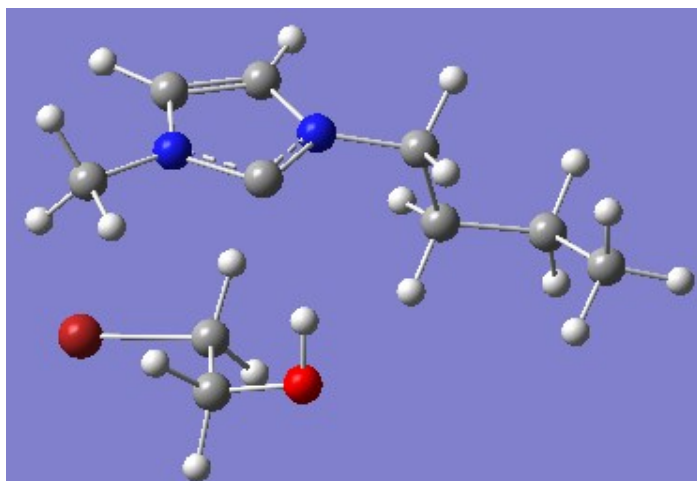
Structure and coordinates of **TS-B1**



Br	-1.68085300	-2.01214300	-1.91506100
C	-2.23321000	-0.37634100	0.79711700
C	-1.62312800	-1.66564900	0.53682700
O	-1.79116200	-0.71627800	2.08087300
H	-1.74168400	0.49129600	0.32157800
H	-3.31810200	-0.31773100	0.66596300
H	-0.54613900	-1.74762900	0.48365600
H	-2.18380400	-2.56288800	0.75235700
C	0.53632700	0.70910600	1.55092100
C	1.02916500	2.82968700	1.17817400
C	1.91234500	2.06168600	0.48212400
N	1.58911000	0.74565000	0.73480400
H	-0.05694600	-0.15249000	1.90056600
H	0.93164000	3.90111900	1.26279500
H	2.73320200	2.33240300	-0.16418400
N	0.17989100	1.96389300	1.83178000
C	2.18488300	-0.43042200	0.07881800
C	1.67163000	-0.58053700	-1.34972700

H	1.92173000	-1.29117700	0.69817000
H	3.27296500	-0.30900900	0.11642500
C	2.25859400	-1.80875200	-2.05062500
H	0.57714500	-0.67086100	-1.34292000
H	1.92218800	0.32755400	-1.91399900
H	1.84012000	-1.83118000	-3.06248600
H	3.34732200	-1.69626300	-2.15599000
C	1.92054400	-3.12755000	-1.35371000
H	2.26802200	-3.97734400	-1.94904700
H	2.39096100	-3.21355200	-0.36674700
H	0.83382400	-3.21841900	-1.24624400
C	-0.98015500	2.31057700	2.65583100
H	-1.61703500	2.99685400	2.09520300
H	-1.52189500	1.38147800	2.86097400
H	-0.64523700	2.77800500	3.58352700

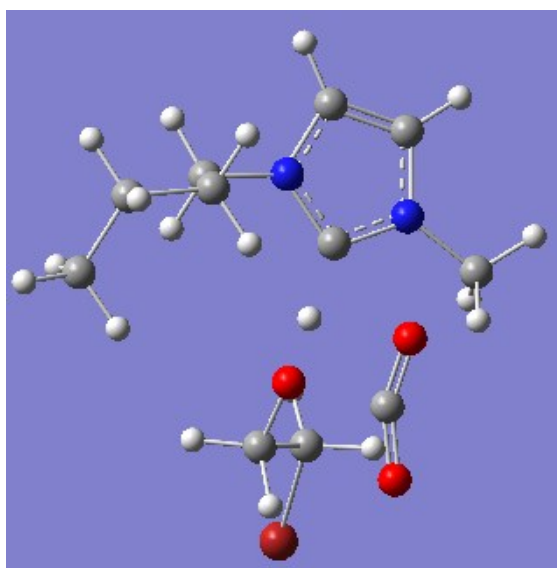
Structure and coordinates of **TS-B1**



C	-2.26307900	-0.77840500	-0.44729200
C	-0.68214100	0.38523600	0.72638500
C	-1.72510800	1.22584600	0.51232500
N	-2.66185700	0.50132700	-0.20447900
H	-3.79155400	-2.06811000	0.07994000
H	0.25964300	0.53631400	1.23303200
H	-1.87420600	2.25734200	0.79699900
N	-1.03123900	-0.81610000	0.13446100
C	-3.99737300	0.99616100	-0.52174100
C	-4.91920200	0.95576300	0.69774900
H	-4.37446300	0.36200700	-1.32734600
H	-3.90500900	2.01938700	-0.90742800
C	-6.27793600	1.60873800	0.43813300
H	-5.05797900	-0.09261700	0.99165500
H	-4.41886600	1.46441200	1.53343600

H	-6.85710100	1.58256000	1.36831400
H	-6.13576200	2.67046800	0.19306400
C	-7.07552500	0.92433600	-0.67308400
H	-8.08709000	1.33583200	-0.74168700
H	-6.60372000	1.05500900	-1.65269000
H	-7.15976000	-0.15184700	-0.48336200
C	-0.18067200	-1.99459500	0.14962400
H	0.01166700	-2.30662500	1.18081900
H	-0.70432000	-2.78763100	-0.38460400
H	0.76717200	-1.78419000	-0.35345700
O	-4.29313000	-2.48763800	0.81506500
C	-3.35970100	-2.72746200	1.84055700
H	-3.77109900	-3.49587200	2.50165600
H	-2.41019500	-3.10469600	1.43785800
C	-3.10297200	-1.45568100	2.64085600
H	-3.97618200	-1.16802200	3.22718000
Br	-1.65178000	-1.76520000	3.90176700
H	-2.78749300	-0.62065300	2.01955700

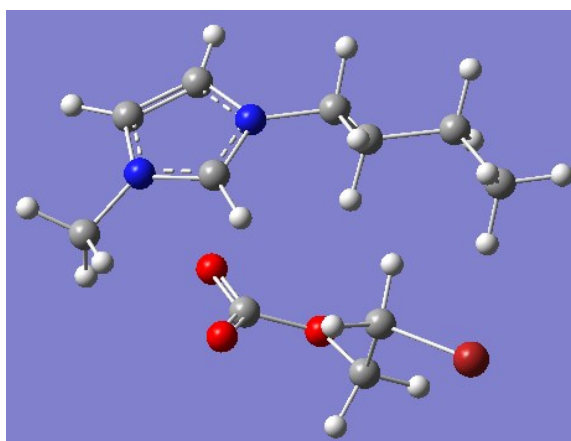
Structure and coordinates of **TS-B2**



O	2.75229500	0.82808700	2.96264900
C	1.39897400	0.68422800	2.62292900
H	0.90159200	0.07833500	3.38906000
H	0.90595400	1.66599100	2.58604200
C	1.28043900	-0.01240200	1.27163300
H	1.81830000	-0.96282100	1.29482500
Br	-0.56470100	-0.43754600	0.86035200
H	1.65023600	0.60394600	0.45078500
C	3.55473500	-0.69610000	3.73756700
O	4.71374200	-0.45749900	3.59828500

O	2.65307100	-1.38752800	4.07567300
C	4.48681000	1.26584500	1.10838800
C	6.23778600	1.11491100	-0.28885200
C	6.15162700	2.40759500	0.12349600
N	5.06558900	2.47168600	0.97212400
H	3.51119500	1.02208000	2.02288700
H	6.93099400	0.62808300	-0.95779500
H	6.75764300	3.26957800	-0.11104000
N	5.20704200	0.43682200	0.33225600
C	4.64024100	3.62346600	1.77069100
C	5.11516100	3.49290400	3.21590200
H	3.54911200	3.66157000	1.71818800
H	5.03662500	4.52650500	1.29454300
C	4.62282200	4.64035700	4.10060200
H	4.74754100	2.53697300	3.61099400
H	6.21162100	3.44858100	3.22385200
H	5.06061300	4.51053500	5.09648700
H	5.00356100	5.59817300	3.71984100
C	3.09835000	4.69438100	4.22374800
H	2.79262100	5.40823100	4.99450200
H	2.62138300	5.00618800	3.28839100
H	2.69828900	3.70974800	4.49126200
C	4.91696400	-0.98463500	0.19185900
H	4.13987100	-1.14280900	-0.55970100
H	5.82808400	-1.50443700	-0.10801900
H	4.59214600	-1.36680700	1.16067200

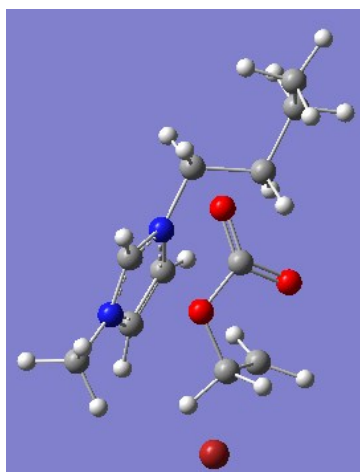
Structure and coordinates of **Int-B2**



O	3.06751900	0.42743300	3.76386400
C	1.66208500	0.46694500	3.62775700
H	1.23942300	-0.53858600	3.53816800
H	1.29291000	0.93783300	4.54310100
C	1.27309600	1.30245600	2.41250700

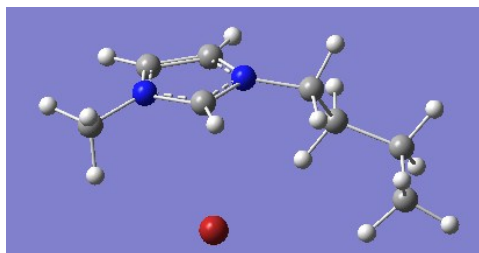
H	1.30298800	0.71398700	1.49947700
Br	-0.53806500	1.99057100	2.57182300
H	1.92449300	2.17381100	2.33630700
C	3.78429400	-0.24319000	2.75259600
O	5.01370700	-0.12923400	2.86355400
O	3.10584800	-0.79167000	1.85339600
C	4.60261800	1.12713400	0.42155400
C	6.76809000	0.78052600	0.37124000
C	6.55773700	2.03617900	0.84788800
N	5.19457100	2.23609100	0.86098200
H	3.53906800	0.93267900	0.40263000
H	7.67938700	0.22454400	0.21646700
H	7.24805200	2.79470500	1.18230500
N	5.53496800	0.23767800	0.09943700
C	4.50977400	3.38251000	1.47084500
C	4.66646000	3.36725000	2.99143300
H	3.46215500	3.31953600	1.16400600
H	4.93035400	4.29391300	1.03207000
C	3.95288900	4.54774000	3.65858000
H	4.29804400	2.41070500	3.38463400
H	5.73777900	3.40524300	3.22521600
H	4.28376900	4.59309900	4.70181000
H	4.27755300	5.48949500	3.19343700
C	2.42665500	4.45267600	3.63123700
H	1.97451600	5.30315000	4.15025400
H	2.02150300	4.44958400	2.61212100
H	2.08543900	3.53914300	4.13141500
C	5.27829600	-1.17691400	-0.16655000
H	4.27572500	-1.28303300	-0.57641300
H	6.02563000	-1.53759100	-0.87492600
H	5.32202900	-1.70147700	0.79004100

Structure and coordinates of **TS-B3**



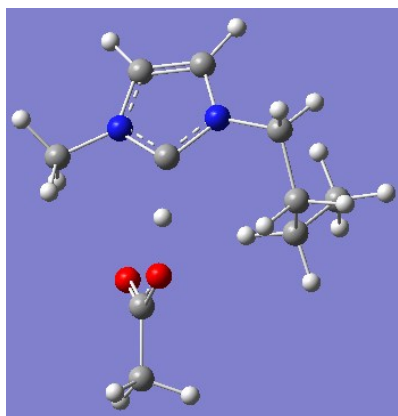
Br	4.79751100	3.50658400	-1.53936200
O	0.15456800	0.02993400	-0.88789800
C	0.77889300	0.96040300	-1.38202900
O	1.34423000	1.05467600	-2.52237200
O	1.01578700	2.06700600	-0.57625900
C	1.81222100	3.01878700	-1.27359100
H	2.27753300	3.65352100	-0.52409400
C	2.81471800	2.25589700	-2.11426200
H	2.96186100	2.48818200	-3.15752900
H	3.34384300	1.40319200	-1.71757600
H	1.18481700	3.62970800	-1.93108600
C	2.70465400	0.08501400	0.63908500
C	4.81378200	0.59681000	0.24542700
C	4.53501100	-0.57384500	-0.39151500
N	3.21222600	-0.87398400	-0.13227400
H	1.66954500	0.14631200	0.94958800
H	5.70361500	1.20671300	0.26016400
H	5.15203300	-1.19619000	-1.01999800
N	3.65717300	0.98821900	0.88292700
C	2.45671400	-2.02539900	-0.66089500
C	2.49882500	-2.06951100	-2.18438300
H	1.43031400	-1.89245400	-0.31457300
H	2.88218500	-2.93169100	-0.21550300
C	1.65913400	-3.22634500	-2.73484500
H	2.11504400	-1.11738900	-2.57021200
H	3.53782900	-2.17933400	-2.52183800
H	1.80156800	-3.25265400	-3.82087900
H	2.04209100	-4.18258500	-2.35124000
C	0.16731200	-3.09023200	-2.42520900
H	-0.40756900	-3.85410000	-2.95773800
H	-0.04534600	-3.20695200	-1.35732600
H	-0.20119200	-2.10273700	-2.71969700
C	3.47997000	2.22440500	1.64467400
H	3.97636400	3.02749800	1.09387800
H	2.41020400	2.42662600	1.71596400
H	3.91439900	2.10934800	2.63952800

Structure and coordinates of **BminBr**



C	-1.87498100	-0.29652500	-0.52648300
C	-0.18015700	0.75605100	0.39277200
C	-1.24913700	1.59307200	0.40411100
N	-2.29136400	0.93026100	-0.21372800
H	-2.47471900	-1.05977200	-0.99549000
H	0.82051200	0.88000600	0.77551500
H	-1.35746900	2.59123700	0.79658800
N	-0.57550400	-0.40339800	-0.24374600
C	-3.70822200	1.31745500	-0.19307600
C	-4.13577700	1.78224800	1.19750300
H	-4.25771000	0.41501100	-0.47163600
H	-3.87876200	2.08692900	-0.95376000
C	-5.65986800	1.86235600	1.33050500
H	-3.74361700	1.05861000	1.92163500
H	-3.69258900	2.76354500	1.41028500
H	-5.88210800	2.26609700	2.32462600
H	-6.06987400	2.58187000	0.60776900
C	-6.34340700	0.50098800	1.17413300
H	-7.38377100	0.54766100	1.51005500
H	-6.35810100	0.16516100	0.13151000
H	-5.81882800	-0.26414600	1.75719900
C	0.12656300	-1.68101000	-0.20582000
H	1.18799200	-1.48995400	-0.04761200
H	-0.29976500	-2.26591200	0.61698800
H	-0.01095700	-2.20005300	-1.15552000
Br	-2.84284800	-1.60669800	1.80665500

