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Stabilization of Glyphosate Zwitterions and Conformational/Tautomerism Mechanism in Aqueous Solution: Insights from *ab initio* and Density Functional Theory-Continuum Model Calculations

OutafFliss[a], Khaled Essalah[a] and Arij Ben Fredj[a,*]

[a]Unité de recherche de Modélisation en Sciences Fondamentales et Didactiques, équipe de Chimie Théorique et Réactivité (UR14ES10). Institut Préparatoire aux études d'Ingénieurs d'El Manar, Université de Tunis El Manar, B.P.244, El Manar II 2092, Tunis, Tunisie.

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1-Structures and energetics of glyphosate conformers in gas-phase, at B3LYP/6-311++G (2d,2p) and B3LYP-D3/6-311++G (2d,2p) levels.

NE1 structure in gas-phase at B3LYP/6-311++G (2d,2p).

E (SCF) = -891.69282824 u.a. ; Zero-point correction = 0.133533 u.a. ; G= -891.596555u.a.at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.37142200	-0.24220100	-0.15360400
C	-0.84211600	1.51036900	-0.05803200
H	-1.53016100	2.03856400	0.60110700
H	-0.96021200	1.93514200	-1.05585400
C	1.60815100	1.15479400	-0.34430400
H	1.35233600	1.10888800	-1.40209600
H	2.49807400	1.78760800	-0.26899500
C	2.04987300	-0.23448800	0.09132300
O	1.64220500	-0.83224400	1.06378200
O	3.02062300	-0.71623000	-0.69578400
H	3.25696500	-1.59722000	-0.37004400
N	0.52082000	1.73877500	0.41204000
H	0.60773300	1.53138300	1.39743500
O	-2.97339000	-0.12732700	-0.22997100
H	-3.34498300	-0.81438500	-0.79504100
O	-1.15793100	-0.82796200	1.32165900
H	-0.21147200	-1.01587700	1.46364400
O	-0.73627500	-1.00830800	-1.24522300

NE1 structure in gas-phase, at B3LYP-D3/6-311++G (2d,2p).

E (SCF) = -891.71111748 u.a.; Zero-point correction = 0.133773 u.a.; G= -891.614367 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.34957000	-0.24538800	-0.14750300
C	-0.85372400	1.51513800	-0.07590400
H	-1.54745400	2.04119700	0.57858900
H	-0.97651800	1.92521700	-1.07903300
C	1.59004600	1.15361800	-0.36533800
H	1.32796000	1.08728700	-1.42013700
H	2.48524400	1.77997600	-0.30364900
C	2.02054300	-0.23037400	0.09557900
O	1.63506300	-0.78570800	1.10225800
O	2.95236600	-0.75411900	-0.70930900
H	3.18313000	-1.63115000	-0.36955200
N	0.50980700	1.75667800	0.38884000
H	0.59979500	1.55135300	1.37490100
O	-2.94992100	-0.17113800	-0.27325000
H	-3.28500300	-0.88020900	-0.83384200
O	-1.15849100	-0.79124100	1.34575300
H	-0.21133000	-0.96217900	1.50342400
O	-0.65928300	-1.01750800	-1.20120900

NE2 structure in gas-phase at B3LYP/6-311++G (2d,2p).
E (SCF) =-891.69085647 u.a.; Zero-point correction = 0.133547 u.a.; G= -891.594432u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.58247600	-0.17409500	0.06788500
C	-0.84985200	1.51154900	0.07293000
H	-1.52642900	2.11571200	-0.53182600
H	-0.92892500	1.88741100	1.09365600
C	1.61257100	1.15246000	0.32445700
H	1.37549500	1.12076100	1.38771000
H	2.49241600	1.79709100	0.23107800
C	2.07647100	-0.23492400	-0.09332900
O	1.63232200	-0.88612600	-1.01363900
O	3.11182100	-0.65588000	0.64793600
H	3.37553000	-1.52899200	0.32160000
N	0.50765700	1.70873700	-0.41879300
H	0.58153900	1.51843200	-1.40783200
O	-1.13334200	-0.84487700	-1.30902000
H	-0.16311400	-0.94825900	-1.37069900
O	-0.68657700	-0.91569400	1.20791600
H	-1.20005700	-1.60102100	1.65158800
O	-3.03148000	-0.23309400	0.30601200

