Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Theoretical predictions of isotope effects versus their experimental values on an example of uncatalyzed hydrolysis of atrazine

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Optimized Cartesian coordinates of all stationary points described in this study:

Alkaline Hydrolysis, Reactant Complex – BP86			
SCF= -1276.167132 SCRF=-1276.5175802	Coordinates		
Atomic Symbol	X	Y	Z
N	0.47058500	1.68018100	0.08679200
C	-0.27452700	0.48948100	-0.00839100
N	0.36954300	-0.72491000	-0.18860000
C	1.69989600	-0.69508000	-0.31027800
N	2.50049000	0.41901600	-0.24089200
C	1.76353400	1.51370700	-0.03434600
Cl	2.74679200	3.02908700	0.09434100
N	2.32626100	-1.89910000	-0.55046700
N	-1.59455700	0.48832200	0.07554100
C	3.76528400	-2.09799700	-0.42922000
C	4.23789200	-2.38732600	1.00833400
C	-2.29949500	1.75820200	0.28638600
C	-2.77550200	2.34001200	-1.06322200
C	-3.48671800	1.52385100	1.24048300
H	4.04597200	-2.93280900	-1.09867100
H	4.25292300	-1.18457000	-0.80629000
H	3.99708000	-1.53516800	1.66544500
H	3.74784800	-3.28907300	1.41626500
H	5.33207100	-2.54715700	1.03334000
H	1.70981400	-2.71093100	-0.47334200
H	-1.91156600	2.53498200	-1.72142600
H	-3.45166600	1.62860800	-1.57207300
H	-3.32205800	3.29097900	-0.91601500

H	-4.02972000	2.46911000	1.42780800
H	-4.19942100	0.79300900	0.81820200
H	-3.13100300	1.12990600	2.20856800
H	-1.61010100	2.49381800	0.74492200
H	-2.41881700	-0.76692500	-0.27949900
O	-5.63118300	-1.84824800	0.14411400
H	-4.67656900	-1.72096800	-0.14045500
H	-5.55152700	-2.31863300	0.99229800
O	-3.00562800	-1.62078700	-0.57011200
H	-2.88988700	-1.67692400	-1.53611000
O	-0.71999500	-3.29346800	0.18867900
H	-0.35460400	-2.36347000	0.10928300
H	-1.66823300	-3.10192600	0.00741200

Alkaline Hydrolysis, Transition State – BP86			
SCF= -1276.1224664 SCRF=-1276.4892219	Coordinates		
Atomic Symbol	X	Y	Z
N	0.93483700	0.28630200	0.68596400
C	0.82696500	-0.97690500	0.21925800
N	-0.32823200	-1.63738600	-0.05030600
C	-1.43762900	-0.90146400	0.19713300
N	-1.47404500	0.38840200	0.59341300
C	-0.24470000	0.93317400	0.69932500
Cl	-0.22171300	2.46219400	1.68415600
N	-2.63710100	-1.58057700	0.06763700
N	1.98472600	-1.69552800	0.02715500
C	-3.92013100	-0.89716000	-0.08006200

C	-5.07894400	-1.81271500	0.33404500
C	3.30969000	-1.06863400	-0.12161800
C	3.98917400	-0.88289600	1.24827900
C	4.15817600	-1.92963900	-1.06938300
H	-3.87926900	-0.00381700	0.56324400
H	-4.06221900	-0.54381200	-1.12309800
H	-5.11485500	-2.72626800	-0.28862200
H	-4.97752400	-2.12412300	1.38820900
H	-6.04440800	-1.29073400	0.21127800
H	-2.51955400	-2.45527800	-0.44535800
H	3.34300000	-0.27804400	1.90451500
H	4.17106300	-1.86060200	1.73342700
H	4.95770200	-0.36186800	1.13329100
H	5.15820700	-1.48188900	-1.19763400
H	4.29602500	-2.95254600	-0.66645200
H	3.68933300	-2.00185300	-2.06632100
H	3.15645000	-0.07384300	-0.58555000
H	1.82133500	-2.59048500	-0.43267600
O	2.58138800	2.09994800	-1.40557100
H	1.55802300	2.00583300	-1.44390500
H	2.71487800	2.10513400	-0.43916800
O	-0.06028900	1.94933100	-1.22795800
H	-0.25134200	2.88093600	-1.00183900
O	-2.38915100	1.42793400	-2.38226300
H	-2.84953200	1.37999000	-1.52370900
H	-1.43067900	1.58721200	-2.05285200

Alkaline Hydrolysis, Product Complex – BP86

SCF= -1276.217194 SCRF=-1276.5811255	Coordinates		
Atomic Symbol	X	Y	Z
N	-1.28347700	0.64437200	0.08384400
C	-1.85541000	-0.57663900	0.14946800
N	-1.22451000	-1.77490000	0.09305700
C	0.12602600	-1.66241400	0.01194500
N	0.83452200	-0.50661000	0.00600800
C	0.06912900	0.61504900	0.01117200
Cl	3.53797600	2.22047500	-0.36001900
N	0.81732600	-2.83830200	-0.09302300
N	-3.22432700	-0.63242400	0.30280700
C	2.27525300	-2.95472200	-0.13071800
C	2.69026400	-4.27475800	-0.78909200
C	-4.10779900	0.52267400	0.11921600
C	-4.40151800	0.79585400	-1.37057700
C	-5.39377300	0.30805000	0.93350300
H	2.66357100	-2.09301000	-0.69663300
H	2.71013400	-2.87361600	0.88452700
H	2.29734000	-5.14776900	-0.23408400
H	2.32400900	-4.33541300	-1.82896000
H	3.78995600	-4.35881500	-0.80213200
H	0.25336200	-3.67313300	0.05828100
H	-3.45858200	0.95559500	-1.91815600
H	-4.93785700	-0.05612900	-1.82939700
H	-5.02667300	1.69946000	-1.48950900
H	-6.06406400	1.17943800	0.83634500
H	-5.94915400	-0.57975300	0.57356800

H	-5.16301000	0.15941300	2.00177500
H	-3.55224300	1.38545400	0.52469500
H	-3.61330200	-1.56550200	0.16333600
O	1.55142800	4.82807400	-0.14852400
H	0.82616500	4.17948200	-0.06204000
H	2.33719400	4.23018900	-0.21966300
O	0.65681200	1.79690700	-0.05612200
H	1.69748700	1.76120700	-0.16553600
O	3.36821500	-0.32099300	1.65359400
H	2.52886400	-0.42473000	1.14599600
H	3.72980400	0.49413000	1.22797600

Alkaline Hydrolysis, Reactant Complex – MPW1K			
SCF= -1275.8720645 SCRF=-1276.2116115	Coordinates		
Atomic Symbol	X	Y	Z
N	0.46888000	1.64191100	0.09958900
C	-0.28152500	0.48332300	-0.00108800
N	0.34256300	-0.71629200	-0.19605800
C	1.65058100	-0.70600100	-0.30370500
N	2.44691400	0.37960400	-0.22177400
C	1.74054900	1.47033600	-0.01728900
Cl	2.71296900	2.93354100	0.11390100
N	2.25829700	-1.89641500	-0.53159600
N	-1.57490100	0.49873800	0.08564100
C	3.67887600	-2.09103800	-0.43715300
C	4.17918400	-2.27181400	0.98655600
C	-2.23760500	1.76363700	0.30516300