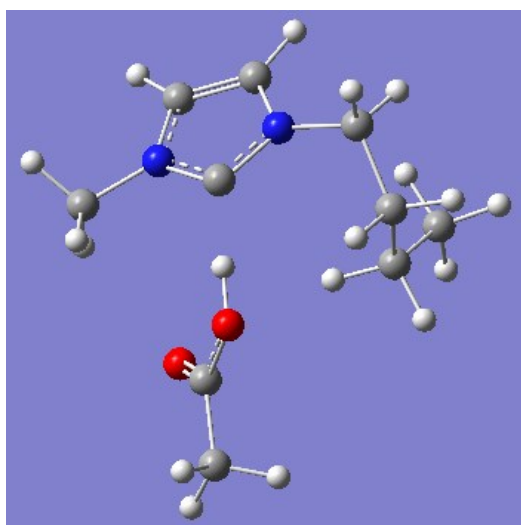
Structure and coordinates of **TS-O1a**



C	-0.53382900	-0.52697200	-0.27799400
C	-1.99599200	-1.68929200	-1.52607000
C	-2.70853100	-0.82011000	-0.76332500
N	-1.78927400	-0.11707800	-0.00824800
H	-2.31316800	-2.41526300	-2.25932500
H	-3.77119000	-0.64411200	-0.69077700

N	-0.66886400	-1.49032500	-1.20667500
C	-2.12624500	0.92274200	0.96935000
C	-1.09140600	2.04526300	1.00242300
H	-2.21998600	0.45679400	1.95569300
H	-3.11026300	1.30944300	0.68700400
C	-0.83753900	2.70872200	-0.35422100
H	-1.46571000	2.79062300	1.71671700
H	-0.14557800	1.66412000	1.40169200
H	-0.12883200	3.52996700	-0.19476600
H	-0.33414000	2.00573400	-1.02894700
C	-2.10464400	3.24416300	-1.02036200
H	-2.77089100	2.43151300	-1.33435400
H	-2.66772000	3.89903900	-0.34330700
H	-1.85945300	3.82059300	-1.91716300
C	0.45906400	-2.14158200	-1.86309600
H	1.33279000	-2.04067800	-1.22016300
H	0.22270800	-3.19742100	-2.01208900
H	0.67172000	-1.64431200	-2.81070300
H	0.65490200	0.02731100	0.03446800
C	2.22053000	0.90920700	-0.99383100
O	1.75685500	0.59589100	0.17821200
O	1.68118700	0.59638100	-2.05905600
C	3.49794700	1.72781600	-0.96883900
H	4.23332500	1.25512900	-0.31221500
H	3.90017100	1.83757000	-1.97654500
H	3.27830900	2.71678200	-0.55293800

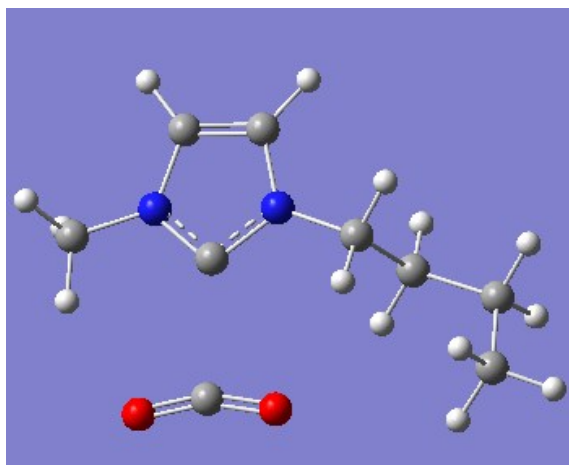
Structure and coordinates of **Int-O1a**



C	-0.27688200	-0.47489200	-0.23037700
C	-1.75095800	-1.56053300	-1.57058700
C	-2.46301800	-0.70504800	-0.79471000

N	-1.54418100	-0.05619900	0.01008500
H	-2.06468200	-2.25009500	-2.33992800
H	-3.52338000	-0.50672500	-0.74414100
N	-0.42822000	-1.40217600	-1.20433200
C	-1.89040600	0.95481500	1.01012100
C	-0.91546700	2.13135200	1.01505600
H	-1.91986400	0.48096700	1.99705200
H	-2.90395600	1.29559000	0.77611100
C	-0.70902100	2.78211100	-0.35560400
H	-1.31706600	2.87064100	1.72112500
H	0.05062700	1.80312400	1.41203000
H	-0.05846000	3.65451900	-0.22038100
H	-0.16438200	2.09290700	-1.01255600
C	-2.01141900	3.21042200	-1.03078700
H	-2.61849100	2.34294800	-1.31488500
H	-2.61545600	3.84403800	-0.36922900
H	-1.81030400	3.77640600	-1.94524700
C	0.68663000	-2.07562400	-1.85368200
H	1.56965000	-1.95186200	-1.22785700
H	0.45533400	-3.13793400	-1.96508800
H	0.88595700	-1.62032700	-2.82585800
H	1.18339100	0.24462100	0.10010500
C	2.62541800	1.02361300	-0.95779300
O	2.09023700	0.76942400	0.22312900
O	2.14841100	0.64836900	-2.01645400
C	3.89578000	1.83567300	-0.86352100
H	4.60383200	1.34051600	-0.19331100
H	4.33343100	1.95895300	-1.85389900
H	3.66831700	2.81536200	-0.43236000

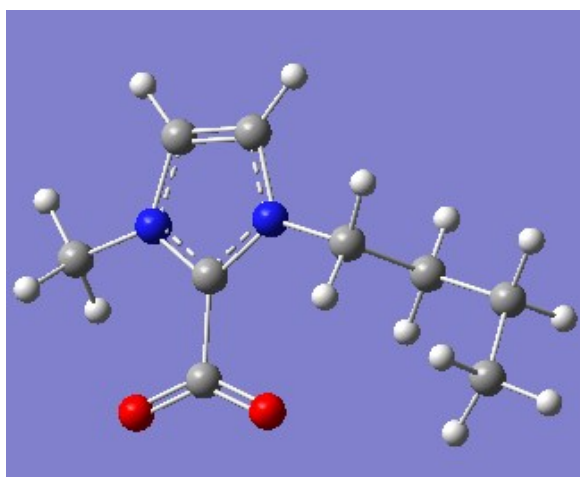
Structure and coordinates of **TS-O2a**



C	-1.96650300	-0.48889300	0.27890200
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C	-0.36769700	0.38502900	-1.08041300
C	-1.49015100	1.12994700	-1.24238600
N	-2.44658200	0.57416900	-0.41297100
H	0.60711800	0.45929100	-1.53919100
H	-1.69145200	1.98566600	-1.87011000
N	-0.68448000	-0.58976800	-0.15136900
C	-3.79289900	1.11203200	-0.23004700
C	-3.84211700	2.13255100	0.90331600
H	-4.44810200	0.26564800	-0.02126800
H	-4.10277400	1.56684900	-1.17854400
C	-5.23233900	2.74486100	1.08795700
H	-3.53090700	1.62859300	1.82702900
H	-3.10779700	2.92327400	0.69991100
H	-5.16627400	3.52592000	1.85452100
H	-5.53715700	3.25002400	0.16064600
C	-6.29553100	1.72480100	1.49784700
H	-7.24618200	2.21953400	1.72019200
H	-6.48496100	0.99021500	0.70839900
H	-5.98048400	1.17099900	2.38859200
C	0.24345000	-1.61478900	0.30249900
H	-0.26879900	-2.22310900	1.04681800
H	0.55026800	-2.24147500	-0.53914500
H	1.12540300	-1.14886100	0.75001900
C	-3.06873700	-1.65792400	1.94460300
O	-4.08191900	-1.05667700	1.97431400
O	-2.25683400	-2.46393300	2.22342700

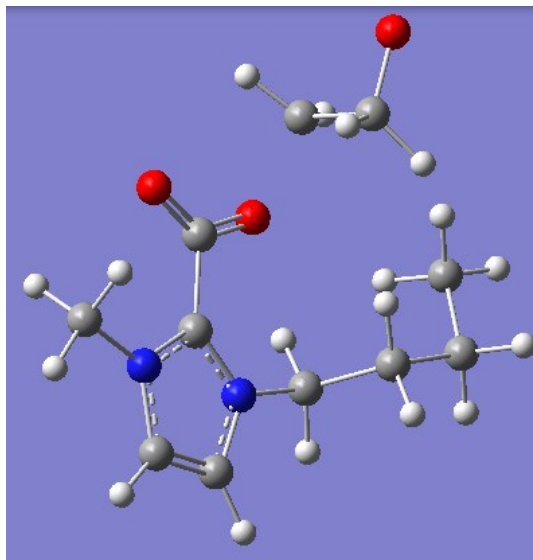
Structure and coordinates of **Int-O2a**



C	3.17918500	0.66820900	1.96597000
O	2.87841700	-0.50545200	1.72231700
O	2.71947400	1.54481000	2.70799900
C	4.43239800	1.13950600	1.14695200

C	6.19791600	1.11097900	-0.20296400
C	6.05807600	2.37728900	0.27322200
N	4.96014100	2.37543400	1.10044500
H	6.92059200	0.68478300	-0.88140000
H	6.63347900	3.27222400	0.09169700
N	5.18416400	0.36128300	0.34620000
C	4.49586700	3.55567600	1.85059900
C	5.07433500	3.57413000	3.26083700
H	3.40915800	3.50878600	1.87844600
H	4.81818000	4.42959900	1.27409000
C	4.59625000	4.78845800	4.06063100
H	4.75138600	2.65583700	3.76385200
H	6.17107000	3.56609500	3.20263400
H	5.07427100	4.75247500	5.04638000
H	4.94776600	5.71338800	3.58211800
C	3.07623500	4.83068100	4.23309500
H	2.78817900	5.59471600	4.96165200
H	2.56529600	5.06691900	3.29416700
H	2.69632500	3.86188200	4.57389700
C	4.98225700	-1.06685100	0.07397600
H	4.01193900	-1.21764600	-0.39497500
H	5.79204700	-1.38279200	-0.58534000
H	4.99980400	-1.62429100	1.00834100

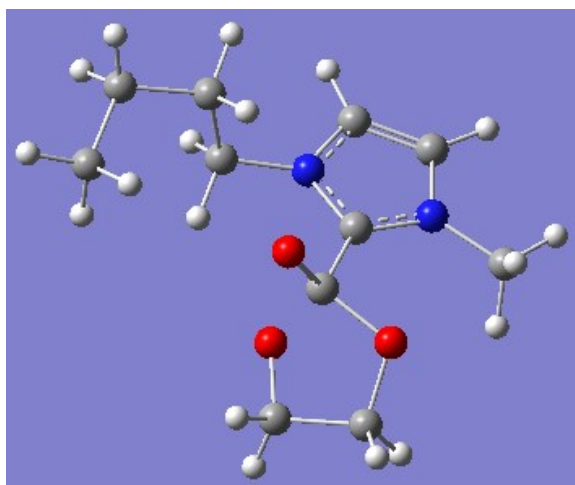
Structure and coordinates of **TS-O3a**



C	-3.15469000	-0.98998600	1.43927100
C	-2.05379700	-1.99858100	1.40559100
O	-2.93543900	-0.69674000	2.73519200
H	-2.98225700	-0.17257100	0.69953000
H	-4.14579400	-1.44322700	1.19365400

H	-1.06085000	-1.57368600	1.49528200
H	-2.23512500	-2.87916000	2.01088900
C	-1.38108000	-2.14898800	-1.06004200
O	-0.52849100	-1.27810300	-1.02109500
O	-1.93400900	-2.81530100	-0.11997600
C	-1.91484700	-2.52771700	-2.43388200
C	-2.18431000	-2.53773900	-4.63019700
C	-3.03988900	-3.45303100	-4.09699600
N	-2.85529100	-3.43856000	-2.73773300
H	-2.00820200	-2.24380200	-5.65334100
H	-3.75673100	-4.11083500	-4.56416300
N	-1.49379400	-1.97526400	-3.58627800
C	-3.64835400	-4.26160700	-1.79974500
C	-4.81799500	-3.47183000	-1.22163600
H	-2.97254900	-4.60707300	-1.02062000
H	-3.99732100	-5.11962400	-2.38270000
C	-5.61048600	-4.29652700	-0.20307200
H	-4.42822100	-2.57076100	-0.73367600
H	-5.47155800	-3.15363300	-2.04454200
H	-6.51098000	-3.73076100	0.05961300
H	-5.95700900	-5.22907500	-0.67073400
C	-4.82413200	-4.60197900	1.07270900
H	-5.44514300	-5.15146100	1.78624200
H	-3.93439400	-5.21059600	0.87737000
H	-4.49707700	-3.67524400	1.55515300
C	-0.47418600	-0.92824700	-3.74480800
H	0.47966700	-1.28183700	-3.35757000
H	-0.40320300	-0.71446600	-4.81140700
H	-0.77054100	-0.04034400	-3.18938500

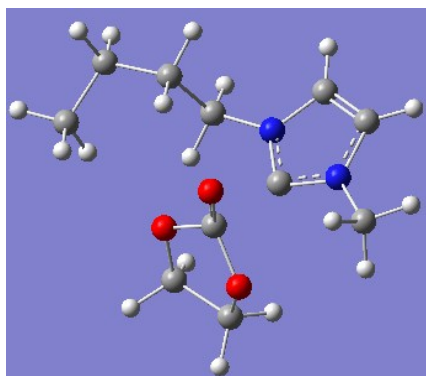
Structure and coordinates of **Int-O3a**



C	3.20903900	0.69106900	2.24979400
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O	2.98761700	-0.74370900	2.05710800
O	3.53891000	1.06326000	3.40800000
C	4.26533800	1.10210800	1.18804500
C	5.88819800	1.18010800	-0.32623600
C	5.69016000	2.44110900	0.13545100
N	4.68115200	2.36995300	1.06917700
H	6.57749400	0.79097600	-1.05907600
H	6.17025600	3.37466500	-0.11493600
N	4.99313500	0.36092200	0.33756500
C	4.19470100	3.49647300	1.88032300
C	5.11242400	3.74836200	3.07220200
H	3.18830400	3.23128100	2.20338800
H	4.14142600	4.36586800	1.21537400
C	4.55019900	4.82308200	4.00592000
H	5.20417200	2.80060200	3.61442400
H	6.10720400	4.04398100	2.71122700
H	5.29716800	5.01926300	4.78402500
H	4.42100500	5.76809800	3.45888700
C	3.23154600	4.40966400	4.66397900
H	2.94677200	5.12165200	5.44532900
H	2.40898100	4.36678600	3.94279400
H	3.31933500	3.41256400	5.10701300
C	4.89602800	-1.08349100	0.11452500
H	3.90567200	-1.33361700	-0.26385100
H	5.65955600	-1.34669100	-0.61900700
H	5.06161800	-1.61403500	1.04999400
C	1.60087900	-0.99259800	1.92415100
H	1.28275200	-1.73623100	2.66175100
H	1.39162600	-1.37372300	0.91365700
C	0.95706600	0.38087700	2.14177000
H	0.05562400	0.54051400	1.54560600
H	0.74021500	0.55708300	3.20293400
O	1.96806100	1.25754700	1.69383800