NE2 structure in gas-phase at B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.70937950 u.a.; Zero-point correction = 0.133839u.a.; G= -891.612361u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.55721900	-0.18339600	0.07124900
C	-0.86929500	1.51754300	0.08655600
H	-1.55282400	2.11178200	-0.51960900
H	-0.95844900	1.88473800	1.10943200
C	1.58374900	1.15255000	0.34805800
H	1.33478000	1.09418000	1.40688700
H	2.46957300	1.79143900	0.27673700
C	2.03848500	-0.22678800	-0.10062200
O	1.62183700	-0.82871200	-1.06659100
O	3.03093200	-0.69664300	0.66778500
H	3.29570800	-1.56114500	0.32036900
N	0.48968100	1.73138300	-0.39648400
H	0.56888400	1.53969000	-1.38541700
O	-1.13573000	-0.80735300	-1.33605800
H	-0.16556200	-0.89240200	-1.41917900
O	-0.58913700	-0.91701800	1.15813300
H	-1.06341900	-1.62742200	1.60543700
O	-2.99237800	-0.29645300	0.36523600

NE3 structure in gas-phase at B3LYP/6-311++G (2d,2p).
E (SCF) = -891.68998350 u.a.; Zero-point correction = 0.133510 u.a.; G= -891.593623u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.39571500	-0.24543100	-0.15104500
C	0.87120900	1.49872300	0.00626400
H	1.02596900	1.96800100	-0.97440600
H	1.54155700	1.97452800	0.72058800
C	-1.56798600	1.12224500	-0.33017400
H	-2.41702900	1.80631500	-0.29446400
H	-1.28507800	1.03200600	-1.38426000
C	-2.09448800	-0.24222700	0.09428600
O	-1.65807500	-0.94542900	0.97432200
O	-3.16137100	-0.59283200	-0.64459300
H	-3.43139200	-1.47985400	-0.36588300
N	-0.49301500	1.60544000	0.51137000
H	-0.67852300	2.53380800	0.85233800
O	2.99948700	-0.13495900	-0.16062000
H	3.37216100	-0.70078200	-0.84597700
O	1.12496800	-0.89872900	1.27350000
H	0.15995600	-0.96925300	1.42357800
O	0.81691100	-0.92728200	-1.32607000

NE3 structure in gas-phase at B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.70754950 u.a.; Zero-point correction = 0.133653 u.a.; G= -891.610867u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.37030000	-0.25072700	-0.14567700
C	0.88205400	1.50347000	-0.01662200
H	1.03723300	1.95207100	-1.00679100
H	1.56449800	1.97838300	0.68653400
C	-1.55304700	1.12683800	-0.34028000
H	-2.41093200	1.79989500	-0.30506800
H	-1.27554800	1.02632400	-1.39461100
C	-2.06136100	-0.23821800	0.10218200
O	-1.64438300	-0.90325800	1.02060300
O	-3.08993100	-0.63220100	-0.66754400
H	-3.35280300	-1.51773900	-0.37818200
N	-0.47920200	1.63003300	0.49159500
H	-0.66153200	2.56828400	0.80564800
O	2.97382500	-0.17471100	-0.21590400
H	3.30624800	-0.76411600	-0.90196100
O	1.13235900	-0.85882100	1.30429300
H	0.16956000	-0.91393300	1.47319000
O	0.73029400	-0.94738700	-1.27975300

NE4 structure in gas-phase at B3LYP/6-311++G (2d,2p).
E (SCF) = -891.68875360 u.a.; Zero-point correction =0.133375u.a.; G= -891.592590u.a. at 298,15K.

Charge = 0;Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.60115900	-0.17878300	-0.05932700
C	-0.86813600	1.49894900	-0.04901700
H	-1.53369800	2.07929400	0.58874600
H	-0.96014700	1.89595400	-1.06780700
C	1.58356500	1.12453300	-0.31287200
H	1.33601300	1.06033100	-1.37805400
H	2.42371800	1.81662100	-0.23830900
C	2.11498500	-0.24151700	0.09866300
O	1.65550400	-0.96961700	0.94544500
O	3.21313100	-0.56316700	-0.60886400
H	3.49984100	-1.44239100	-0.32192000
N	0.47899400	1.57613600	0.50252800
H	0.65636700	2.48450100	0.89674400
O	-1.12011900	-0.88369500	1.27975200
H	-0.14396600	-0.88725600	1.36627400
O	-0.73907300	-0.87043100	-1.25365800
H	-1.23132400	-1.59429100	-1.65811300
O	-3.05505000	-0.22005900	-0.26717400

NE4 structure in gas-phase at B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.70652149 u.a.; Zero-point correction =0.133584 u.a.; G= -891.609894u.a. at 298,15K.