C	-2.51081200	2.47078600	-1.01700800
C	-3.53139100	1.51675000	1.06482300
H	3.93120700	-2.96435200	-1.03901200
H	4.16313700	-1.22958700	-0.88919300
H	3.96008200	-1.38207000	1.57243700
H	3.69946400	-3.12483600	1.46466000
H	5.25752900	-2.43373000	0.99892400
H	1.65195300	-2.69439000	-0.46292000
H	-1.57394200	2.67648200	-1.53058700
H	-3.12911900	1.84232800	-1.65887000
H	-3.03143200	3.41706000	-0.85930100
H	-4.04655700	2.45556500	1.27228400
H	-4.20229600	0.87910100	0.48967100
H	-3.32526200	1.02023600	2.01198400
H	-1.60160200	2.42041800	0.90385800
H	-2.43952400	-0.83488400	-0.29923600
O	-5.60720800	-1.86235400	0.18524200
H	-4.69078400	-1.78761900	-0.13420200
H	-5.55620100	-1.64437100	1.11063300
O	-2.97964900	-1.64167500	-0.60131100
H	-2.81033000	-1.71023400	-1.53692100
O	-0.67582300	-3.29344800	0.20803700
H	-0.37698800	-2.36836500	0.12198900
H	-1.61778400	-3.19582800	0.05933900

Alkaline Hydrolysis, Transition State – MPW1K	
SCF= -1275.825414 SCRF=-1276.1833209	Coordinates

Atomic Symbol	X	Y	Z
N	0.91603100	0.23554800	0.71666100
C	1.05374700	-0.98662400	0.22776800
N	0.06208800	-1.82880100	-0.07161300
C	-1.14495000	-1.38155000	0.28260600
N	-1.41757600	-0.18480200	0.77752300
C	-0.35585100	0.61636700	0.80911600
Cl	-0.59846100	2.09483000	1.70936600
N	-2.16421700	-2.26529000	0.14080200
N	2.30887000	-1.46451000	0.03360700
C	-3.55444800	-1.89102300	0.18848000
C	-4.09150000	-1.33691200	-1.11965500
C	3.49005400	-0.63218000	-0.00168700
C	4.69289700	-1.47725400	0.37964700
C	3.67492600	0.04974200	-1.34911000
H	-4.11876900	-2.77392200	0.49289000
H	-3.66123400	-1.15025600	0.97596200
H	-3.60641200	-0.39468600	-1.36935300
H	-3.93959500	-2.04587100	-1.93446400
H	-5.16189600	-1.14534300	-1.03743500
H	-1.90670000	-3.09012400	-0.36566600
H	4.55466900	-1.93067400	1.35932800
H	4.85273800	-2.27730300	-0.34625300
H	5.59612300	-0.86985200	0.40019800
H	4.58649800	0.64784100	-1.35459700
H	3.75427400	-0.69289300	-2.14538100
H	2.84416600	0.71971100	-1.56155500
H	3.33760300	0.13421900	0.75493700

H	2.32874800	-2.33085200	-0.47138800
O	1.68601500	2.92949100	-1.15274900
H	0.79294300	2.49183400	-1.18430100
H	1.95980800	2.75583800	-0.25601800
O	-0.58225700	1.60127700	-1.04917600
H	-0.46652300	0.87963100	-1.66644000
O	-3.17706300	2.03386700	-1.02449300
H	-3.32204200	1.79380200	-0.11308600
H	-2.18973800	1.94129800	-1.10711400

Alkaline Hydrolysis, Product Complex – MPW1K			
SCF=-1275.9361704 SCRF=-1276.286785	Coordinates		
Atomic Symbol	X	Y	Z
N	0.37551600	0.10666300	0.13067200
C	0.15900200	-1.20716500	0.18624800
N	-1.04543500	-1.78660700	0.26090700
C	-2.06062400	-0.92936900	0.28301900
N	-1.96646600	0.39985800	0.22607600
C	-0.71155100	0.85028000	0.15975700
Cl	4.44218600	1.52872200	-0.00401000
N	-3.29237300	-1.47344000	0.38410400
N	1.22469800	-2.01590000	0.17513300
C	-4.52583700	-0.73820400	0.27820300
C	-4.93825700	-0.43394700	-1.15117200
C	2.59222100	-1.57299700	-0.03534800
C	3.53256900	-2.40206600	0.81592800
C	2.96900600	-1.61592800	-1.50583700

H	-5.29488100	-1.32810400	0.77645900
H	-4.42458200	0.18731500	0.83824600
H	-4.18296200	0.17687500	-1.63870200
H	-5.06892000	-1.35120000	-1.72496300
H	-5.87547000	0.12029800	-1.16583200
H	-3.30404200	-2.47182500	0.31589800
H	3.25693000	-2.34328900	1.86707600
H	3.52623600	-3.45271800	0.51375000
H	4.54469800	-2.01987100	0.70791400
H	3.95359700	-1.17372600	-1.63955400
H	2.97530900	-2.64093800	-1.88466800
H	2.26255400	-1.03100500	-2.09062900
H	2.65094000	-0.53731300	0.28827400
H	1.01290300	-2.99510900	0.14183100
O	1.83415900	3.02519600	0.00081600
H	2.62809800	2.44120800	0.11535400
H	2.04917100	3.53623700	-0.77444200
O	-0.57687700	2.14702600	0.11549100
H	0.39294200	2.40867200	0.07022000
O	-3.70423700	2.69145400	0.19597000
H	-3.17060200	1.88071700	0.19465000
H	-3.04418000	3.37844600	0.23602600

Acidic Hydrolysis, Reactant Complex – BP86			
SCF= -1277.0927642 SCRF=-1277.4488336	Coordinates		
Atomic Symbol	X	Y	Z
N	-0.86829600	-1.80761000	-0.16554200

C	-0.96638400	-0.48097100	0.04998100
N	0.14578300	0.34038000	0.00355600
C	1.38919800	-0.23317100	-0.17217200
N	1.52124700	-1.55399100	-0.40583200
C	0.37300700	-2.24238100	-0.41278300
Cl	0.51746400	-3.93449100	-0.76503300
N	2.47297600	0.55767400	-0.12025300
N	-2.15259300	0.09119900	0.30079600
C	3.85073800	0.05194400	-0.30102100
C	4.51313600	-0.36576400	1.01793500
C	-3.44292800	-0.64157500	0.40216300
C	-3.77491100	-0.93112500	1.87563100
C	-4.53189100	0.17549000	-0.30755400
H	3.79672000	-0.79825700	-0.99699200
H	4.41747300	0.85985100	-0.79325100
H	4.56821700	0.47441100	1.73083900
H	3.96134300	-1.19506800	1.48880300
H	5.54236600	-0.70890000	0.82125300
H	2.35789800	1.52856300	0.19768000
H	-2.97982900	-1.52708900	2.35196900
H	-3.90807700	0.00441600	2.44719600
H	-4.71534600	-1.50285600	1.94047000
H	-5.48908800	-0.36847700	-0.26685300
H	-4.68701300	1.15265700	0.18540000
H	-4.28122800	0.34843300	-1.36697300
H	-3.28043200	-1.59280700	-0.12938900
H	-2.15109300	1.09035000	0.52709500
H	-0.00150200	1.39849500	0.04928100

O	-0.45137400	2.93996600	0.22852200
H	-0.75179600	3.51348700	-0.52987800
H	0.33706700	3.38572500	0.61857400
O	2.20735500	3.44309600	1.07946700
H	2.70522800	4.17260500	0.66168400
H	2.41343700	3.50974000	2.03225800
O	-1.23313300	4.61626100	-1.78178700
H	-1.21672200	4.45750400	-2.74319800
H	-1.91091500	5.30073900	-1.63220100

Acidic Hydrolysis, Transition State – BP86			
SCF= -1277.0414081 SCRF=-1277.4073869	Coordinates		
Atomic Symbol	X	Y	Z
N	0.92960500	0.27464200	0.23337500
C	1.02934700	-1.01519200	-0.04196900
N	-0.10210000	-1.80348500	-0.26094700
C	-1.36635900	-1.21880500	-0.12579700
N	-1.50754500	0.05337000	0.18483900
C	-0.35722300	0.78101200	0.33177200
Cl	-0.48739700	1.96073900	1.71874600
N	-2.43925600	-2.02277000	-0.29085700
N	2.22504400	-1.64501300	-0.09563700
C	-3.83061300	-1.53227500	-0.20124100
C	-4.79633000	-2.70583600	-0.03294900
C	3.53644400	-0.98918900	0.12915000
C	4.46468000	-1.97735700	0.84980000
C	4.12799800	-0.48015100	-1.19723900