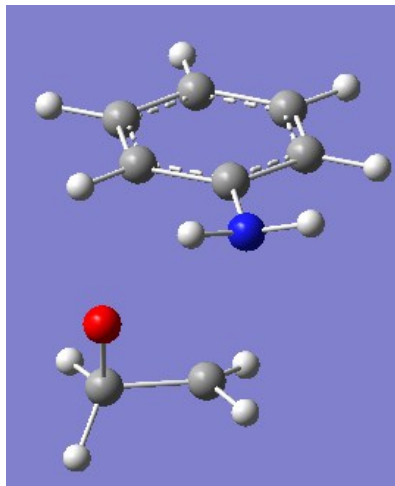
Structure and coordinates of **TS-O4a**



C	3.84450400	0.19057700	2.76831300
O	3.06683500	-0.91725900	2.42128500
O	4.98774600	0.05574000	3.16685400
C	4.10997000	1.00843600	1.00152700
C	5.53497400	1.16912800	-0.73912800
C	5.27425000	2.42964800	-0.30822400
N	4.39441300	2.30480900	0.75129500
H	6.15516400	0.80901400	-1.54597000
H	5.62101900	3.38856400	-0.66308000
N	4.80880900	0.32022500	0.07323100
C	3.96180200	3.41268000	1.60173900
C	4.93498300	3.64600200	2.75468100
H	2.97046600	3.15842800	1.97722600
H	3.87254900	4.30343100	0.96888200
C	4.43990200	4.72414700	3.72174400
H	5.07086200	2.69570000	3.28536200
H	5.91085400	3.93103100	2.33987400
H	5.23396500	4.91972800	4.45147600
H	4.28055600	5.66788400	3.18059100
C	3.16422000	4.32774400	4.46837600
H	2.91283100	5.07022600	5.23249100
H	2.30292300	4.24805500	3.79537600
H	3.29063000	3.35490700	4.95379900
C	4.89363000	-1.13584700	0.05098200
H	3.90000900	-1.56669600	-0.07648300
H	5.53392900	-1.43106200	-0.78168600
H	5.31515500	-1.48108100	0.99748300
C	1.75998600	-0.46687300	2.14427700
H	1.05336300	-1.22027800	2.49777500
H	1.63194900	-0.32119400	1.06367600
C	1.66083300	0.87419400	2.90744600
H	1.32996100	1.68841400	2.24955000
H	0.99964200	0.82688300	3.77661200
O	2.97743700	1.11414500	3.36327200

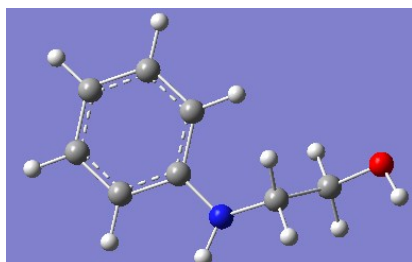
Cartesian coordinates of structures in Figure 2

Structure and coordinates of **TS-N1**



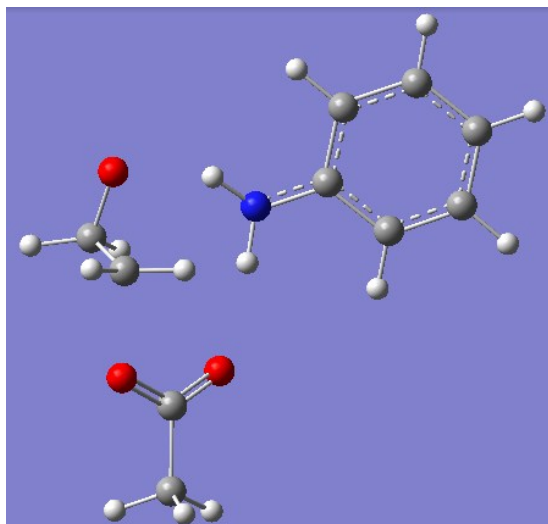
O	1.61577300	1.39341500	-1.44237700
C	2.86087700	1.99613500	-1.44221600
H	3.53460900	1.67341300	-2.25614400
C	2.25434900	3.30348800	-1.69908000
H	1.67547900	3.73682700	-0.89076100
H	2.55822100	3.96746100	-2.50458600
H	3.40988100	1.92966600	-0.48635800
H	0.49797100	2.14238000	-2.64225100
C	1.18756900	2.87797500	-4.44900100
C	1.90300600	1.71308700	-4.75996500
C	2.52969100	1.60133600	-5.99681000
C	2.46095900	2.63925900	-6.92744200
C	1.75756700	3.79972000	-6.60908800
C	1.12669500	3.92565200	-5.37388500
H	1.94819700	0.91252700	-4.02417400
H	3.07580700	0.69341000	-6.23606500
H	2.94985800	2.54308200	-7.89181900
H	1.69564300	4.61376700	-7.32557700
H	0.57657400	4.83123800	-5.12759700
N	0.62827300	3.01275600	-3.17088500
H	-0.12592600	3.68690800	-3.08598900

Structure and coordinates of **Pro-C2**



H	2.34432600	-1.00035900	-2.14761800
O	1.91915700	-1.77376800	-1.75230300
C	0.51367500	-1.61394100	-1.80629600
H	0.09303100	-2.40182000	-1.17567000
H	0.19663300	-0.65111900	-1.38283200
C	-0.01871000	-1.74393800	-3.23497100
H	0.37449600	-2.66611700	-3.68581700
H	0.35750700	-0.90842600	-3.83724900
C	-2.52136300	-5.20577500	-2.59762300
C	-1.70463800	-4.08095800	-2.70731600
C	-2.23603700	-2.86581400	-3.16494200
C	-3.59997400	-2.81583600	-3.50237900
C	-4.40164100	-3.94264600	-3.38722700
C	-3.87070300	-5.15180400	-2.93286800
H	-2.08735900	-6.13598500	-2.24106500
H	-0.65763300	-4.15672500	-2.43205900
H	-4.02513900	-1.87816900	-3.85456000
H	-5.45204700	-3.87617800	-3.65738800
H	-4.49871400	-6.03245400	-2.84473000
N	-1.46689600	-1.71088900	-3.26997000
H	-1.87725500	-0.98943000	-3.84491800

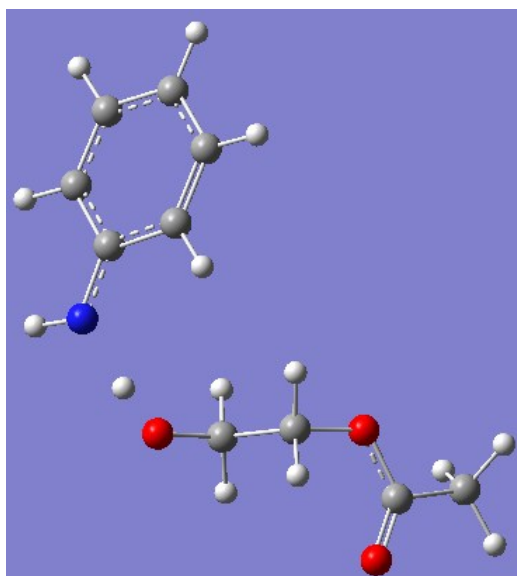
Structure and coordinates of **TS-O4**



C	-2.27502500	-0.61402800	1.83603500
C	-2.00034900	-1.91981200	1.24662900
O	-1.26255200	-1.00885500	2.70433200
H	-2.05716900	0.25624000	1.19675100
H	-3.27251700	-0.50238400	2.29026100
H	-1.08410200	-2.03790300	0.68840400
H	-2.40920600	-2.78418500	1.75130200
C	-2.65723700	-1.62053200	-1.34459500

O	-3.07454700	-2.24527000	-0.30837100
O	-1.66159500	-0.88175900	-1.41569100
C	-3.50045300	-1.85579600	-2.59998900
H	-3.44068500	-2.91237900	-2.88126300
H	-4.55024500	-1.63260500	-2.38713100
H	-3.14262900	-1.23528900	-3.42410500
N	0.43745000	0.02376400	0.57963600
C	1.76218800	-0.10519900	0.27165500
C	2.74752400	-0.19054200	1.27923500
C	2.19729400	-0.11507400	-1.07193400
C	4.09590800	-0.26921700	0.95198300
H	2.42929100	-0.19461700	2.31904200
C	3.54884400	-0.19263900	-1.38253300
H	1.44818800	-0.06508800	-1.85896000
C	4.51904500	-0.26834200	-0.37942500
H	4.82986500	-0.33582100	1.75290700
H	3.85018600	-0.19882700	-2.42832400
H	5.57465800	-0.32980900	-0.62828300
H	-0.23391000	-0.17598900	-0.16326700
H	0.11192800	-0.27365900	1.50802700

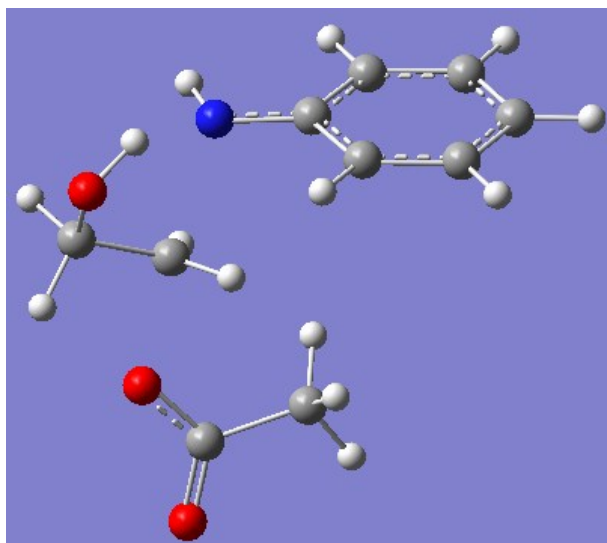
Structure and coordinates of **Int-O4**



H	-2.15843800	-0.50739000	2.26758900
N	-0.75296100	0.07599600	2.60136600
C	-0.50781300	1.22531200	3.24347600
C	-1.57942700	2.13624700	3.52264000
C	0.78083000	1.65393900	3.70234400
C	-1.37599200	3.32918400	4.19513600
H	-2.57222900	1.86135800	3.17099100
C	0.96469400	2.85470600	4.37339200

H	1.63536300	1.00396900	3.51290400
C	-0.10326000	3.71946700	4.63900200
H	-2.23079900	3.98014400	4.37913900
H	1.96951400	3.12523200	4.69910500
H	0.04785300	4.65824400	5.16429000
H	0.09853100	-0.47040800	2.48128300
O	-3.12005000	-0.91456400	2.20982100
C	-3.54704200	-1.10699200	3.51987400
H	-3.72641300	-2.17461900	3.73840500
H	-2.80047200	-0.73403000	4.24028700
C	-4.85511700	-0.35163700	3.72648500
H	-5.62144500	-0.70860800	3.03481400
H	-4.69862400	0.72033100	3.59412100
C	-6.13842300	-1.52119100	5.36265700
O	-5.32684700	-0.50093700	5.08632200
O	-6.57512500	-2.30478000	4.54919600
C	-6.44791700	-1.57273900	6.84089900
H	-6.80389200	-0.59848800	7.18534600
H	-7.19779000	-2.34135700	7.02821800
H	-5.53208300	-1.80389200	7.39261300

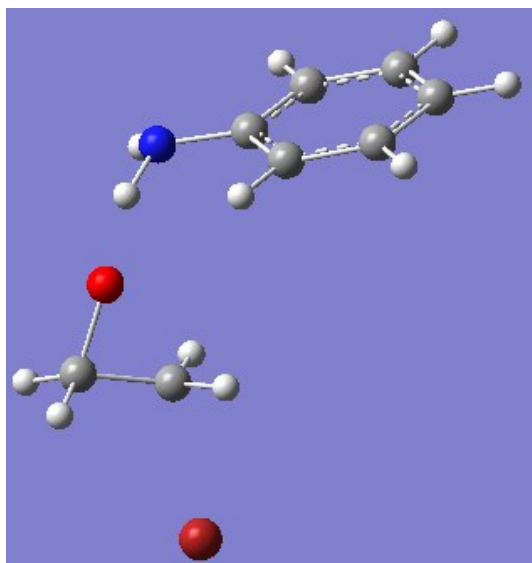
Structure and coordinates of **TS-O5**



O	0.95152800	2.26443300	-0.26247400
C	2.28132900	1.83536700	-0.44107900
H	2.31433300	0.82539500	-0.88228900
C	3.07183500	2.78003000	-1.33190700
H	2.92387200	3.84598900	-1.22438200
H	3.71826400	2.41382800	-2.11522800
H	2.75740500	1.79648200	0.53914300
H	0.69368800	2.53295800	-1.17655100
C	2.17479000	5.29158700	-5.49474100

C	2.07016200	4.07356200	-4.83281000
C	1.68294300	3.99584400	-3.46942300
C	1.41802800	5.23244900	-2.82147600
C	1.53755200	6.44307300	-3.48968400
C	1.91513800	6.49533000	-4.83553400
H	2.47348600	5.30113900	-6.54173300
H	2.28748800	3.14769000	-5.36414800
H	1.10051400	5.20756500	-1.78082400
H	1.32627400	7.36605600	-2.95278700
H	2.00624000	7.44597600	-5.35293700
N	1.58707200	2.83307700	-2.76065300
C	5.58715200	3.60369200	-0.40781900
O	6.65433600	3.56066000	0.20631800
O	4.59212600	2.80831100	-0.18825900
C	5.39991600	4.67834100	-1.48636200
H	5.07020800	4.25112300	-2.43950600
H	4.62708300	5.39257500	-1.17969400
H	6.34166200	5.21037900	-1.62902900
H	1.78628500	2.03720000	-3.36913800