Charge = 0;Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.57305700	-0.18885600	-0.06468200
C	-0.88682500	1.50506700	-0.06529400
H	-1.56579100	2.07403700	0.56829700
H	-0.98537800	1.88931700	-1.08838700
C	1.55843700	1.13022600	-0.32394200
H	1.31143500	1.05073600	-1.38783500
H	2.40804900	1.81147400	-0.25693400
C	2.07306400	-0.23471400	0.10872700
O	1.63586100	-0.92209300	1.00011200
O	3.13158800	-0.60262700	-0.63531900
H	3.41610300	-1.47718800	-0.33298600
N	0.45901500	1.60565000	0.48527200
H	0.63499900	2.52818100	0.84551900
O	-1.12730400	-0.84452800	1.31081400
H	-0.15343200	-0.83218400	1.41910100
O	-0.63430200	-0.87970800	-1.20141800
H	-1.08808800	-1.62589500	-1.60961300
O	-3.01374400	-0.27962600	-0.33678900

NE5 structure in gas-phase at B3LYP/6-311++G (2d,2p).
E (SCF) = -891.68839245 u.a.; Zero-point correction = 0.133055 u.a.; G=-891.593266u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.78343500	-0.17633900	0.13279400
C	-0.45853000	0.92445600	0.74790300
H	0.02814200	0.38987500	1.56386500
H	-0.92160700	1.81497100	1.18172500
C	1.90465200	1.16873800	0.01087300
H	2.46993700	1.75127800	-0.71812700
H	2.16629400	1.57861000	0.99632000
C	2.45001300	-0.25027100	-0.04577300
O	1.81661400	-1.24211400	-0.31730300
O	3.76001900	-0.28732600	0.25496800
H	4.04864600	-1.21044200	0.20415500
N	0.50374800	1.21279900	-0.31054900
H	0.24510800	2.01266000	-0.86224200
O	-1.01357200	-1.44837200	-0.42297800
H	-0.05602600	-1.31299500	-0.56477000
O	-2.29977300	0.60958800	-1.18905100
H	-3.25737400	0.71020500	-1.14803700
O	-2.87261900	-0.46130300	1.08074200

NE5 structure in gas-phase at B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.70468771u.a.; Zero-point correction = 0.133256 u.a.; G=-891.609106u.a. at298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.77565800	-0.18056400	0.12970500
C	-0.43267000	0.87391500	0.77886600
H	0.07497200	0.28274700	1.54101200
H	-0.87473600	1.73828000	1.28182000
C	1.90230800	1.17376900	0.00237200
H	2.45664300	1.74265500	-0.74554300
H	2.18533500	1.59290100	0.97831900
C	2.43726800	-0.24857500	-0.04745900
O	1.79506600	-1.23666300	-0.31273400
O	3.74699900	-0.29134900	0.25252500
H	4.03403700	-1.21505000	0.20526500
N	0.49658500	1.21284800	-0.29341900
H	0.21414100	2.02798500	-0.81007800
O	-1.02266600	-1.43125400	-0.49319300
H	-0.06122500	-1.30162200	-0.60996400
O	-2.29121800	0.67404400	-1.15006300
H	-3.24525300	0.79373500	-1.08647900
O	-2.86150300	-0.49449800	1.07238100