H	-3.87906700	-0.84365600	0.65686200
H	-4.06881500	-0.94639400	-1.10799700
H	-4.75100900	-3.40061600	-0.89049300
H	-4.59041800	-3.26980200	0.89199200
H	-5.82880600	-2.32677100	0.02375400
H	-2.30006500	-2.96002600	-0.66741500
H	4.03707800	-2.30363400	1.81160400
H	4.66095400	-2.86964100	0.22733800
H	5.43678900	-1.49948500	1.05055900
H	5.06584300	0.06927200	-1.00990800
H	4.36164800	-1.32011500	-1.87454600
H	3.42504200	0.19166800	-1.71765900
H	3.32427300	-0.13711000	0.79666500
H	2.24950100	-2.60863500	-0.43039900
H	-0.01418900	-2.82020100	-0.25222900
O	-0.41958200	1.88460900	-1.04129700
H	0.44470800	2.43263100	-0.97690600
H	-1.21868200	2.51198300	-0.92813200
O	-2.50866900	3.46698400	-0.74709900
H	-2.70211000	3.69405300	0.18240600
H	-2.61945500	4.28793800	-1.26181100
O	1.91289500	2.94221500	-0.58995000
H	2.19134900	2.12135600	-0.12444600
H	2.59613100	3.14370800	-1.25572900

Acidic Hydrolysis, Product Complex – BP86	
SCF= -1277.0918003 SCRF=-1277.4633078	Coordinates

Atomic Symbol	X	Y	Z
N	1.14896500	0.46547200	-0.53969400
C	1.11924100	-0.84736500	-0.29273000
N	-0.06535200	-1.56814700	-0.41041400
C	-1.23471000	-0.90848100	-0.78311100
N	-1.22406100	0.40047000	-1.03370500
C	-0.04700500	1.02493700	-0.84261100
Cl	-1.37707300	0.20191500	2.47995900
N	-2.36140800	-1.62576600	-0.89152500
N	2.22343300	-1.51208600	0.08302800
C	-3.69071500	-1.05329800	-1.20506000
C	-4.76758200	-1.65728100	-0.30094300
C	3.56090100	-0.89073500	0.28570000
C	4.24469500	-1.58743500	1.47010200
C	4.38580100	-0.95647200	-1.01022200
H	-3.60611400	0.03432600	-1.06828500
H	-3.90800000	-1.24557800	-2.27125100
H	-4.84532700	-2.75174500	-0.42791400
H	-4.56946300	-1.43472100	0.75987500
H	-5.74725700	-1.22835100	-0.56600400
H	-2.32633000	-2.62891300	-0.70683700
H	3.64439900	-1.50429200	2.39059000
H	4.42648400	-2.65694600	1.25728000
H	5.22551900	-1.12255400	1.65793900
H	5.35839300	-0.45859300	-0.86092800
H	4.58623600	-2.00213500	-1.30191300
H	3.86392200	-0.45488300	-1.84132600
H	3.35420800	0.16105100	0.54232900

H	2.16996600	-2.52488700	0.20129900
H	-0.10969700	-2.53045700	-0.07102200
O	-0.10530000	2.34413500	-0.97034200
H	0.80737100	2.78653900	-0.84175200
H	-1.80868700	2.75699700	0.24772900
O	-2.41010300	2.56436900	1.00050400
H	-1.86797300	1.29803600	1.84009900
H	-2.48225800	3.38692100	1.52067100
O	2.09870200	3.71132500	-0.66525500
H	2.97233500	3.29718000	-0.79008700
H	2.13133000	4.56900800	-1.12964200

Acidic Hydrolysis, Reactant Complex – MPW1K			
SCF=-1276.8170059 SCRF=-1277.1598103	Coordinates		
Atomic Symbol	X	Y	Z
N	0.95617000	-1.66951600	0.23435800
C	0.92442200	-0.35638800	0.05166900
N	-0.24933000	0.27609900	-0.20676400
C	-1.38258500	-0.45791900	-0.36149400
N	-1.37425600	-1.77105200	-0.18983100
C	-0.20162500	-2.28496900	0.11776000
Cl	-0.17691700	-3.96513900	0.38487600
N	-2.48567700	0.18239100	-0.68924200
N	2.02509600	0.36245600	0.12330900
C	-3.78405600	-0.46239100	-0.83359400
C	-4.59551100	-0.42178200	0.44410500
C	3.34607100	-0.21041100	0.39849000

C	4.01588500	-0.65213200	-0.88963900
C	4.16391800	0.80946700	1.16470800
H	-4.29860800	0.04938800	-1.64269600
H	-3.60664800	-1.48568100	-1.14698200
H	-4.08974700	-0.96167500	1.24085200
H	-4.77223100	0.60048600	0.77236900
H	-5.56198200	-0.89231700	0.28011500
H	-2.41924400	1.17981400	-0.81040900
H	3.41074000	-1.39048900	-1.40943700
H	4.18500800	0.19457600	-1.55384700
H	4.98102400	-1.10306000	-0.67108800
H	5.13285500	0.38795800	1.41791100
H	4.34439500	1.70218300	0.56561800
H	3.67111700	1.10152600	2.08916800
H	3.17005400	-1.08091900	1.02433200
H	1.98240900	1.33539600	-0.14690800
H	-0.33556700	1.30745300	-0.23995400
O	-0.84163800	2.88051700	-0.44058600
H	-0.06571600	3.33117900	-0.78618400
H	-1.25672200	3.46518900	0.21424800
O	-2.09151400	4.52771900	1.34194500
H	-2.02513200	4.56547800	2.29334900
H	-2.69897200	5.21517500	1.07759600
O	1.89374900	3.24757300	-1.12694900
H	2.39798200	3.94757500	-0.71364600
H	2.15466300	3.24816000	-2.04742700

Acidic Hydrolysis, Transition State 1 – MPW1K

SCF= -1276.7653742 SCRF=-1277.1189228	Coordinates		
Atomic Symbol	X	Y	Z
N	0.96929800	0.22469300	0.43992500
C	1.21095600	-0.98065200	0.02413000
N	0.19126300	-1.87035900	-0.21523100
C	-1.09353100	-1.50854600	0.10605000
N	-1.37255000	-0.31373800	0.52754100
C	-0.33578900	0.56052000	0.57246000
Cl	-0.57663200	1.80011000	1.80469500
N	-2.03292900	-2.44258900	-0.00611400
N	2.45171100	-1.41540500	-0.16279300
C	-3.44094100	-2.18705300	0.25807500
C	-4.18202200	-1.65989500	-0.95281300
C	3.63711500	-0.57771200	0.02010500
C	4.79417800	-1.46728600	0.42706000
C	3.92917400	0.22404500	-1.23500900
H	-3.86899400	-3.12518900	0.60170900
H	-3.49062700	-1.48359700	1.08319900
H	-3.76693700	-0.70936700	-1.27840500
H	-4.13672200	-2.36228500	-1.78260200
H	-5.23019700	-1.50634600	-0.70547300
H	-1.78450200	-3.33557700	-0.38606400
H	4.57402100	-2.01289700	1.34171500
H	5.03876700	-2.18341100	-0.35828700
H	5.68117600	-0.86406400	0.59989400
H	4.78421300	0.87625400	-1.07090000
H	4.16410900	-0.43211800	-2.07189500