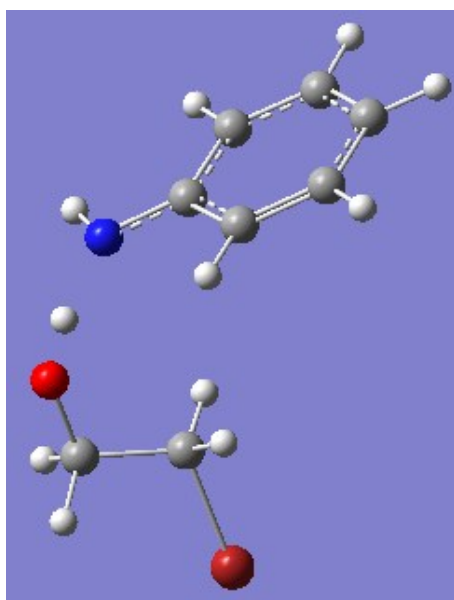
Structure and coordinates of **TS-B4**



Br	-1.89347700	-3.62783200	0.47373200
C	-2.04644900	-0.43153800	0.81556100
C	-1.10464600	-1.46596700	1.22762700
O	-1.15741400	0.39337100	1.49124500
H	-2.12273500	-0.27459000	-0.27088300
H	-3.04969800	-0.51062100	1.25760900
H	-0.17055800	-1.55211800	0.68975200
H	-1.11938300	-1.77732700	2.26116500
N	1.49429500	1.04078900	0.86259300

C	2.22230100	0.46952500	1.88993000
C	1.58986600	0.15647200	3.10989600
C	3.60348400	0.23277800	1.77422100
C	2.32888100	-0.35958400	4.16671800
H	0.51733700	0.31934000	3.18844000
C	4.32900800	-0.28909800	2.84126700
H	4.10459700	0.46735700	0.83667500
C	3.70307300	-0.58912300	4.05051100
H	1.81890900	-0.59841600	5.09738300
H	5.39601300	-0.46530900	2.72177600
H	4.26928100	-1.00099000	4.88105800
H	1.87515200	0.89899500	-0.06392600
H	0.47312100	0.88935000	0.92600300

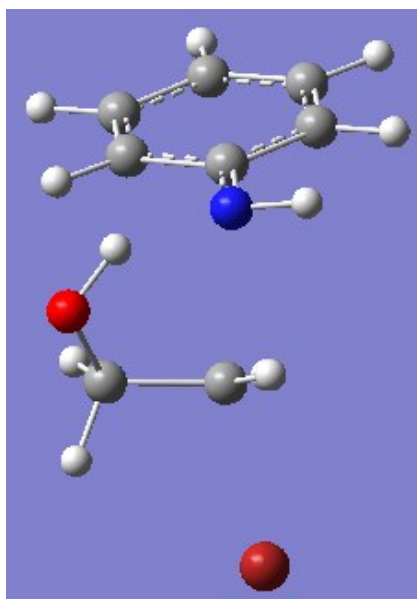
Structure and coordinates of **Int-B4**



H	-2.23421300	-0.55725400	1.87757400
O	-3.20142500	-0.89602700	1.69921600
C	-3.44755700	-1.91284800	2.61656400
H	-4.45343300	-2.31491800	2.43802800
H	-2.73307300	-2.74959100	2.52486800
C	-3.36951500	-1.36569900	4.03915300
H	-4.02322200	-0.50273200	4.16215800
Br	-4.00917000	-2.70569000	5.32504000
H	-2.35071100	-1.10578300	4.32530200
N	-0.83267100	-0.07633600	2.43472000
C	-0.74276200	0.96069100	3.28297600
C	-1.91527100	1.71403100	3.62084100
C	0.46281300	1.39828900	3.91998800
C	-1.86606200	2.79340200	4.48736600

H	-2.84951300	1.43325400	3.13871500
C	0.48884400	2.48116400	4.78796700
H	1.38415500	0.85808900	3.70150400
C	-0.67035300	3.20152100	5.09631700
H	-2.78686100	3.33736200	4.69811200
H	1.43839800	2.77005800	5.23928900
H	-0.64428700	4.04838300	5.77613400
H	0.07802200	-0.50531800	2.27714300

Structure and coordinates of **TS-B5**

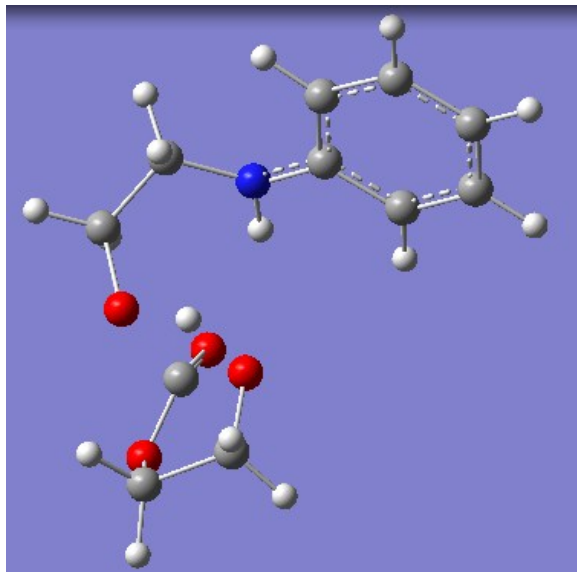


Br	4.03229200	4.54980700	-0.03064800
O	1.73110500	1.15563600	-0.89687300
C	2.87856200	1.93103700	-1.14649600
H	3.44745500	1.54672100	-2.00899600
C	2.53167200	3.38491700	-1.43393800
H	1.71287000	3.83284300	-0.89206400
H	2.93407400	3.90266700	-2.29115000
H	3.51655700	1.86593700	-0.26497400
H	1.09107800	1.49306800	-1.57648400
C	1.33933800	2.64172200	-4.07996500
C	2.03330800	1.46012000	-4.46209600
C	2.51064400	1.28239400	-5.75255900
C	2.32446600	2.25803600	-6.73903100
C	1.64192800	3.42543400	-6.38893600
C	1.16632600	3.61963500	-5.09746200
H	2.16132200	0.67986000	-3.71481100
H	3.03426600	0.36031800	-5.99927800
H	2.70044100	2.11173400	-7.74757300
H	1.48352000	4.20332400	-7.13428800

H	0.64315200	4.54149100	-4.84591600
N	0.90518000	2.78427400	-2.79645800
H	0.36427600	3.64500900	-2.70881800

Cartesian coordinates of structures in Figure 4

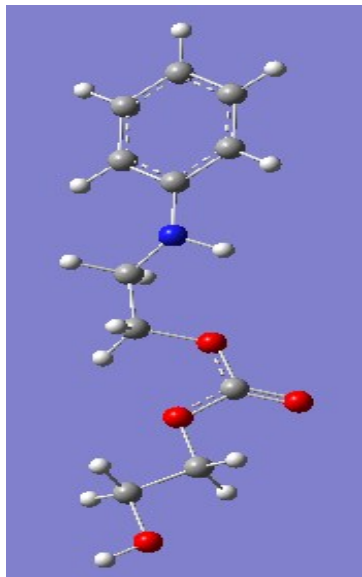
Structure and coordinates of TS-N2



H	-0.85497700	-0.08604900	0.75335300
C	3.67482500	-1.32950700	-1.18503000
C	2.91902700	-1.33760100	-0.01264000
C	2.35907100	-0.14609900	0.47579500
C	2.58893000	1.04590100	-0.23709400
C	3.35042200	1.03890800	-1.39628300
C	3.89868700	-0.14961400	-1.88754600
H	4.10035100	-2.26360800	-1.54245900
H	2.78945000	-2.26691500	0.53369000
H	2.14898900	1.97080300	0.12876100
H	3.51271200	1.97286200	-1.92784300
H	4.49257400	-0.15054200	-2.79587600
N	1.60487200	-0.10954400	1.63224500
H	1.23551100	0.79359900	1.91254600
C	0.98153200	-1.27161800	2.21674400
H	1.61527000	-1.75249900	2.97816600
H	0.78734500	-2.02031100	1.43502800
C	-0.34343100	-0.88475700	2.85449400
H	-0.82044300	-1.75420800	3.31473200
H	-0.19697200	-0.10937900	3.61494200
O	-1.24431800	-0.36901600	1.87571000
C	-2.09919800	1.17004500	-0.55316200
C	-3.21154900	1.03464600	0.49232900
H	-2.16350600	0.41742300	-1.34263400
H	-2.07763800	2.17064800	-0.99290300
H	-3.47251100	-0.01095500	0.68406500
H	-4.10593300	1.61104400	0.25640800

O	-2.63888900	1.60239700	1.66627200
O	-0.90419300	0.99384400	0.19616000
C	-1.33073500	1.30065500	1.78758500
O	-0.53844200	1.87822000	2.47607100

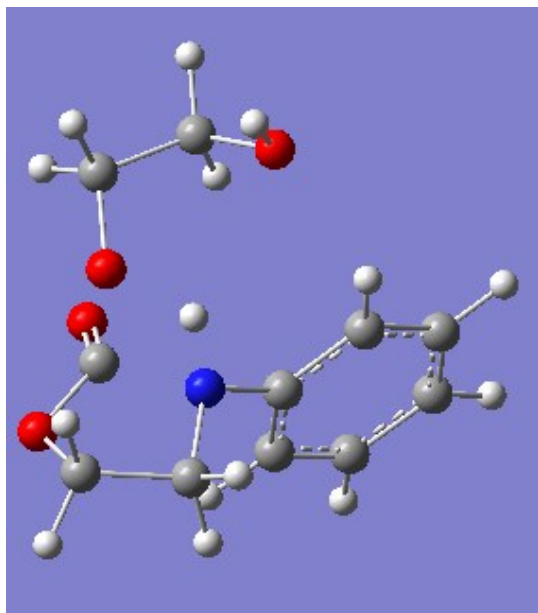
Structure and coordinates of **Int-N2**



C	-6.02797500	-1.89305300	-0.21490500
C	-6.60447100	-0.63886500	-0.04532800
C	-5.76967600	0.47128000	0.10608300
C	-4.39002200	0.32640900	0.09470700
C	-3.80293400	-0.93973500	-0.07350100
C	-4.64175100	-2.05044800	-0.23574400
H	-6.65900800	-2.76884500	-0.34067700
H	-7.68349800	-0.52317700	-0.03398800
H	-6.19879000	1.46088500	0.23669600
H	-3.74710600	1.19407700	0.22556200
H	-4.22350400	-3.04075700	-0.38211200
N	-2.41074100	-1.05173100	-0.03436000
H	-1.93441300	-0.21671300	-0.36046300
C	-1.77011700	-2.26200200	-0.50070200
H	-2.10119700	-3.10887500	0.11126200
H	-2.01222900	-2.49059000	-1.55198100
C	-0.27136900	-2.14452400	-0.33144800
H	-0.01155700	-1.97015900	0.71666700
H	0.23578200	-3.04455000	-0.68983300
O	0.13928100	-1.01301700	-1.11590900
C	1.42281400	-0.63842600	-1.13269900
O	1.80962800	0.32242800	-1.73891500
O	2.19629900	-1.45912800	-0.40476600
C	3.58782200	-1.11342900	-0.37604600

H	3.99072900	-1.11960900	-1.39222700
H	3.71103000	-0.11211700	0.04470500
C	4.26575700	-2.15646900	0.48858000
H	4.11174100	-3.15278100	0.05252000
H	3.82500500	-2.14282800	1.49475700
O	5.63417500	-1.80292600	0.51299400
H	6.12334800	-2.43512900	1.05532200

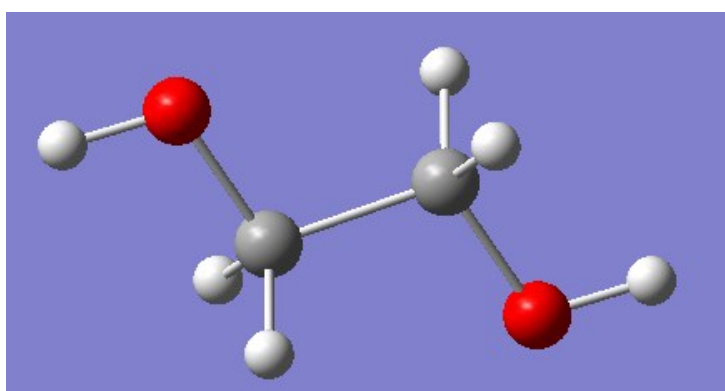
Structure and coordinates of **TS-N3**



N	-0.07673200	-0.72690400	-0.66783900
C	0.02442700	-1.88463700	-1.58196500
H	-0.81821500	-2.55739400	-1.39710700
H	0.01413900	-1.55484100	-2.62266100
C	1.35035200	-2.51645000	-1.14866100
O	1.38789600	-2.30044800	0.25599500
C	0.84713600	-1.09312600	0.55565700
O	0.62907400	-0.68531400	1.66157600
C	2.37787900	1.18604100	0.38421600
H	1.38141300	-3.59245000	-1.32028000
H	2.20928700	-2.02310700	-1.61124500
O	2.03241300	0.08100100	-0.39307900
H	3.32449700	1.60827300	0.00631800
H	2.54337100	0.88324500	1.43078100
C	1.29296300	2.25732800	0.36373800
H	0.38863700	1.88334200	0.85588600
H	1.63090200	3.15564900	0.90002800
O	0.89730400	2.58422500	-0.96678400
H	1.69340300	2.76183400	-1.48877600
H	0.76225400	0.05396500	-0.91610200

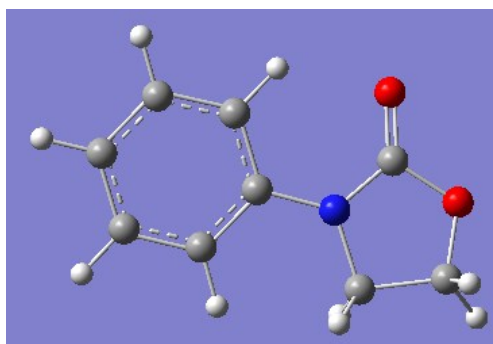
C	-1.40039700	-0.26047400	-0.32917300
C	-1.81928700	0.98323800	-0.78915800
C	-2.22765500	-1.05693200	0.46145100
C	-3.10171400	1.42654500	-0.46463900
H	-1.13488400	1.60227100	-1.36420400
C	-3.50422400	-0.60583100	0.77817800
H	-1.86255400	-2.00647900	0.84482000
C	-3.94392700	0.63439800	0.31189000
H	-3.43614500	2.39788800	-0.81592000
H	-4.15152500	-1.21650200	1.40003600
H	-4.93997600	0.98556700	0.56455500

Structure and coordinates of **Pro-C3**



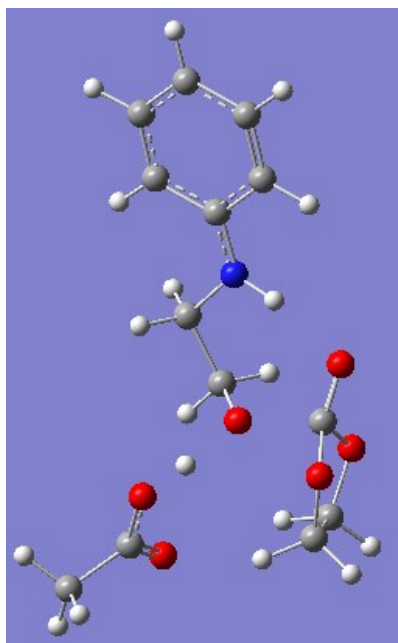
C	0.56915500	-0.49949100	0.00005400
H	0.48976200	-1.13556100	-0.89161300
H	0.48983400	-1.13544100	0.89181200
C	-0.56915500	0.49949100	0.00002700
H	-0.48983500	1.13548500	0.89175300
H	-0.48976100	1.13551600	-0.89167200
O	1.77143500	0.25159100	-0.00004400
H	2.52583600	-0.35122600	0.00005800
O	-1.77143500	-0.25159100	-0.00004200
H	-2.52583600	0.35122600	0.00032200

Structure and coordinates of **Pro-C3**



C	-2.77171700	-1.21757500	-0.16985400
C	-1.37960400	-1.27210400	-0.14967900
C	-0.63086300	-0.10477500	0.04342700
C	-1.29447700	1.11757100	0.22180100
C	-2.68456300	1.15288000	0.19541700
C	-3.43432400	-0.00650100	0.00044200
H	-3.33386400	-2.13423400	-0.32339400
H	-0.88772300	-2.22871900	-0.29042800
H	-0.72487900	2.02520800	0.37048200
H	-3.18532800	2.10674100	0.33360800
H	-4.51889100	0.03468200	-0.01650100
C	1.48089800	-1.46294100	0.02929900
C	2.92140300	-0.99579700	0.24569200
H	1.34283700	-1.94713500	-0.94691300
H	1.14011400	-2.14108500	0.81628900
H	3.20364700	-1.03187700	1.30255500
H	3.65192600	-1.54132300	-0.35158800
N	0.77735800	-0.19327400	0.08556400
O	2.91944300	0.36593400	-0.17748300
C	1.64989300	0.85485700	-0.15815700
O	1.39696900	2.01614200	-0.33529800

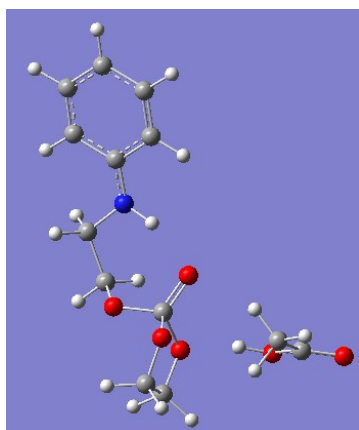
Structure and coordinates of **TS-O6**



H	-0.54254600	-0.24210600	0.88144400
C	6.38109900	-0.43445900	1.21306200
C	5.08833600	0.08610300	1.18019000
C	4.34760900	0.09279300	-0.02164400
C	4.95883800	-0.45923200	-1.17399000
C	6.24330200	-0.97315100	-1.11990600

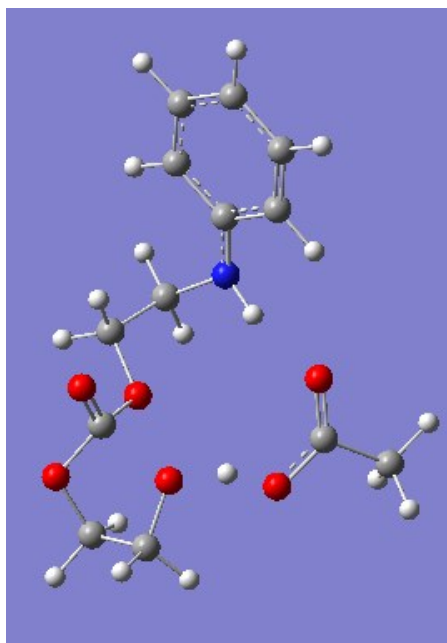
C	6.97814700	-0.96690200	0.07330300
H	6.92655100	-0.42391400	2.15477000
H	4.64779100	0.48851300	2.08689300
H	4.39180600	-0.46945500	-2.10175800
H	6.68218300	-1.38994200	-2.02400900
H	7.98540100	-1.37158700	0.10945600
N	3.09820300	0.62508800	-0.11159400
H	2.54280600	0.42895500	-0.95423600
C	2.33281100	1.03814500	1.03818600
H	2.84082200	1.86570400	1.55934000
H	2.21528300	0.21176100	1.76084000
C	0.95326200	1.50588200	0.58471400
H	0.38974400	1.87910600	1.45537900
H	1.06402500	2.33563200	-0.12826500
O	0.24013200	0.46519900	-0.02276700
C	-2.12992500	0.21291700	-1.48616400
C	-1.79303400	1.71700500	-1.35422000
H	-2.47399800	-0.20154700	-0.53225900
H	-2.87761100	0.00981800	-2.26126400
H	-1.81414300	2.02761200	-0.30451500
H	-2.44682500	2.35786000	-1.95344900
O	-0.48406600	1.81021400	-1.87786600
O	-0.91279500	-0.38917500	-1.88113900
C	0.11775000	0.54761400	-1.73052100
O	1.21827400	0.35208600	-2.24711400
C	-2.03272800	-0.07976700	2.19676200
O	-1.08124500	-0.78593800	1.64140400
O	-2.32101500	1.07237600	1.90540600
C	-2.78239200	-0.85410600	3.26504900
H	-3.52202700	-0.21172100	3.74416400
H	-3.27759900	-1.71513800	2.80537700
H	-2.07667600	-1.24055200	4.00584100

Structure and coordinates of **Int-O6**



H	1.16295300	5.19516700	-2.30896700
C	5.52223700	-1.65109100	1.24283800
C	4.65179900	-0.56485100	1.32072000
C	4.26798700	0.13288300	0.15522500
C	4.78729900	-0.31866200	-1.08231700
C	5.64920100	-1.40073700	-1.13909500
C	6.03299400	-2.08418800	0.02222700
H	5.80072900	-2.16690800	2.15968100
H	4.27036600	-0.25069000	2.28722900
H	4.49204200	0.20570300	-1.98785400
H	6.02864500	-1.72241000	-2.10654100
H	6.70881600	-2.93273000	-0.02928000
N	3.44832100	1.22004200	0.18826700
H	3.04983100	1.58180900	-0.69124400
C	2.71960800	1.60778100	1.36886900
H	3.41107200	1.95253400	2.15582400
H	2.14656000	0.75959100	1.78213900
C	1.75115300	2.73805700	1.04132400
H	1.28776400	3.08662000	1.97406600
H	2.29312300	3.57621900	0.58682500
O	0.72043100	2.29979400	0.18427400
C	-1.42753200	2.83930800	-1.34585800
C	-0.94162100	4.26934200	-0.98282400
H	-1.82339000	2.32312000	-0.46198300
H	-2.18545900	2.83668900	-2.13681200
H	-1.22342300	4.54094000	0.04277200
H	-1.32825400	5.03240500	-1.67056300
O	0.45677200	4.20635400	-1.11808400
O	-0.28008900	2.19328500	-1.83268100
C	0.85559200	2.75821300	-1.18164800
O	1.97308100	2.59574200	-1.73802300
C	1.26799500	5.45726600	-4.22622800
O	1.52759300	6.18100100	-5.16503200
O	1.39444100	5.89949900	-2.97298200
C	0.77198400	4.03736500	-4.37264300
H	1.36829500	3.34841900	-3.76220900
H	-0.25480700	3.96568000	-3.99462300
H	0.79120000	3.75742100	-5.42644500

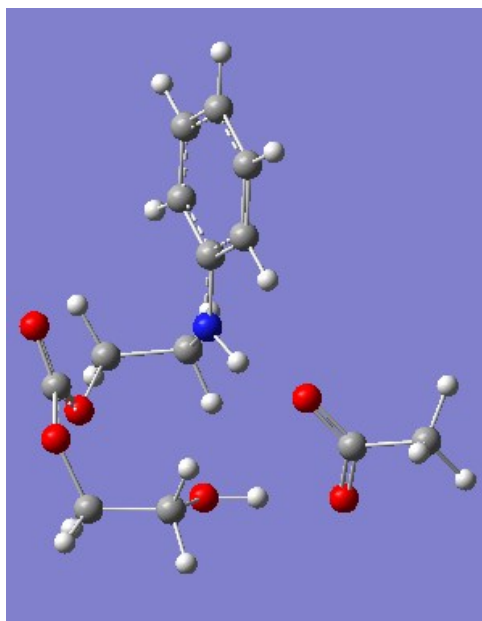
Structure and coordinates of **TS-O7**



C	-2.01657000	-0.37527600	2.86063500
O	-0.88414700	0.05091500	2.64985200
O	-2.87134100	-0.75351900	1.96418300
C	-2.54645200	-0.51157100	4.28025800
H	-1.81594200	-0.12950000	4.99438100
H	-3.49104700	0.03180400	4.37628800
H	-2.75242800	-1.56615200	4.48849700
C	-3.91588500	-1.14047900	-0.74551900
C	-3.51465600	-2.53623400	-1.21583200
H	-4.41039600	-0.58982700	-1.55879000
H	-4.57504500	-1.16529400	0.13280200
H	-4.26572800	-3.02929300	-1.84141800
H	-3.26439800	-3.17363600	-0.35514100
O	-2.37834600	-2.29433400	-2.00807100
O	-2.68895700	-0.54083100	-0.42888400
C	-1.48018000	-1.40082100	-1.36817500
O	-0.80578900	-0.67469000	-2.07631300
H	-2.59345500	-0.63020100	0.86164300
O	-0.90025000	-2.05337200	-0.24868300
C	0.40871300	-2.52550600	-0.50228800
H	0.36702200	-3.45360700	-1.09653800
H	0.97394700	-1.77079100	-1.06093000
C	1.05257900	-2.78885100	0.85201300
H	1.97289400	-3.37148600	0.72998400
H	0.36786200	-3.39913100	1.45239200
C	4.58910500	-0.30795100	0.33303500
C	3.51347500	-1.17167100	0.53882300
C	2.39819800	-0.75843700	1.29136500

C	2.39723700	0.55972100	1.79938000
C	3.47260600	1.40578700	1.58261500
C	4.58892300	0.98343800	0.85136400
H	5.43512000	-0.65547900	-0.25630500
H	3.54337500	-2.16341800	0.09952700
H	1.52452400	0.89393200	2.35511800
H	3.43664700	2.41686400	1.98221500
H	5.42662700	1.65287800	0.67811700
N	1.33458400	-1.58221800	1.60040700
H	0.49577000	-1.07102300	1.87879400

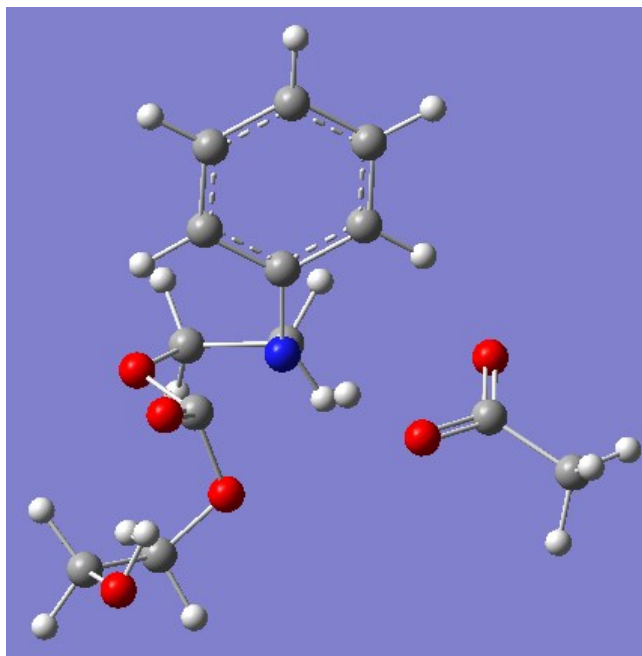
Structure and coordinates of **Int-O7**



C	-1.03278500	-3.18022100	1.30659600
C	-2.29958800	-3.80211300	0.73636300
H	-1.19843200	-2.10538700	1.47860200
H	-0.85559700	-3.65118700	2.28949200
H	-2.98141700	-4.06741200	1.54848300
H	-2.05228000	-4.69591600	0.15735100
O	-3.09816300	-2.90219100	-0.05692100
O	0.06125000	-3.39875300	0.45766200
C	-2.76649300	-2.60341600	-1.31514400
O	-3.36544600	-1.77489000	-1.95200700
O	-1.77701600	-3.38209300	-1.77711200
C	-1.03643400	-2.86952600	-2.88470400
H	-0.71410500	-3.74272600	-3.45951800
H	-1.69567300	-2.24485100	-3.49341000
C	0.17071600	-2.10053400	-2.34915200
H	0.79728700	-1.78763200	-3.20154900
H	0.74706900	-2.78288500	-1.72143600

C	-1.00969200	1.75192800	-3.90659300
C	-0.71065000	0.47629800	-3.42827500
C	-0.49284300	0.25868000	-2.05424500
C	-0.58207800	1.36950600	-1.18389000
C	-0.88234400	2.62807900	-1.67841300
C	-1.10144600	2.84062100	-3.04563500
H	-1.17925200	1.88646100	-4.97304600
H	-0.66263900	-0.35130500	-4.12872500
H	-0.38958600	1.20555900	-0.12635100
H	-0.94252000	3.46411700	-0.98474400
H	-1.33969000	3.83075400	-3.42410800
N	-0.20634300	-0.97927700	-1.52995200
H	0.09653100	-0.99331600	-0.54921500
H	0.84634200	-2.94334600	0.88235500
C	1.64579400	-0.89906300	1.77607300
O	0.66472200	-0.39266500	1.17662500
O	2.00142900	-2.10896500	1.73233800
C	2.47328800	0.04242300	2.65896100
H	2.72547800	0.94686700	2.09723100
H	1.86497900	0.34920300	3.51706500
H	3.38158500	-0.44731300	3.01707700

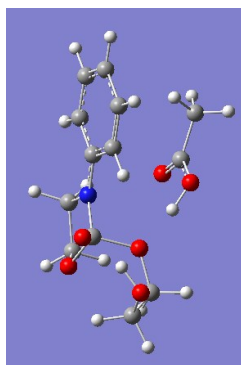
Structure and coordinates of **TS-O8**



N	0.12285700	-0.08339100	-0.41229600
C	0.47013500	-1.13794100	-1.39168200
H	-0.38113000	-1.34956300	-2.03932000
H	1.28812200	-0.76146900	-2.00582800
C	0.89954200	-2.33224000	-0.50451600