H	3.07624400	0.84155300	-1.50522600
H	3.39679400	0.10245400	0.83351400
H	2.59587700	-2.34297000	-0.51585400
H	0.40256500	-2.82679500	-0.43141000
O	-0.62045600	1.50727200	-0.87519100
H	-0.04680300	2.30817300	-0.88882200
H	-1.56373500	1.79998300	-0.87645700
O	-3.17146900	2.20315700	-0.76276700
H	-3.53677000	2.08614700	0.11260600
H	-3.55835900	2.99593700	-1.12851500
O	0.79678100	3.74901900	-0.86558800
H	1.18479500	4.05031600	-0.04648600
H	1.28658600	4.14760600	-1.58132200

Acidic Hydrolysis, Intermediate – MPW1K			
SCF= -127 6.7735851 SCRF=-1277.1275449	Coordinates		
Atomic Symbol	X	Y	Z
N	0.93104900	0.34450400	-0.14397600
C	1.15858900	-0.89222400	0.14118000
N	0.12806500	-1.74691400	0.47149600
C	-1.16616900	-1.33584500	0.26985200
N	-1.43927100	-0.10425200	-0.01214500
C	-0.36173100	0.77192800	0.06819400
Cl	-0.44694000	1.65764100	1.73825700
N	-2.11283500	-2.26940500	0.39042100
N	2.38570300	-1.41312900	0.14032100
C	-3.52996300	-1.99013200	0.24680600

C	-3.99831200	-1.96493800	-1.19410300
C	3.58437200	-0.63569500	-0.16132300
C	4.76199400	-1.27026300	0.55100800
C	3.80165400	-0.52253400	-1.65981100
H	-4.05800100	-2.75450200	0.81122800
H	-3.72418300	-1.04361400	0.74423600
H	-3.47218300	-1.20450700	-1.76589500
H	-3.83602100	-2.92665400	-1.67611700
H	-5.06382100	-1.74989700	-1.23630700
H	-1.82964900	-3.23043800	0.37568200
H	4.59759500	-1.31774000	1.62483300
H	4.94934700	-2.27918200	0.18202100
H	5.66265500	-0.68969800	0.37034800
H	4.67109600	0.09750500	-1.86781100
H	3.97915700	-1.50188500	-2.10244900
H	2.93810700	-0.07365000	-2.14393600
H	3.40131600	0.35436400	0.25022300
H	2.47979000	-2.41190300	0.13793900
H	0.31972700	-2.64775400	0.86710000
O	-0.62260300	1.82759100	-0.86813100
H	0.01992200	2.61764400	-0.75127700
H	-1.63134400	2.08966600	-0.82718900
O	-3.05121800	2.10211400	-0.70895800
H	-3.15754700	1.22754500	-0.31693800
H	-3.49511800	2.74385800	-0.15599500
O	0.84565600	3.81334400	-0.52651000
H	1.14908100	3.91321000	0.37602200
H	1.57179600	4.02593800	-1.11094200

Acidic Hydrolysis, Transition State 2 – MPW1K			
SCF=-1276.7716986 SCRF=-1277.1314676	Coordinates		
Atomic Symbol	X	Y	Z
N	0.90385900	0.30778800	-0.35831600
C	1.15822100	-0.87210100	0.12384400
N	0.13572900	-1.68049000	0.56191700
C	-1.16157800	-1.33190300	0.28263300
N	-1.44317100	-0.15334400	-0.18804400
C	-0.38304700	0.69495300	-0.23578200
Cl	-0.46541200	1.72717300	1.65793500
N	-2.10000200	-2.24226600	0.51937400
N	2.39297300	-1.34561800	0.21683900
C	-3.51894700	-2.00178800	0.31114700
C	-3.95343100	-2.18726100	-1.12774500
C	3.58377400	-0.58583400	-0.16457200
C	4.74580700	-1.05824100	0.68560600
C	3.85507000	-0.71444400	-1.65235700
H	-4.04839600	-2.68517900	0.96970700
H	-3.73125900	-0.99592200	0.66173200
H	-3.43269700	-1.49583600	-1.78516300
H	-3.75982100	-3.20159400	-1.46981400
H	-5.02199800	-2.00552800	-1.21787000
H	-1.81430300	-3.18384000	0.70913500
H	4.53935100	-0.93480200	1.74608700
H	4.97575500	-2.10659100	0.49291800
H	5.63686000	-0.48492500	0.44496700
H	4.71810800	-0.11244500	-1.92797400

H	4.07101900	-1.74746800	-1.92134700
H	3.00270000	-0.37370500	-2.23451400
H	3.35717300	0.45087000	0.07275500
H	2.52353500	-2.31587900	0.43686100
H	0.33654600	-2.52902800	1.05792900
O	-0.66040100	1.78188700	-1.05858500
H	0.02114100	2.57302400	-0.87767900
H	-1.66077200	2.08780900	-0.90011000
O	-2.99723000	2.33060700	-0.60040100
H	-3.27692300	1.50777700	-0.19172500
H	-3.14800300	3.03000300	0.03696900
O	0.77719400	3.63792700	-0.42219100
H	0.83297300	3.49262400	0.53001200
H	1.65357700	3.80257300	-0.76738000

Acidic Hydrolysis, Product Complex – MPW1K			
SCF=-1276.8201913 SCRF=-1277.1314676	Coordinates		
Atomic Symbol	X	Y	Z
N	0.79653000	0.27749000	-0.84734200
C	1.09789200	-0.82052100	-0.19513600
N	0.11172200	-1.59676600	0.35415500
C	-1.19391900	-1.21151400	0.23414800
N	-1.50950300	-0.11795200	-0.41754600
C	-0.49098100	0.59218300	-0.89268600
C	0.45250400	1.15865200	2.56450500
N	-2.12331200	-1.96634500	0.78999700
N	2.34829100	-1.20927800	-0.05411200

C	-3.54952500	-1.66938500	0.71324100
C	-4.21484700	-2.32471600	-0.47787200
C	3.50050800	-0.46998800	-0.58356000
C	4.67596800	-0.69665500	0.34474900
C	3.78669800	-0.88540600	-2.01407400
H	-3.98820600	-2.00875800	1.64780500
H	-3.64989800	-0.59016200	0.67139900
H	-3.78747400	-1.96049000	-1.40870200
H	-4.11379300	-3.40760700	-0.44739700
H	-5.27663900	-2.09018800	-0.47908100
H	-1.85125100	-2.82380500	1.23307200
H	4.45101300	-0.37387200	1.35857700
H	4.96870100	-1.74696600	0.36518100
H	5.53445800	-0.13122700	-0.00683300
H	4.62070200	-0.30835200	-2.40661100
H	4.05340500	-1.93975800	-2.07009600
H	2.92446000	-0.70690300	-2.65141700
H	3.21318800	0.57776900	-0.56207000
H	2.54182500	-2.06927500	0.42608900
H	0.35455100	-2.37537500	0.93991300
O	-0.75567000	1.72839100	-1.46239000
H	0.28534600	3.17115200	-0.29490500
H	-1.72221000	1.94166000	-1.46687600
O	-3.23616200	2.55877600	-1.55303300
H	-3.61363700	2.83359800	-2.38641700
H	-3.53800500	3.17581200	-0.88904400
O	0.30853600	3.45648200	0.62040600
H	0.42326500	2.19477400	1.75909900

H	0.90714600	4.19765200	0.68294300

Neutral Hydrolysis, Reactant Complex – BP86			
SCF= -1276.690904	Coordinates		
Atomic Symbol	X	Y	Z
N	1.04611300	0.41809500	0.61082700
C	1.08494400	-0.82088600	0.01040800
N	0.01484200	-1.59861400	-0.24130000
C	-1.17460400	-1.05959500	0.10626400
N	-1.33780000	0.14353300	0.75682900
C	-0.18638800	0.77717700	0.96107300
Cl	-0.31370500	2.32531100	1.79464200
N	-2.28466700	-1.77902400	-0.17350100
N	2.29981100	-1.29629200	-0.37132200
C	-3.66734200	-1.35067600	0.07001300
C	-4.61668300	-2.54837300	-0.01932000
C	3.60821000	-0.74788700	0.02405100
C	4.08600800	-1.35347800	1.35842500
C	4.61349400	-0.97851400	-1.11499900
H	-3.70776100	-0.89383900	1.07295500
H	-3.95654800	-0.56741900	-0.65546500
H	-4.58598700	-3.01376800	-1.02080800
H	-4.36711900	-3.31763900	0.73139400
H	-5.65269200	-2.21746500	0.15794700
H	-2.11853000	-2.60884200	-0.74275500
H	3.35101500	-1.16377500	2.15755100
H	4.22993400	-2.44511500	1.26662400
H	5.04837800	-0.90640200	1.66204200