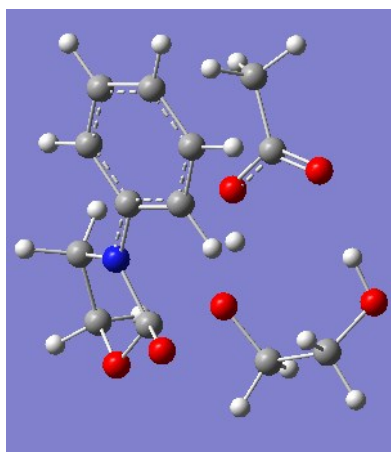
O	0.97546100	-1.85485600	0.81937500
C	1.07512700	-0.40326500	0.81432000
O	0.79074700	0.14705300	1.90665200
C	3.47434600	-0.62821100	0.82625800
H	0.16402800	-3.14488900	-0.52608000
H	1.86973300	-2.72710000	-0.83803700
O	2.33075700	-0.06695200	0.20942400
H	4.31549700	-0.07619600	0.39315500
H	3.57365100	-1.69380700	0.55623900
C	3.51288800	-0.50645000	2.34949300
H	2.78986600	-1.20494600	2.79106200
H	4.51964600	-0.79439900	2.68265000
O	3.27397500	0.80559300	2.79183700
H	2.32616700	0.94975900	2.56937300
H	0.41752300	0.96561200	-0.90492800
C	-1.29416900	-0.06959800	-0.09114100
C	-2.14501900	0.51778600	-1.03130700
C	-1.81621900	-0.64135600	1.07068700
C	-3.51916400	0.54047100	-0.80529600
H	-1.71674800	0.93032800	-1.94262600
C	-3.19446400	-0.61160700	1.28316400
H	-1.14474100	-1.07488600	1.80140400
C	-4.05039900	-0.02216400	0.35436000
H	-4.17410900	1.00007600	-1.54118300
H	-3.59849800	-1.05086500	2.19180700
H	-5.12278200	-0.00216300	0.53266500
C	0.51652900	2.08531200	-2.79026000
O	0.72079700	2.10225000	-1.52484500
O	-0.01219400	1.16092100	-3.42775300
C	0.98373100	3.34305700	-3.51846600
H	0.74870700	3.28273400	-4.58290200
H	0.50397700	4.22133800	-3.07548000
H	2.06336000	3.45934200	-3.38000800

Structure and coordinates of **Int-O8**



N	0.00401000	-0.86325700	-0.49239400
C	0.14269200	-1.86433500	-1.52214400
H	-0.59296400	-2.67595000	-1.38688600
H	0.03440100	-1.43398100	-2.52363400
C	1.56446300	-2.35728200	-1.25739000
O	1.72413300	-2.21896400	0.13532400
C	1.10064300	-0.97559300	0.52095900
O	0.80891200	-0.87258100	1.74380100
C	3.42764300	-0.06448100	0.42495200
H	1.71285200	-3.40784300	-1.52321100
H	2.28664300	-1.72959600	-1.80010100
O	2.07329900	0.08138500	0.04223500
H	3.88865900	0.91267000	0.23375800
H	3.92270800	-0.81776800	-0.21100100
C	3.63474300	-0.44374500	1.89011900
H	3.33096200	-1.48791500	2.03979500
H	4.70787700	-0.35775400	2.11128700
O	2.94086700	0.40735800	2.76766700
H	1.99961700	0.15073700	2.61364700
H	1.50751400	1.28438100	-0.88736400
C	-1.12770300	-0.10821800	-0.35555000
C	-2.20907300	-0.27612800	-1.24987000
C	-1.24325800	0.90200800	0.63058700
C	-3.35047300	0.51813400	-1.15543400
H	-2.14733600	-1.02238400	-2.03478900
C	-2.38678500	1.68157700	0.70466600
H	-0.42088700	1.04965600	1.31961600
C	-3.45845100	1.50595500	-0.18093200
H	-4.15925100	0.36090600	-1.86634600
H	-2.44119700	2.45342400	1.46955600
H	-4.34703100	2.12747600	-0.11189600
C	0.39567300	1.72786800	-2.40623400
O	1.00089300	2.06338000	-1.27631400
O	0.68785000	0.76031500	-3.08349800
C	-0.72057800	2.68442500	-2.74619700
H	-1.08930700	2.48771400	-3.75340200
H	-1.52780200	2.52976900	-2.01980900
H	-0.37669600	3.71828900	-2.65176500

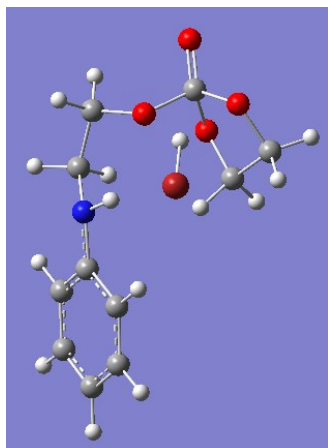
Structure and coordinates of **TS-O9**



N	0.26683500	-1.06981200	-0.48167500
C	0.73311700	-1.25492800	-1.83443600
H	-0.01236200	-1.78673700	-2.44690200
H	0.96591000	-0.29333400	-2.31184500
C	1.99439300	-2.10573300	-1.60817800
O	1.79813100	-2.71696800	-0.35345100
C	1.08686100	-1.81028800	0.46923700
O	0.67142500	-2.20525600	1.55400600
C	3.29767000	-1.04213000	1.63449200
H	2.11685200	-2.89116000	-2.35895000
H	2.88800900	-1.47070700	-1.58144800
O	2.32806800	-0.62015300	0.71342000
H	4.30398200	-0.83623600	1.23353500
H	3.19437500	-2.12830700	1.77604000
C	3.15275500	-0.35022800	2.98035400
H	2.11504800	-0.47925200	3.32177500
H	3.81810600	-0.83217100	3.70969800
O	3.52257800	1.01271700	2.94603600
H	2.24280600	0.61100800	0.09327100
C	-0.65762700	-0.11052100	-0.14398600
C	-1.49129500	0.44644000	-1.13575000
C	-0.79247500	0.35814800	1.18021300
C	-2.43860400	1.41478500	-0.81037500
H	-1.40113000	0.11095700	-2.16451600
C	-1.73188500	1.33437500	1.48044400
H	-0.13962600	-0.04592000	1.94468400
C	-2.57161200	1.87146100	0.49864400
H	-3.07114500	1.82027400	-1.59754100
H	-1.79599800	1.69636000	2.50361400
H	-3.30149100	2.63638900	0.74908900
C	1.55594300	2.46707000	0.23447400
O	1.98947200	1.47576100	-0.50095900
O	1.73168800	2.57340000	1.44329400

C	0.76215900	3.48993300	-0.54328000
H	0.70783500	4.42753700	0.01166500
H	1.19524200	3.64401800	-1.53470600
H	-0.24984900	3.08736200	-0.67130800
H	2.86512600	1.50550200	2.41320900

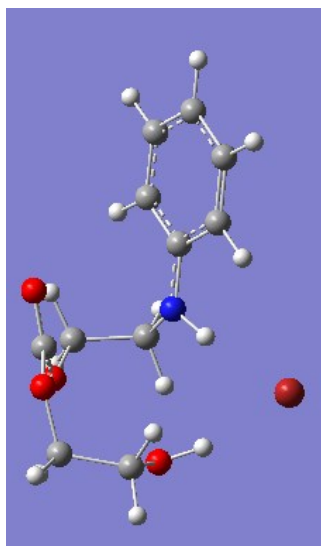
Structure and coordinates of **TS-B6**



H	3.08622100	1.05692100	-4.29803300
C	8.32945000	-0.28344800	-0.37629400
C	7.91973900	0.44263600	-1.49342600
C	6.72333500	0.11403000	-2.15640500
C	5.93556100	-0.93166500	-1.62948600
C	6.36630800	-1.65544000	-0.52824400
C	7.56835400	-1.34230700	0.11440800
H	9.26065500	-0.01177900	0.11616000
H	8.53025400	1.26117400	-1.86311000
H	4.99012900	-1.16500800	-2.11341300
H	5.74404600	-2.46367800	-0.15060700
H	7.89581800	-1.90548200	0.98345300
N	6.31105000	0.76586700	-3.29660100
H	5.34585500	0.56972000	-3.54909100
C	6.65464200	2.15675500	-3.55707000
H	7.70258500	2.23715000	-3.87966800
H	6.51542800	2.77064500	-2.65475000
C	5.73772200	2.66806200	-4.67051400
H	5.86196900	3.74814100	-4.81711000
H	5.98685300	2.15239900	-5.60828700
O	4.39785600	2.38504700	-4.36917100
C	2.19115500	2.51803700	-2.21481200
C	3.60841600	2.65605600	-1.65592600
H	1.77439700	1.51028200	-2.09453000
H	1.51416100	3.24828900	-1.74618800
H	4.18008200	1.72117500	-1.78282500

H	3.63546200	2.94927700	-0.60135000
O	4.13788200	3.69238200	-2.43834600
O	2.34670800	2.81317900	-3.58181800
C	3.62472300	3.54045500	-3.79449000
O	3.61707600	4.56625700	-4.48315100
Br	2.92262200	-0.40428700	-4.15726200

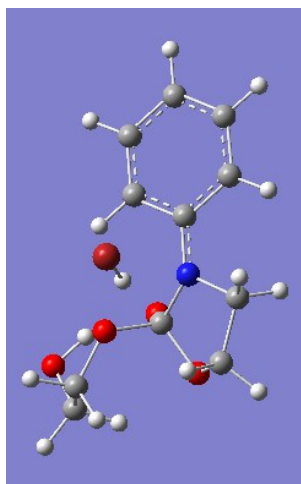
Structure and coordinates of **Int-B6**



C	-1.07926100	-3.21627100	1.56820900
C	-2.45925600	-3.50738700	1.00590900
H	-1.07892600	-2.22514300	2.04322300
H	-0.88028000	-3.96702000	2.35248800
H	-3.12453300	-3.83425800	1.80993300
H	-2.39849900	-4.28545500	0.24034400
O	-3.12381700	-2.34378000	0.48555500
O	-0.10455100	-3.29247400	0.56032600
C	-2.89771300	-1.89513200	-0.75253100
O	-3.39746200	-0.87902500	-1.16006300
O	-2.14623700	-2.74202700	-1.47260900
C	-1.54239900	-2.19621100	-2.64461300
H	-1.43066400	-3.03407600	-3.33890100
H	-2.21433800	-1.44684800	-3.07056800
C	-0.17446300	-1.61565200	-2.28478700
H	0.31340700	-1.27032600	-3.21328800
H	0.43065100	-2.42023300	-1.85676300
C	-1.28612800	2.50468700	-3.09565300
C	-1.01449600	1.15709800	-2.85662500
C	-0.51623200	0.74346100	-1.60921400
C	-0.29151400	1.72364900	-0.61777900
C	-0.58132500	3.05416900	-0.86862600

C	-1.07853400	3.46584600	-2.11156600
H	-1.67489500	2.79849600	-4.06849200
H	-1.20292000	0.43043000	-3.64066900
H	0.11580300	1.40508200	0.33919800
H	-0.40510700	3.78849700	-0.08589900
H	-1.30178400	4.51185500	-2.30210300
N	-0.25265200	-0.57229400	-1.29938300
H	0.30800500	-0.71159000	-0.45579100
Br	1.70340800	-0.82471700	1.48741100
H	0.61596200	-2.66597800	0.80681600

Structure and coordinates of **TS-B7**

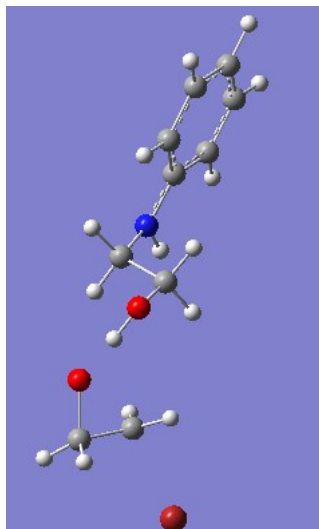


N	0.03574000	-0.88581600	-0.41443200
C	0.26364000	-1.77458400	-1.52524600
H	-0.37175400	-2.67564300	-1.47964800
H	0.09965000	-1.26478700	-2.48465300
C	1.72694500	-2.13589300	-1.28196300
O	1.81103000	-2.25146600	0.11649400
C	1.02247400	-1.18630000	0.71500900
O	0.55698700	-1.45239300	1.85695100
C	3.17112100	-0.07539200	1.16900400
H	2.01968500	-3.08865300	-1.73284900
H	2.38342600	-1.33346900	-1.65691700
O	1.86040800	0.02128500	0.64975400
H	3.51267100	0.96156700	1.26862000
H	3.82820300	-0.59684100	0.45229500
C	3.26287800	-0.78006700	2.52158300
H	3.09263500	-1.85589700	2.38130500
H	4.27985400	-0.63643300	2.91234100
O	2.35889800	-0.25406200	3.46186400
H	1.48545800	-0.56064400	3.11706900
C	-1.20316800	-0.33351300	-0.16286400

C	-2.32441500	-0.63855400	-0.95229000
C	-1.36274100	0.58032100	0.89907900
C	-3.55884400	-0.04119200	-0.69754700
H	-2.23064500	-1.33671200	-1.77851100
C	-2.60052700	1.14981000	1.15352000
H	-0.50237400	0.81589400	1.51606600
C	-3.71333800	0.85029600	0.35904000
H	-4.40768700	-0.28990000	-1.33098300
H	-2.69831400	1.84894400	1.98074400
H	-4.67750700	1.30980000	0.55954900
Br	1.06947100	1.72490900	-2.03843900
H	1.06407800	0.71624200	-0.96209800

Cartesian coordinates of structures in Figure 6

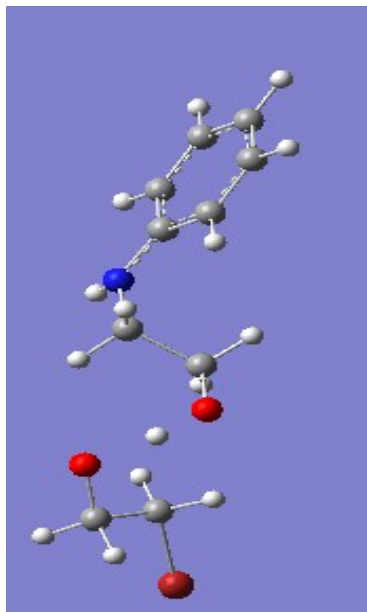
Structure and coordinates of TS-B8



Br	-3.97222600	-1.27763800	0.83964600
C	-0.86973900	-0.50709100	1.30398400
C	-1.99779200	0.13777000	0.64615900
O	-0.24330100	0.67511500	0.91618600
H	-0.97072200	-0.64909400	2.38730100
H	-0.50587200	-1.42430800	0.82254400
H	-2.50020500	0.93789500	1.16742100
H	-2.03755300	0.11646700	-0.43351200
H	0.44581300	1.00538900	-0.59708100
O	0.65978300	1.48787700	-1.44079100
C	-0.21283700	2.58477900	-1.48649500
H	-0.02058300	3.12680500	-2.42079600
H	-1.26938300	2.26624900	-1.50353700
C	-0.00992900	3.51257600	-0.28341600
H	1.04750800	3.79276000	-0.21228900
H	-0.25136400	2.95921100	0.62873400
C	0.77574700	6.95135300	-2.80288300
C	0.57881500	5.86778900	-1.95223200
C	-0.61643400	5.74491800	-1.21744900
C	-1.59515000	6.74756200	-1.38102200
C	-1.38397800	7.82132000	-2.23445600
C	-0.19419100	7.94071800	-2.95645900
H	1.70712300	7.01462900	-3.36055400
H	1.34693000	5.10651800	-1.86819900
H	-2.52585200	6.67076000	-0.82228400
H	-2.16111000	8.57487300	-2.33830200
H	-0.03237800	8.77913200	-3.62694800
N	-0.82624000	4.71667400	-0.32496900