H	5.59281800	-0.54473100	-0.85405200
H	4.76686100	-2.05853300	-1.29640000
H	4.26635200	-0.51845100	-2.05495200
H	3.45592200	0.33473800	0.16683200
H	2.27025400	-2.23850900	-0.76411200
O	-0.94173900	1.46419600	-2.47942200
H	-0.18451000	1.99781700	-2.14657300
H	-1.72383200	1.77025000	-1.96533500
O	-3.12842700	1.95285300	-0.58965800
H	-2.63109000	1.39222100	0.06062800
H	-3.18500100	2.83551400	-0.18182800
O	1.56821900	2.55429300	-1.40823200
H	1.61807800	1.90995300	-0.66172800
H	2.20808400	2.23248200	-2.06860000

Neutral Hydrolysis, Transition State – BP86			
SCF= -1276.6547402	Coordinates		
Atomic Symbol	X	Y	Z
N	0.96531700	0.36438700	-0.13340900
C	0.97437300	-0.99203000	-0.17389600
N	-0.11471700	-1.79313500	-0.12790600
C	-1.29400000	-1.12797600	-0.07665300
N	-1.44558400	0.21752300	-0.01976800
C	-0.27342000	0.90451700	0.00146300
Cl	-0.27795500	2.19113100	1.51336400
N	-2.41981300	-1.89732000	-0.06223300
N	2.18067900	-1.62972900	-0.28949900
C	-3.78599600	-1.38023800	-0.06864200

C	-4.78933300	-2.51775400	0.14235500
C	3.49333200	-1.01185800	-0.05273000
C	3.74288300	-0.73430100	1.44296800
C	4.57570300	-1.91313900	-0.66638400
H	-3.88128000	-0.63036900	0.73714300
H	-3.99653300	-0.85693200	-1.02282900
H	-4.71706500	-3.27245300	-0.66118800
H	-4.62342500	-3.02208900	1.10983500
H	-5.81768000	-2.12175700	0.13465300
H	-2.25807300	-2.89445100	-0.19220400
H	2.95033200	-0.08952300	1.85536700
H	3.76200600	-1.67927400	2.01502200
H	4.71219200	-0.22532500	1.58672900
H	5.57154000	-1.45820700	-0.53774300
H	4.59617500	-2.90003100	-0.16737500
H	4.39943800	-2.07300800	-1.74330200
H	3.49122900	-0.04842900	-0.59327400
H	2.10784400	-2.64309300	-0.19215000
O	-0.41837700	2.04926800	-1.23644000
H	0.43211900	2.61964900	-1.17908300
H	-1.30999700	2.52941500	-1.03202500
O	-2.84797800	2.50638600	-0.56126400
H	-2.67505400	1.55593800	-0.26912700
H	-2.92317900	3.00875200	0.27286000
O	2.05723200	2.73243400	-0.98745500
H	2.00947000	1.80138100	-0.60125400
H	2.54573800	2.65045500	-1.82713900

Neutral Hydrolysis, Product Complex – BP86			
SCF= -1276.7253745	Coordinates		
Atomic Symbol	X	Y	Z
N	1.56786300	0.63505800	-0.28216400
C	1.74119300	-0.70627400	-0.07474000
N	0.75459600	-1.62528500	-0.05106200
C	-0.49083700	-1.13274800	-0.25710400
N	-0.78955200	0.18532400	-0.46806800
C	0.27904600	1.00045300	-0.46568600
Cl	-4.99953900	1.13291500	1.26712600
N	-1.50580700	-2.02710200	-0.25334700
N	3.00656100	-1.17420600	0.10833100
C	-2.93278300	-1.71291200	-0.40444000
C	-3.75531400	-3.00239500	-0.44619500
C	4.22089300	-0.36449200	0.28718000
C	4.32519600	0.20488600	1.71554400
C	5.44016700	-1.22091800	-0.08805600
H	-3.27087100	-1.07433200	0.43228400
H	-3.07631800	-1.13704600	-1.33578400
H	-3.46672800	-3.64023800	-1.30000400
H	-3.63778500	-3.58445000	0.48506600
H	-4.82323200	-2.75437600	-0.54927600
H	-1.22655200	-2.98703600	-0.05456300
H	3.43655700	0.80673100	1.96494500
H	4.41211200	-0.61208100	2.45356900
H	5.21515200	0.85090200	1.81006400
H	6.36529600	-0.62960400	0.00742100
H	5.53334200	-2.09174000	0.58706800

H	5.36693100	-1.58976800	-1.12466300
H	4.14804000	0.47438500	-0.42800300
H	3.04978500	-2.16913100	0.33115300
O	0.00285400	2.29580800	-0.66383500
H	0.86965000	2.82266000	-0.64876300
H	-2.72747200	2.57830200	-0.77372800
O	-3.07854200	1.66890500	-0.82445600
H	-2.26448000	1.07669400	-0.69105300
H	-4.07825900	1.42510200	0.25964900
O	2.50526800	3.16679900	-0.53038600
H	2.56390100	2.16874400	-0.43603800
H	2.96547800	3.40451300	-1.35592100

Neutral Hydrolysis, Reactant Complex – MPW1K			
SCF=-1276.4116927 SCRF=-276.7039051	Coordinates		
Atomic Symbol	X	Y	Z
N	1.03370000	0.42092700	0.58690800
C	1.06850300	-0.80871000	0.02722200
N	0.01051900	-1.57206500	-0.19457200
C	-1.15735800	-1.03386600	0.13710600
N	-1.30670500	0.16359000	0.74632300
C	-0.17528700	0.79317300	0.92416900
Cl	-0.29217200	2.33583600	1.69413000
N	-2.25335400	-1.74427700	-0.11650200
N	2.26114800	-1.29377200	-0.33373300
C	-3.60945400	-1.29877300	0.11411800

C	-4.56006700	-2.47264200	0.04067100
C	3.54743500	-0.72105700	0.01105800
C	3.98124600	-1.13198100	1.40925100
C	4.55981900	-1.12326300	-1.04429500
H	-3.65209700	-0.83503800	1.09676100
H	-3.88646700	-0.53688700	-0.61476300
H	-4.53290400	-2.94388100	-0.94128600
H	-4.31820900	-3.22390000	0.79012800
H	-5.57926900	-2.13642500	0.21262500
H	-2.09786200	-2.57741100	-0.65218900
H	3.24218900	-0.82286400	2.14434800
H	4.10272100	-2.21285400	1.47354700
H	4.93171400	-0.66782500	1.66683800
H	5.52800100	-0.67789100	-0.82845400
H	4.69460300	-2.20531800	-1.06348800
H	4.24433500	-0.80198700	-2.03449000
H	3.42494200	0.35936500	-0.00493400
H	2.23270800	-2.22504500	-0.70638300
O	-0.90242700	1.13897100	-2.39113500
H	-0.16160600	1.72865400	-2.22940300
H	-1.67568500	1.56244500	-2.01017900
O	-3.08753200	1.97977900	-0.65162700
H	-2.63084600	1.44378200	0.00913500
H	-3.13291400	2.86396100	-0.29881900
O	1.51405900	2.49239800	-1.52149900
H	1.61444700	1.91500500	-0.75796700
H	2.28014900	2.35760600	-2.07191400