H	-1.78184600	4.60243800	-0.01495900
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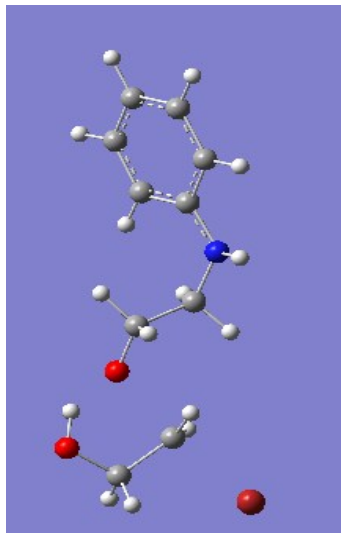
Structure and coordinates of **Int-B8**



Br	-2.02521000	-3.90438900	0.67946100
C	0.46860700	-2.68005900	1.64779900
C	-0.64030400	-2.48996900	0.60646100
O	1.31377100	-1.61655900	1.56234600
H	-0.01895800	-2.77496800	2.64156800
H	0.94512600	-3.66676500	1.44872900
H	-1.17620400	-1.55767800	0.78773500
H	-0.24662600	-2.50727500	-0.41068100
H	1.74029900	-1.32197900	0.18470800
O	1.90206200	-0.93782200	-0.78180600
C	1.13895700	0.22482400	-0.83476700
H	1.24504000	0.68216300	-1.82934600
H	0.05840900	0.02534700	-0.69002400
C	1.57398800	1.21380800	0.25439500
H	2.64658900	1.41983500	0.15530200
H	1.42962200	0.72657800	1.22379100
C	2.15639300	4.42138600	-2.60474800
C	2.02391400	3.40508600	-1.66413100
C	0.96787900	3.42766100	-0.73029700
C	0.05726900	4.50430000	-0.79708700
C	0.20149500	5.50825700	-1.74481800
C	1.25475100	5.48366300	-2.66201000
H	2.97978000	4.37172700	-3.31351200
H	2.73067300	2.58237500	-1.65904600
H	-0.76547100	4.54144700	-0.08545000
H	-0.52027500	6.32181800	-1.76666400

H	1.36475500	6.26831400	-3.40435200
N	0.83956400	2.47324800	0.24980100
H	-0.05186900	2.45747900	0.72604300

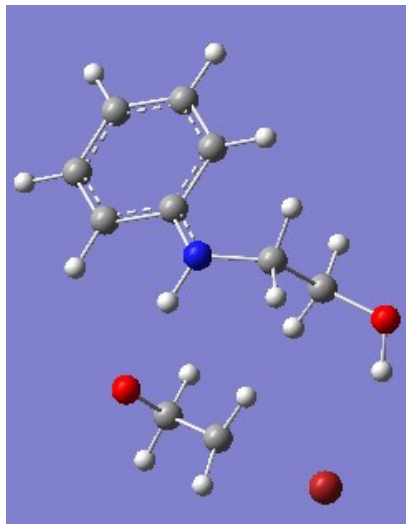
Structure and coordinates of **TS-B9**



Br	4.72767800	2.77523200	-3.64609500
O	2.95861200	1.59302400	0.07932800
C	3.52800500	1.57365600	-1.20451300
H	3.39172700	0.59880000	-1.69857600
C	2.95315800	2.64743900	-2.13533000
H	3.04473900	3.68884100	-1.85187900
H	2.31111400	2.39225500	-2.95825100
H	4.60103600	1.74315500	-1.09746200
H	2.03459700	1.93340600	-0.09848800
O	1.08944200	2.65263000	-1.18593300
C	0.69924000	3.94093700	-0.93191400
H	-0.10287800	3.98964400	-0.16789800
H	1.52462700	4.57678400	-0.52948200
C	0.18919200	4.62860600	-2.21030400
H	-0.61072500	4.02418100	-2.65270100
C	-3.63868100	5.72260300	-0.48222700
C	-2.44819700	5.34944200	-1.09845500
C	-1.44885800	6.30743700	-1.35828500
C	-1.69586900	7.63851700	-0.96283100
C	-2.88659700	7.99399500	-0.34445300
C	-3.87803300	7.04163900	-0.09863500
H	-4.38903500	4.95884900	-0.29214000
H	-2.28201500	4.31016500	-1.36076800
H	-0.93472800	8.39314600	-1.15208400
H	-3.04140800	9.02963200	-0.05040100
H	-4.80811900	7.32006500	0.38744200

N	-0.28368200	5.99614900	-2.02655800
H	0.99595300	4.65785900	-2.95114300
H	0.44959900	6.68680200	-1.93200600

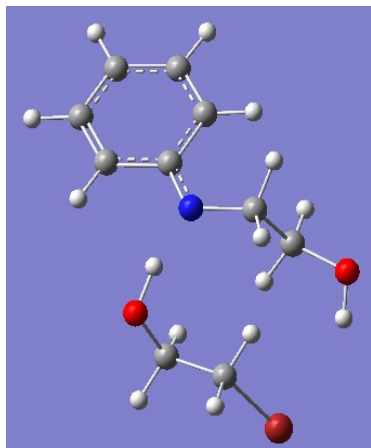
Structure and coordinates of **TS-B10**



Br	-1.52895500	1.08270700	-1.91476800
C	-1.23640000	0.13148200	1.15534900
C	-1.25593500	-0.49276900	-0.17276200
O	-0.96118900	-1.13942100	1.62591300
H	-0.44171400	0.88296900	1.30597500
H	-2.20335100	0.55581000	1.46600400
H	-0.31913800	-0.84577700	-0.57683200
H	-2.13170300	-1.07735300	-0.41956300
H	0.89480100	0.74487400	-2.35745300
O	1.83652400	0.59933300	-2.14461600
C	1.96053200	0.65694900	-0.73492900
H	2.78040100	1.34305900	-0.48789300
H	1.04738600	1.06449100	-0.28350600
C	2.22876800	-0.74084500	-0.14520700
H	3.28723900	-1.00894700	-0.27048500
H	1.66323200	-1.47121800	-0.73268500
C	4.30510900	1.00369000	3.24338100
C	3.71421700	0.37760100	2.14783700
C	2.43962400	-0.21430700	2.26256000
C	1.78120800	-0.12996900	3.51189800
C	2.38541100	0.49841100	4.58962800
C	3.65807400	1.07090300	4.47521900
H	5.28985500	1.45079000	3.12348500
H	4.24084100	0.35148400	1.19858200
H	0.78725800	-0.56585500	3.59539700
H	1.85200600	0.54931200	5.53654400

H	4.12457900	1.56493700	5.32250800
N	1.83079100	-0.89271300	1.23814700
H	0.83594700	-1.13016200	1.40394900

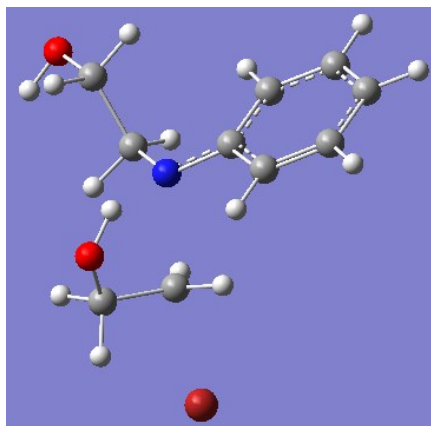
Structure and coordinates of **Int-B10**



Br	-1.70057500	1.30350200	-1.76183200
C	-1.38225400	0.09307400	0.87347700
C	-1.35841500	-0.26310800	-0.61073400
O	-0.96262000	-1.02260900	1.58539700
H	-0.72847300	0.96191000	1.05233300
H	-2.40505800	0.37331600	1.16135900
H	-0.38469100	-0.64091300	-0.91886700
H	-2.13017800	-0.99110000	-0.86091700
H	0.88060400	0.86064400	-2.32692400
O	1.77558700	0.58489500	-2.08131700
C	1.90603900	0.73037200	-0.66341400
H	2.77054100	1.37556500	-0.46811600
H	1.02609400	1.23863500	-0.24835600
C	2.05758400	-0.62783900	0.04776800
H	3.10496700	-0.97067200	-0.04321400
H	1.46203200	-1.35606100	-0.52244600
C	4.42629500	0.93118000	3.25274000
C	3.68221500	0.44034400	2.18299000
C	2.37004100	-0.09840900	2.36615000
C	1.88325700	-0.07230700	3.71395200
C	2.63647200	0.42636900	4.75956900
C	3.92953400	0.93709100	4.55610600
H	5.42210700	1.32852100	3.05568500
H	4.11389800	0.47934100	1.18667500
H	0.88574900	-0.47045400	3.88940700
H	2.21272600	0.41845500	5.76353500
H	4.51706900	1.32869600	5.38181300
N	1.58381100	-0.61892900	1.40710300

H	0.09659600	-0.95358900	1.60072700
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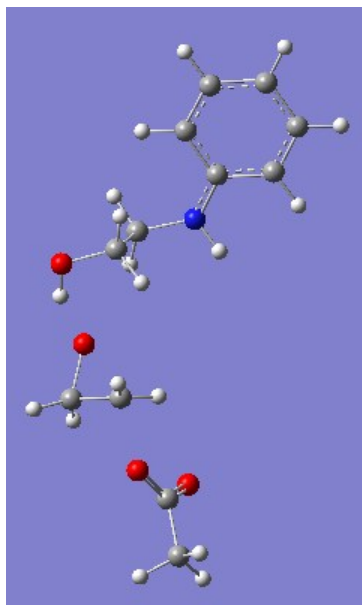
Structure and coordinates of **TS-B11**



Br	4.94841000	3.16241000	-0.03037400
O	0.79423600	2.44373400	-0.53430300
C	2.16426800	2.14380000	-0.41820800
H	2.36160200	1.07342800	-0.60149200
C	3.04089800	2.95623200	-1.37463800
H	2.91678500	4.02931100	-1.42528800
H	3.67212700	2.48692200	-2.11174000
H	2.45495000	2.35975100	0.60935500
H	0.69116500	2.59188400	-1.51319900
H	1.55010500	-0.75110300	-4.54636800
O	1.10056100	-0.15913000	-5.16622800
C	0.75292200	1.02717300	-4.45495300
H	0.35923900	1.72149000	-5.20202600
H	-0.04504000	0.82695000	-3.72599400
C	1.94666100	1.64021900	-3.72310100
H	2.76761200	1.79638400	-4.44730300
C	1.65490600	5.43435100	-5.64577900
C	1.76172100	4.18160200	-5.04504500
C	1.50395000	4.00202300	-3.66020500
C	1.13075000	5.16939700	-2.93510100
C	1.03345800	6.40776900	-3.54731900
C	1.29492100	6.56434300	-4.91455000
H	1.85895400	5.52302800	-6.71166900
H	2.03813100	3.33188100	-5.66190600
H	0.91409200	5.06316100	-1.87396000
H	0.74547000	7.27062100	-2.94975900
H	1.21413400	7.53730000	-5.39075700
N	1.59301600	2.82038300	-2.97910300
H	2.31483600	0.88607800	-3.00448600

Cartesian coordinates of structures in Figure 7

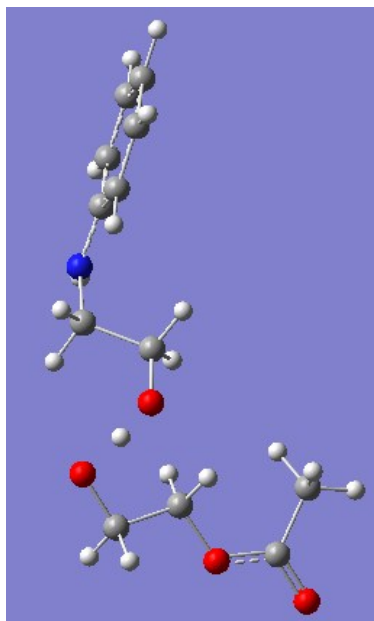
Structure and coordinates of TS-O10



C	-0.87953400	-0.61373500	1.00010400
C	-2.03540600	0.18783700	0.63485200
O	-0.26628600	0.57234600	0.57645000
H	-0.76449400	-0.83770500	2.06702100
H	-0.67738900	-1.49714000	0.38072000
H	-2.37752000	0.92958700	1.34027700
H	-2.28644900	0.26856100	-0.41301100
H	0.29731500	0.88503200	-0.99152100
O	0.46641500	1.39701400	-1.82959000
C	-0.24195200	2.59686400	-1.66530300
H	-0.18409800	3.15620200	-2.60752400
H	-1.30836200	2.41096100	-1.45426500
C	0.33305500	3.42310800	-0.50885800
H	1.38238400	3.66941000	-0.70994100
H	0.31182600	2.80207500	0.39143300
C	0.49917000	7.05924500	-2.88487500
C	0.51802300	5.91179000	-2.09701200
C	-0.42997500	5.73431500	-1.07027300
C	-1.39299600	6.74816400	-0.88261000
C	-1.40084100	7.88447900	-1.67905700
C	-0.45326700	8.05845400	-2.69092900
H	1.24378100	7.16635900	-3.67011200
H	1.26369800	5.14597600	-2.28266600
H	-2.13587700	6.62820400	-0.09673600
H	-2.15952600	8.64451600	-1.50795500
H	-0.46230500	8.94733600	-3.31416800

N	-0.40935200	4.64345100	-0.23129100
H	-1.23918700	4.51646700	0.33294400
C	-4.23350300	-0.74876900	2.02998400
O	-3.69990600	-0.86214200	0.87149300
O	-3.84407500	-0.02751700	2.95906400
C	-5.48752200	-1.61150400	2.22665700
H	-5.87103400	-1.50728500	3.24410000
H	-6.25545000	-1.30392700	1.50894000
H	-5.25012900	-2.65990300	2.02021500