Neutral Hydrolysis, Transition State – MPW1K			
SCF=-1276.3679158 SCRF=-1276.6514096	Coordinates		
Atomic Symbol	X	Y	Z
N	0.96047800	0.35522700	-0.06965100
C	0.95625500	-0.97046500	-0.14989300
N	-0.11966700	-1.75560700	-0.13241500
C	-1.27725300	-1.09781600	-0.05665900
N	-1.42581900	0.21674800	0.04459300
C	-0.26559200	0.91375700	0.05873100
Cl	-0.26761500	2.14731600	1.46770200
N	-2.38792700	-1.85232900	-0.07158000
N	2.13916300	-1.60587100	-0.26717500
C	-3.72831700	-1.33444900	-0.00000300
C	-4.72391500	-2.47014900	0.08507400
C	3.43701900	-0.99860400	-0.07645000
C	3.71150000	-0.67652400	1.38474800
C	4.49106500	-1.91987500	-0.66097300
H	-3.81777400	-0.68954100	0.87444100
H	-3.94060800	-0.71692700	-0.87499800
H	-4.66236900	-3.11506400	-0.79060600
H	-4.55164400	-3.07749500	0.97215300
H	-5.73690500	-2.07944200	0.13746100
H	-2.23417500	-2.83664000	-0.16960100
H	2.93951400	-0.02339800	1.78306600
H	3.73276600	-1.59026500	1.97796800
H	4.67342100	-0.17749900	1.49433900

H	5.47893700	-1.47554000	-0.56515900
H	4.50853900	-2.87348100	-0.13186400
H	4.30080900	-2.11613000	-1.71406000
H	3.44273900	-0.06872400	-0.64437800
H	2.06599800	-2.60487200	-0.22267000
O	-0.39629300	1.95554200	-1.16429400
H	0.42448400	2.51762800	-1.18585300
H	-1.26523600	2.43498300	-1.05314100
O	-2.83709000	2.44981100	-0.62830400
H	-2.69330600	1.54443100	-0.28161500
H	-3.03279300	2.99921600	0.12756100
O	2.04731000	2.69602400	-1.00156300
H	2.04454200	1.81122700	-0.58279900
H	2.59291200	2.63971400	-1.78174100

Neutral Hydrolysis, Product Complex – MPW1K			
SCF= -1276.4424012 SCRF=-1276.7237287	Coordinates		
Atomic Symbol	X	Y	Z
N	0.52916700	-0.52188500	-0.63327200
C	0.01264200	-1.58471500	0.00238700
N	-1.25456600	-1.70431500	0.38413400
C	-2.02646300	-0.66022600	0.08933800
N	-1.62585400	0.45193000	-0.53976300
C	-0.35485000	0.43571800	-0.87919800
Cl	2.51340800	3.47215900	1.06182400
N	-3.31256400	-0.74352500	0.44968700

N	0.82097700	-2.61813400	0.27023200
C	-4.29102400	0.29898100	0.26307400
C	-5.68829000	-0.28116700	0.26664300
C	2.24049000	-2.67603700	-0.00620100
C	3.05274600	-2.00734700	1.09262300
C	2.64290800	-4.12538300	-0.20305800
H	-4.19536500	1.05532500	1.04581000
H	-4.07890600	0.79307600	-0.68085900
H	-5.81406900	-1.00081100	-0.53974000
H	-5.91052300	-0.78090200	1.20925000
H	-6.42314200	0.50927900	0.13511600
H	-3.55872700	-1.56625000	0.96609400
H	2.72685200	-0.98141700	1.24853000
H	2.93683300	-2.54272200	2.03435100
H	4.11099500	-1.99597000	0.83693300
H	3.70247500	-4.19438500	-0.43703200
H	2.46917200	-4.70511700	0.70435300
H	2.08145100	-4.58097700	-1.01558300
H	2.39791600	-2.14143000	-0.94142900
H	0.39139200	-3.36382500	0.78477300
O	0.07378200	1.51151500	-1.51852900
H	1.05285000	1.45393300	-1.65168600
H	-0.31437500	3.07395100	-0.62875200
O	-0.19892200	3.82034000	-0.02288600
H	-0.94177300	3.80797900	0.57576500
H	1.27622500	3.67910500	0.61737600
O	2.66688100	1.15685000	-1.43761400
H	2.99450900	1.75425800	-0.76184400

H	2.40527700	0.34312200	-0.99096200

Atrazine unprotonated – BP86			
SCF= -1047.360175 SCRF=-1047.5641773	Coordinates		
Atomic Symbol	X	Y	Z
N	0.79060600	0.85293700	0.10663300
C	0.86517100	-0.51021400	-0.00461700
N	-0.18377900	-1.34273500	-0.20117100
C	-1.38172200	-0.71937400	-0.27882200
N	-1.58779000	0.62997100	-0.17287200
C	-0.45669200	1.30442500	0.01191700
Cl	-0.63734700	3.05688700	0.15219000
N	-2.47113000	-1.50617100	-0.49681500
N	2.09347000	-1.08393800	0.10642900
C	-3.85740700	-1.03637000	-0.50791400
C	-4.53781200	-1.10877400	0.86883300
C	3.36799200	-0.35682300	0.20972500
C	4.34526200	-1.17956700	1.06368000
C	3.94049800	-0.02730700	-1.18267800
H	-3.84425400	0.00244100	-0.87254600
H	-4.40773800	-1.64637700	-1.24631400
H	-4.55087600	-2.14167600	1.25847800
H	-4.00910700	-0.46904300	1.59434000
H	-5.58229700	-0.75839500	0.79651600
H	-2.27835000	-2.50678900	-0.49730700
H	3.93267900	-1.37148200	2.06810700
H	4.56908000	-2.15262600	0.58726300

H	5.30044800	-0.64060500	1.17691200
H	4.87362000	0.55523700	-1.08887300
H	4.16827100	-0.95112900	-1.74479800
H	3.21972200	0.56917300	-1.76508800
H	3.13185900	0.58883100	0.72591600
H	2.11046700	-2.09107300	-0.05600800

Atrazine protonated at N1 position – BP86			
SCF= -1047.7323899 SCRF=-1048.0057371	Coordinates		
Atomic Symbol	X	Y	Z
N	0.77945500	-0.25206000	1.16986600
C	0.90407500	-1.18418600	0.13380800
N	-0.17286700	-1.61439700	-0.52102000
C	-1.37523900	-1.11495900	-0.13456000
N	-1.56348300	-0.19669000	0.89191700
C	-0.48504600	0.19049500	1.49456900
Cl	-0.55376700	1.32795600	2.78858100
N	-2.46093700	-1.53524600	-0.79095500
N	2.12162300	-1.64864100	-0.18131600
C	-3.86185500	-1.14397000	-0.54525800
C	-4.73342700	-2.35566800	-0.19364700
C	3.43702800	-1.25803700	0.39106700
C	4.40041500	-2.44246600	0.22695800
C	3.96787100	0.03218300	-0.26115100
H	-3.85343300	-0.40129800	0.26485800
H	-4.23123500	-0.64582300	-1.45949900
H	-4.73300700	-3.10808100	-1.00069100

H	-4.39262400	-2.83760500	0.73693400
H	-5.77463400	-2.02469700	-0.04938200
H	-2.27313500	-2.21541500	-1.53205300
H	4.01529800	-3.34956700	0.71984400
H	4.57495100	-2.66191000	-0.84138400
H	5.37434100	-2.19349300	0.67593900
H	4.91785200	0.32807800	0.21315500
H	4.15748000	-0.12721400	-1.33577100
H	3.26225000	0.87479100	-0.16250300
H	3.28369500	-1.09951900	1.47722600
H	2.11597200	-2.30768500	-0.96408100
H	1.59083100	0.10073300	1.68068500

Atrazine protonated at N3 position – BP86			
SCF= -1047.7246834 SCRF=-1048.0089796	Coordinates		
Atomic Symbol	X	Y	Z
N	-0.046280	0.131828	0.012272
C	-0.032823	-0.075151	1.337958
N	1.179537	-0.177514	2.021237
C	2.377047	-0.052876	1.318950
N	2.367462	0.153693	-0.005301
C	1.155053	0.224753	-0.573016
Cl	1.140997	0.474724	-2.279377
N	3.530623	-0.144434	1.993138
N	-1.173423	-0.196274	2.024872
C	4.878156	-0.042561	1.379879
C	5.741508	-1.257543	1.729338

C	-2.542689	-0.085823	1.432351
C	-3.415674	-1.204774	2.015998
C	-3.107502	1.320732	1.684691
H	4.722582	0.052723	0.296117
H	5.337857	0.893788	1.742433
H	5.885196	-1.362733	2.818820
H	5.302481	-2.189283	1.337563
H	6.739046	-1.132888	1.278068
H	3.499825	-0.301355	3.002012
H	-2.993913	-2.201286	1.806996
H	-3.542515	-1.091861	3.108270
H	-4.419517	-1.158230	1.564832
H	-4.102093	1.406117	1.217308
H	-3.226241	1.519563	2.764386
1	-2.458795	2.097313	1.248582
1	-2.400559	-0.240606	0.351351
1	-1.130017	-0.317343	3.039042
1	1.188318	-0.348735	3.029279

Atrazine protonated at N5 position – BP86			
SCF= -1047.7329717 SCRF=-1048.0061891	Coordinates		
Atomic Symbol	X	Y	Z
N	1.87621000	0.04181300	0.31959700
C	1.78157300	-1.31442600	0.02513400
N	0.64080100	-1.94672300	-0.36120000
C	-0.45836800	-1.20549700	-0.46137200
N	-0.42724100	0.16408500	-0.17852400

C	0.77727800	0.71576600	0.20587500
Cl	0.73627900	2.40734600	0.53712000
N	-1.62467600	-1.75251500	-0.83607600
N	2.89223600	-2.04667900	0.13005000
C	-2.92041000	-1.06123400	-0.99074300
C	-3.99977400	-2.05246200	-1.43195500
C	4.24788600	-1.59078600	0.52970600
C	4.66724900	-2.31691900	1.81885900
C	5.22531100	-1.82630500	-0.63397500
H	-3.20423300	-0.60212900	-0.02411500
H	-2.81562500	-0.25858300	-1.74604200
H	-3.75143800	-2.50758600	-2.40506400
H	-4.13973500	-2.85065400	-0.68427500
H	-4.95916500	-1.52460400	-1.54326800
H	-1.57547000	-2.75555900	-1.02717200
H	3.95765200	-2.12394800	2.63958000
H	4.73616900	-3.40789100	1.66103900
H	5.66222600	-1.96294400	2.13381600
H	6.22758800	-1.46548000	-0.35164000
H	5.31321600	-2.90092700	-0.87341800
H	4.90888200	-1.28790900	-1.54190700
H	4.15186300	-0.51125900	0.72383700
H	2.77255800	-3.03836100	-0.09657500
H	-1.26015600	0.75181700	-0.24935300

Water molecule – BP86			
SCF= -76.4339484	Coordinates		
Atomic Symbol	X	Y	Z

O	0.000264	0.000000	0.001531
H	0.034843	0.000000	0.974899
H	0.932009	0.000000	-0.282155

Hydroxide Ion – BP86			
SCF= -75.8065688 SCRF=-75.9816243	Coordinates		
Atomic Symbol	X	Y	Z
O	0.00000000	0.00000000	0.10886800
H	0.00000000	0.00000000	-0.87094100

Atrazine nonprotonated – MPW1K			
SCF= -1047.1685231 SCRF=-1047.3647164	Coordinates		
Atomic Symbol	X	Y	Z
N	0.76562800	0.81919900	0.10577700
C	0.85683500	-0.51848100	0.00071200
N	-0.16957300	-1.34231900	-0.19011100
C	-1.35515300	-0.74687800	-0.26873600
N	-1.56571000	0.57702300	-0.16599300
C	-0.46332500	1.25827300	0.01355700
Cl	-0.65679000	2.97078600	0.14736000
N	-2.42084700	-1.52928700	-0.47563900
N	2.07139400	-1.06818800	0.10462900
C	-3.78584800	-1.06131500	-0.51205300
C	-4.42461400	-0.96691500	0.86068400
C	3.31190500	-0.32943800	0.23366400

C	4.32247900	-1.19683600	0.95936000
C	3.82414700	0.13751800	-1.11938100
H	-3.79028600	-0.08761500	-0.99337300
H	-4.34447400	-1.74482000	-1.14888400
H	-4.42816200	-1.93350300	1.36173800
H	-3.88201700	-0.25812100	1.48147900
H	-5.45493200	-0.62547000	0.77594400
H	-2.22913300	-2.51221400	-0.48800100
H	3.95297800	-1.49495800	1.93814700
H	4.54840000	-2.09778100	0.38715700
H	5.25522900	-0.65487300	1.09576000
H	4.73548200	0.72165600	-1.00196200
H	4.04589800	-0.71293900	-1.76375000
H	3.08206500	0.76167500	-1.61074900
H	3.08709300	0.54558500	0.83957700
H	2.10249000	-2.06056200	-0.03567900

Atrazine protonated at N1 position – MPW1K			
SCF= -1047.5429836 SCRF= -1047.8107468	Coordinates		
Atomic Symbol	X	Y	Z
N	-0.75645300	0.80842500	-0.11032000
C	-0.85047200	-0.55614200	0.00744600
N	0.22727400	-1.28005500	0.18544700
C	1.39953900	-0.64266000	0.24127200
N	1.54865000	0.71288900	0.12163300
C	0.47522100	1.37440000	-0.04698600
Cl	0.50767200	3.05937300	-0.20775500

N	2.48127800	-1.35999100	0.42494100
N	-2.03581400	-1.12601100	-0.07119600
C	3.85198700	-0.87758700	0.49631800
C	4.67190300	-1.34550000	-0.68772300
C	-3.33669200	-0.47695400	-0.23835800
C	-4.29236500	-1.48711900	-0.84219800
C	-3.84910200	0.08299800	1.07867800
H	3.81452100	0.20429200	0.54719500
H	4.27532700	-1.24106200	1.43056800
H	4.70445700	-2.43144000	-0.74973500
H	4.27003300	-0.95814000	-1.62074900
H	5.69429700	-0.99079900	-0.58506600
H	2.32121800	-2.35108900	0.49296000
H	-3.92384200	-1.86486400	-1.79262700
H	-4.44708200	-2.32613900	-0.16479000
H	-5.25913800	-1.02285500	-1.01316900
H	-4.79149400	0.60167200	0.92068200
H	-4.02116600	-0.72050000	1.79148900
H	-3.15354200	0.78631900	1.53375500
H	-3.20863400	0.32839800	-0.96573800
H	-2.01188800	-2.12597400	0.03857900
H	-1.56815200	1.38742200	-0.23576300

Atrazine protonated at N3 position – MPW1K			
SCF= -1047.5337477 SCRF=-1047.8121995	Coordinates		
Atomic Symbol	X	Y	Z
N	0.84279000	0.88309100	0.05482900