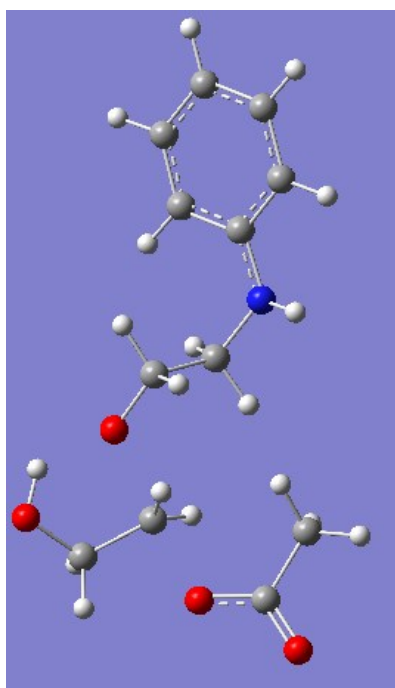
Structure and coordinates of **Int-O10**



C	0.38405100	-2.60815300	1.56286700
C	-0.79777800	-2.42376700	0.60758600
O	1.15516200	-1.47873800	1.54898100
H	-0.02847000	-2.83774800	2.56761000
H	0.92129200	-3.52785300	1.23851600
H	-1.39437600	-1.56385600	0.93740500
H	-0.40744100	-2.23137200	-0.39749500
H	1.58964800	-1.20606400	0.23402300
O	1.78555100	-0.84745600	-0.76373200
C	1.11612000	0.36721200	-0.82583900
H	1.23173800	0.80552000	-1.82918200
H	0.02465200	0.25502600	-0.65041800
C	1.64681500	1.33736100	0.23967600
H	2.72344600	1.48856400	0.09812200
H	1.51440100	0.86052400	1.21585900
C	2.29263300	4.53635700	-2.62059500
C	2.14457700	3.52272100	-1.67939800
C	1.11702500	3.58492200	-0.71616200

C	0.25135000	4.69949600	-0.75283500
C	0.41060400	5.70071000	-1.70115300
C	1.43523900	5.63597000	-2.64827100
H	3.09243100	4.45519200	-3.35303000
H	2.81487600	2.67034800	-1.69719500
H	-0.54779100	4.76873000	-0.01708400
H	-0.27587800	6.54443000	-1.69916100
H	1.55696000	6.41864700	-3.39082600
N	0.97681600	2.63263700	0.26447600
H	0.09834300	2.65284800	0.76431700
O	-1.63322800	-3.60594500	0.60198700
C	-2.61495500	-3.74995500	-0.28714300
O	-3.32942500	-4.72909200	-0.25179600
C	-2.79023400	-2.66437300	-1.33142400
H	-2.88609000	-1.67790600	-0.86926300
H	-1.91942900	-2.62641700	-1.99308300
H	-3.68237700	-2.89574600	-1.91260800

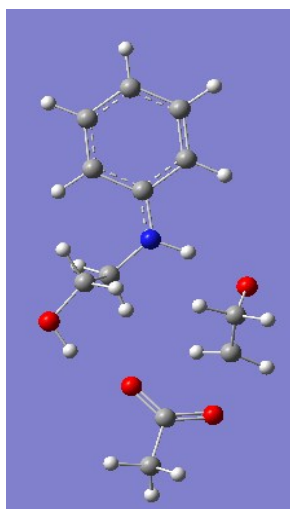
Structure and coordinates of **TS-O11**



O	3.03979000	1.36898400	-0.06313500
C	3.29604400	1.40668400	-1.44893700
H	2.69702100	0.64925300	-1.97709600
C	2.97205000	2.76644600	-2.04261800
H	3.19022300	3.65275600	-1.46020500
H	2.42376900	2.84139400	-2.96755600
H	4.35386100	1.19204700	-1.60289700
H	2.17260200	1.82876300	0.00111400

O	1.20789700	2.76866900	-1.15645300
C	0.73395400	4.04896400	-1.06782700
H	0.09543900	4.19771500	-0.17470000
H	1.54896600	4.80886900	-0.97156300
C	-0.08011700	4.43687100	-2.31590600
H	-0.90245700	3.72538100	-2.45070600
C	-3.55235500	5.74638100	-0.05722800
C	-2.49002300	5.28884900	-0.83111500
C	-1.63556500	6.20130500	-1.47903200
C	-1.89023300	7.57736000	-1.30631300
C	-2.95125400	8.01834500	-0.52778800
C	-3.80052800	7.10863200	0.10571000
H	-4.19160100	5.01704800	0.43464400
H	-2.30897300	4.22278000	-0.91732800
H	-1.23954800	8.29811800	-1.79792200
H	-3.11573600	9.08734400	-0.41409300
H	-4.62911800	7.45322900	0.71679700
N	-0.60968700	5.79512200	-2.30791600
H	0.55735600	4.34184000	-3.20205500
H	0.07693500	6.51279700	-2.50279000
C	4.82055200	3.93282400	-3.75936800
O	5.88168200	4.11871300	-4.35499700
O	4.59304200	2.93962700	-2.96696300
C	3.67462100	4.93257500	-3.98182800
H	2.86283600	4.45398600	-4.54240900
H	3.25313600	5.28315100	-3.03316100
H	4.04806400	5.78170700	-4.55623400

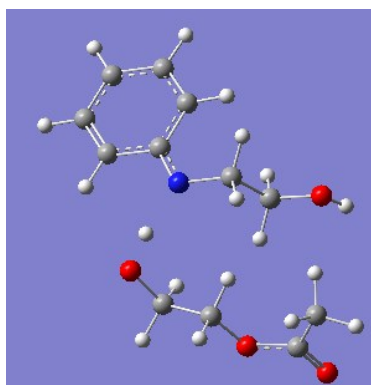
Structure and coordinates of **TS-O12**



C	-1.53741800	-1.80715400	1.43508800
C	-2.07979100	-2.34589200	0.19480600

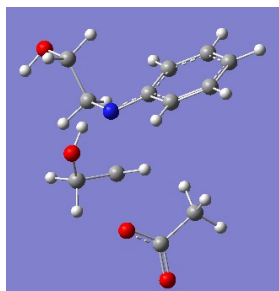
O	-0.42530000	-2.54207400	1.02685600
H	-1.40630400	-0.71448400	1.45942800
H	-2.01899300	-2.15539600	2.36079200
H	-1.73638300	-1.91278300	-0.73183400
H	-2.40287500	-3.37694300	0.19718500
C	-3.96057900	-0.53618200	-0.49834000
O	-3.88940000	-1.74743900	-0.10351300
O	-2.99430900	0.20374000	-0.75872300
C	-5.38163300	-0.00218900	-0.67325700
H	-5.36903700	1.07541200	-0.84779000
H	-5.84627600	-0.50305000	-1.52917700
H	-5.98005100	-0.23865000	0.21087700
H	-2.02133300	1.77588400	-1.01397100
O	-1.25053700	2.36871900	-0.91364400
C	-0.36633100	1.70691400	-0.03380800
H	0.40099900	2.43222100	0.26178900
H	-0.88592400	1.37854400	0.87759800
C	0.26898700	0.48123600	-0.69976800
H	0.85685700	0.80272700	-1.57285600
H	-0.54979100	-0.14269100	-1.07124100
C	4.36882900	1.31818900	0.46883300
C	3.04336900	1.10215400	0.09850200
C	2.35377400	-0.05131800	0.53547500
C	3.05826700	-0.96070700	1.36364200
C	4.37481500	-0.72509300	1.72259600
C	5.05462600	0.41732200	1.28097600
H	4.87009000	2.21693900	0.11441900
H	2.53594200	1.83119700	-0.52572400
H	2.53528700	-1.85092400	1.70618200
H	4.88423700	-1.44648100	2.35846300
H	6.08699000	0.59773000	1.56616200
N	1.06547800	-0.32492700	0.19497200
H	0.64966400	-1.22042200	0.50939500

Structure and coordinates of **Int-O12**



C	-1.58511000	-0.03597600	1.03926000
C	-1.63973500	-0.51529800	-0.40692400
O	-1.08746500	-1.06481200	1.83786100
H	-0.94554900	0.86103800	1.08203400
H	-2.59102400	0.24732300	1.37640900
H	-0.64901200	-0.88662000	-0.67890800
H	-2.36739800	-1.32920900	-0.51429800
H	2.17532500	1.11429900	-2.60144600
O	2.18048800	0.26859700	-2.13357800
C	1.80893300	0.50029100	-0.76882600
H	2.44734700	1.27164300	-0.31876800
H	0.76775300	0.85335000	-0.71093000
C	1.93985000	-0.80156500	0.01998000
H	2.98669400	-1.14949100	-0.05369300
H	1.33766100	-1.56781600	-0.49500500
C	4.40908700	0.90862600	3.05036600
C	3.63116800	0.36017200	2.03290200
C	2.29574600	-0.09514100	2.27131400
C	1.82739700	0.07276000	3.61562800
C	2.61445800	0.62514900	4.60754900
C	3.92741100	1.05536000	4.35038000
H	5.42156400	1.23495500	2.81200200
H	4.06115100	0.28129800	1.03822300
H	0.81389200	-0.25821400	3.83354000
H	2.20115000	0.72653500	5.61061800
H	4.54192700	1.49034700	5.13363300
N	1.46849300	-0.65934900	1.36990600
H	-0.05635900	-1.00635400	1.73162900
O	-2.02305300	0.57853600	-1.25738200
C	-1.71898400	0.58220700	-2.56405800
O	-2.06220400	1.52051600	-3.24724500
C	-0.94162300	-0.59044600	-3.12123600
H	0.10080200	-0.55698200	-2.77682100
H	-1.37106800	-1.54702000	-2.81074300
H	-0.95668600	-0.50994900	-4.20814000

Structure and coordinates of **TS-O13**



O	0.86801500	2.40181400	-0.38792100
C	2.21509100	1.98712500	-0.38452800
H	2.30019900	0.91960500	-0.64653800
C	3.07814200	2.80167100	-1.33768000
H	2.98282600	3.87848700	-1.33728300
H	3.75828400	2.32735100	-2.03185500
H	2.60691200	2.11563200	0.62444100
H	0.70188800	2.57342500	-1.34590400
H	1.36650500	-0.76650800	-4.55560900
O	1.05183400	-0.09698100	-5.17960800
C	0.78513100	1.09347300	-4.44231400
H	0.50765300	1.84820300	-5.18319300
H	-0.07101200	0.95305100	-3.76729300
C	1.98926000	1.55536200	-3.62176000
H	2.86687500	1.64076700	-4.29019500
C	2.12956100	5.38394200	-5.47946100
C	2.10056400	4.11849500	-4.89647500
C	1.74041900	3.94280000	-3.53599500
C	1.40133900	5.12242000	-2.81796400
C	1.44151700	6.37483600	-3.40950800
C	1.80828300	6.52760700	-4.75169700
H	2.41211200	5.47159600	-6.52708900
H	2.35752400	3.25866300	-5.50750400
H	1.09006800	5.01629900	-1.78060600
H	1.17497400	7.24812400	-2.81758900
H	1.83695300	7.51002400	-5.21413900
N	1.71643000	2.74804500	-2.86097400
H	2.23048700	0.75021200	-2.90677600
C	5.58168600	3.61376000	-0.34685000
O	6.60043200	3.61102000	0.34527800
O	4.54096000	2.88465200	-0.10944900
C	5.51658400	4.55153300	-1.55934400
H	5.24863700	4.01397000	-2.47531800
H	4.74848900	5.31884500	-1.40884200
H	6.48512900	5.03643400	-1.68990500

An input file of Gaussian09

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H      -6.80753600    1.60781600    1.41382000
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C      -7.08453100    0.48069000   -0.40261100
H      -8.14932600    0.73078100   -0.43647800
H      -6.72383800    0.45177100   -1.43619400
H      -6.98395300   -0.52789600    0.01404700
C       0.00293300   -1.67520500    0.09744300
H       0.20892500   -1.89603500    1.14945700
H      -0.47718400   -2.53521200   -0.36966100
H       0.94061200   -1.45661800   -0.42063500
O      -4.08914700   -2.32158400    0.99025000
C      -3.16175600   -2.60000200    2.01139400
H      -3.59918900   -3.35922400    2.66671400
H      -2.22094900   -3.00043400    1.60284400
C      -2.84856000   -1.34622700    2.82583800
H      -3.73805800   -1.00412000    3.36194100
H      -2.47191400   -0.54359900    2.18563100
C      -2.13725800   -2.16763000    4.93399100
O      -1.78717200   -1.60699100    3.76023000
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O	-3.27375600	-2.44643600	5.22963800	
C	-0.93206000	-2.38780500	5.80991000	
H	-0.41307800	-1.43951600	5.97286500	
H	-1.25104300	-2.81095600	6.76171700	
H		-0.23446500	-3.06808200	5.31341100

Table S1 Calculated free energies ΔG_{sol} for all the transition states and intermediates in Figure 1,2,4 and 6, with using the M06-2X/6-31+G* method and SMD model. All the values of free energies are in the units of kcal/mol.

	TS-B1	Int-B1	TS-B2	Int-B2	TS-B3	Pro-C1
ΔG_{sol}	25.7	12.1	20.4	-8.6	16.2	-6.8
	TS-O1	Int-O1	TS-O2	Int-O2	TS-O3	Pro-C1
ΔG_{sol}	27.5	-2.7	4.8	-19.9	18.7	-10.8
	TS-O1a	Int-O1a	TS-O2a	Int-O2a	TS-O3a	Int-O3a
ΔG_{sol}	9.7	6.5	22.4	-8.6	21.4	2.3
	TS-O4a	Pro-C1	TS-B4	Int-B4	TS-B5	Pro-C2+Br⁻
ΔG_{sol}	14.3	-1.1	16.6	4.2	26.4	-25.8
	TS-N1	Pro-C2	TS-O4	Int-O4	TS-O5	Pro-C2+OAc⁻
ΔG_{sol}	46.5	-13.3	30.1	7.0	37.3	-31.6
	TS-N2	Int-N2	TS-N3	Pro-C3	TS-B6	Int-B6
ΔG_{sol}	46.7	-5.9	35.8	-25.3	24.8	-8.9
	TS-B7	Pro-C3+Br⁻	TS-O6	Int-O6	TS-O7	Int-O7
ΔG_{sol}	26.6	-37.7	14.5	12.1	15.9	-1.0
	TS-O8	Int-O8	TS-O9	Pro-C3+OAc⁻	TS-B8	Int-B8
ΔG_{sol}	16.9	11.6	11.9	-57.1	25.0	1.5
	TS-B9	Pro+C4	TS-B10	Int-B10	TS-B11	Pro+C4a
ΔG_{sol}	27.5	-14.2	24.6	16.3	33.9	-12.9
	TS-O10	Int-O10	TS-O11	Pro-C4	TS-O12	Int-O12
ΔG_{sol}	23.7	-5.0	26.8	-31.0	27.9	8.7
	TS-O13	Pro-C4a				
ΔG_{sol}	32.5	-30.7				