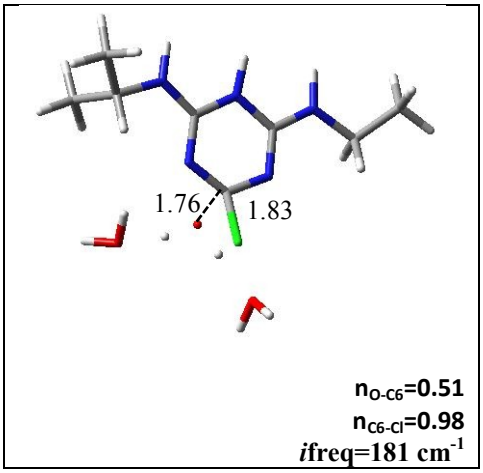
C	0.91190700	-0.44658300	-0.03602200
N	-0.24317800	-1.18327700	-0.16524100
C	-1.46097000	-0.54657900	-0.20596800
N	-1.51980600	0.78170200	-0.11488800
C	-0.36563700	1.41018000	0.01463200
Cl	-0.44774300	3.09803100	0.14017100
N	-2.56204500	-1.28417100	-0.33491700
N	2.07805800	-1.08623500	-0.00117100
C	-3.92202300	-0.74707100	-0.38843700
C	-4.81755400	-1.44094100	0.61288800
C	3.39321800	-0.43536900	0.12414900
C	4.16433300	-1.10550400	1.24378000
C	4.11556200	-0.48669500	-1.20833000
H	-3.84916500	0.31569300	-0.19151900
H	-4.29222200	-0.87501800	-1.40396700
H	-4.88368300	-2.51153600	0.42496800
H	-4.46703300	-1.28636700	1.63037300
H	-5.82353400	-1.03694600	0.53738000
H	-2.47243000	-2.28216200	-0.40541200
H	3.62924600	-1.04516000	2.18829100
H	4.36296700	-2.15363000	1.01930000
H	5.12538700	-0.61401500	1.36886600
H	5.07372400	0.01980000	-1.12462100
H	4.31157200	-1.51383800	-1.51419500
H	3.54109600	0.00669400	-1.98842000
H	3.18092500	0.59586300	0.38628100
H	2.08716900	-2.08703300	-0.09484200
H	-0.19613800	-2.18526600	-0.22581700

Atrazine protonated at N5 position – MPW1K			
SCF= -1047.5436126 SCRF= -1047.8111903	Coordinates		
Atomic Symbol	X	Y	Z
N	-0.90017600	0.89423000	-0.00000300
C	-0.87523400	-0.47552200	-0.00000100
N	0.24463300	-1.20734100	0.00000000
C	1.38551400	-0.56733600	0.00000200
N	1.41657100	0.80472700	0.00000200
C	0.23336500	1.47065900	-0.00000200
Cl	0.35234600	3.15935400	-0.00000400
N	2.53045400	-1.22169800	0.00000300
N	-2.02172800	-1.10678700	0.00000000
C	3.86286700	-0.63843300	0.00000400
C	4.90678000	-1.73206300	-0.00000200
C	-3.36319200	-0.52220700	-0.00000200
C	-4.09283500	-0.94117700	-1.26305800
C	-4.09283000	-0.94115300	1.26306400
H	3.98499700	-0.01406200	-0.88672700
H	3.98500000	-0.01406900	0.88674000
H	4.82146800	-2.35738000	0.88587600
H	4.82146600	-2.35737200	-0.88588500
H	5.89838100	-1.28994000	-0.00000100
H	2.43665300	-2.22285500	0.00000400
H	-3.55735800	-0.62394500	-2.15444000
H	-4.22385300	-2.02196500	-1.30341000
H	-5.08145800	-0.48973300	-1.28224900
H	-5.08145400	-0.48971000	1.28225000

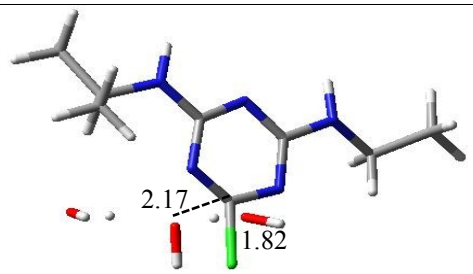
H	-4.22384700	-2.02194000	1.30343800
H	-3.55735100	-0.62390300	2.15443800
H	-3.22025700	0.55375100	-0.00001300
H	-1.94859000	-2.11136100	0.00000200
H	2.28143300	1.31693800	0.00000400

Water Molecule – MPW1K			
SCF= -76.4038462	Coordinates		
Atomic Symbol	X	Y	Z
O	0.00000000	0.11440300	0.00000000
H	0.76212500	-0.45761700	0.00000000
H	-0.76212500	-0.45761000	0.00000000

Hydroxide Ion – MPW1K			
SCF= -75.7614861 SCRF=-75.9411019	Coordinates		
Atomic Symbol	X	Y	Z
O	0.00000000	0.00000000	0.10635300
H	0.00000000	0.00000000	-0.85082500

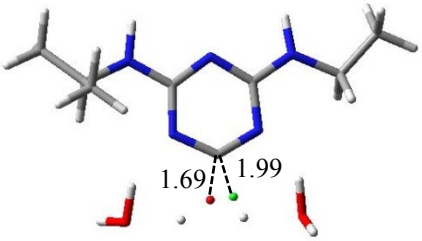


Acidic hydrolysis



$n_{O\text{-}C6}$=0.26
$n_{C6\text{-}Cl}$=0.97
*i*freq=162 cm^{-1}

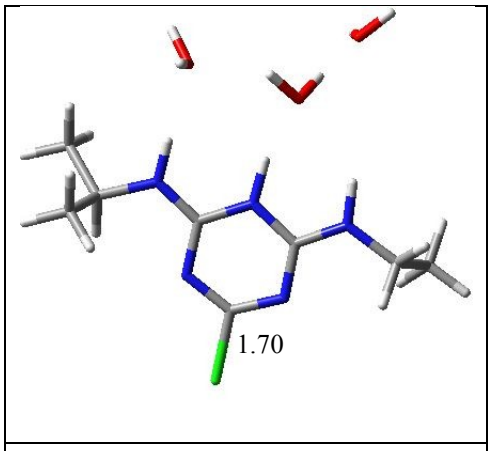
Alkaline



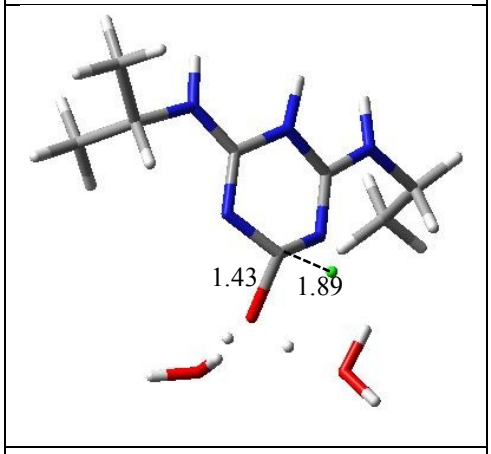
$n_{O\text{-}C6}$=0.57
$n_{C6\text{-}Cl}$=0.78
*i*freq=255 cm^{-1}

Neutral

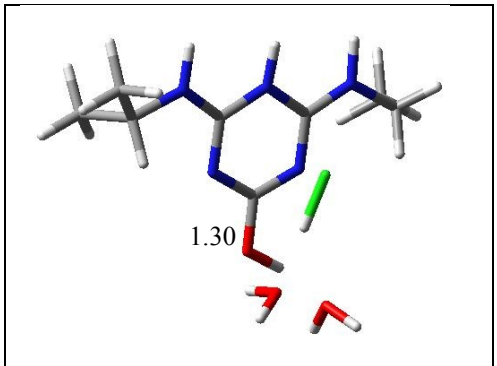
Figure S1. Key parameters for the transition state structures located for acidic, alkaline and neutral hydrolysis using the BP86 level of calculations. The interatomic distances are given in Å.



Acidic hydrolysis – Reactants Complex



Acidic hydrolysis – Intermediate



Acidic hydrolysis – Products Complex

Figure S2. Key parameters for the other stationary points structures located for acidic hydrolysis using the MPW1K level of calculations. The interatomic distances are given in Å.

Alkaline Hydrolysis – a model with none explicit water molecules			
C6 – KIE	N – KIE	Cl – KIE	ΔG_{act} (kcal/mol)
1.0021	1.0017	1.0017	30.9