NE6 structure in gas-phase at B3LYP/6-311++G (2d,2p).
E (SCF) = -891.68857938 u.a.; Zero-point correction = 0.133215 u.a.; G=-891.593259u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.76580100	-0.07324400	-0.06912000
C	-0.44940200	0.92478800	0.71288700
H	0.00635300	0.32405100	1.49942900
H	-0.89129500	1.80676600	1.18554000
C	1.92983800	1.16757700	0.02745200
H	2.51545300	1.75131800	-0.68427700
H	2.18069300	1.56085200	1.02273500
C	2.45605900	-0.25866400	-0.03773900
O	1.81380900	-1.23941900	-0.32835900
O	3.76135700	-0.31696900	0.28143500
H	4.03820800	-1.24314600	0.22241000
N	0.53683200	1.23497600	-0.31748100
H	0.29156500	2.04534900	-0.86016900
O	-2.69315500	-0.56152400	1.15819400
H	-3.60290100	-0.28013900	1.01180200
O	-1.02998800	-1.42569600	-0.46727000
H	-0.07074500	-1.31907100	-0.61707700
O	-2.52166200	0.64431300	-1.11110500

NE6 structure in gas-phase at B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.70474117 u.a.; Zero-point correction = 0.133393 u.a.; G= -891.609031u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.75888300	-0.06933100	-0.06813900
C	-0.42631000	0.88422400	0.73580400
H	0.04644200	0.23687600	1.47377100
H	-0.85142200	1.74035400	1.26740400
C	1.92983100	1.17205800	0.02036300
H	2.50975300	1.74326900	-0.70596300
H	2.19820700	1.57077000	1.00922600
C	2.44245800	-0.25836200	-0.03913100
O	1.78951000	-1.23406500	-0.32354400
O	3.74739700	-0.32494500	0.27882700
H	4.02073800	-1.25230100	0.22375300
N	0.53281700	1.23928800	-0.30525000
H	0.27052500	2.06760200	-0.81198300
O	-2.67649800	-0.59863600	1.14997200
H	-3.58198600	-0.29298900	1.02869300
O	-1.03649500	-1.40757800	-0.53172700
H	-0.07316400	-1.30447900	-0.65455400
O	-2.51909500	0.69876500	-1.07024300

NE7 structure in gas-phase at B3LYP/6-311++G (2d,2p).
E (SCF) = -891.68813094 u.a.; Zero-point correction = 0.133365 u.a.; G=-891.593644u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
C	1.46411800	0.07733700	0.85716700
H	0.98677900	1.05273700	0.77701500
H	1.86502600	0.01407000	1.87140900
C	2.65027100	0.02052600	-0.09441000
O	3.43224300	1.11454500	0.02248900
O	2.89365600	-0.89051700	-0.84299700
N	0.48846300	-0.98092600	0.64972300
H	-1.44735800	-0.78599500	1.71453500
C	-0.34350800	-0.83545300	-0.55734700
H	0.16664600	-0.36650900	-1.40180500
H	-0.66893400	-1.82189400	-0.88462900
P	-1.88130800	0.07702500	-0.17728800
O	-2.96582500	0.02566700	-1.16639700
O	-1.33894600	1.58178600	0.09775000
O	-2.26182100	-0.49665200	1.26790500
H	0.96917700	-1.87021000	0.61073100
H	-1.95352800	2.23346200	-0.25935100
H	4.18282600	1.00235800	-0.57909700

NE7 structure in gas-phase at B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.609031u.a. ; Zero-point correction = 0.133615 u.a; G= -891.609728u.a. at298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
C	1.44668300	-0.01796300	0.88947400
H	0.95860200	0.95512800	0.91034900
H	1.87788800	-0.16900000	1.88119600
C	2.60151100	0.02990600	-0.09974700
O	3.37760300	1.11577500	0.10037700
O	2.82145000	-0.80031900	-0.94354200
N	0.47758600	-1.06598400	0.61161800
H	-1.42203200	-0.85543600	1.67437000
C	-0.34384100	-0.84725200	-0.59194100
H	0.18362600	-0.35703100	-1.41292500
H	-0.69822900	-1.80887800	-0.95953400
P	-1.85176400	0.09518300	-0.17208800
O	-2.94236100	0.10754700	-1.15571400
O	-1.26326900	1.57484700	0.14462700
O	-2.23246700	-0.51021800	1.25982300
H	0.96158200	-1.94949300	0.52100400
H	-1.84989700	2.25195200	-0.21156800
H	4.10804700	1.07769900	-0.53417600

NE8 structure in gas-phase at B3LYP/6-311++G (2d,2p).
E (SCF) =-891.68860826 u.a.; Zero-point correction = 0.133134 u.a.; G=-891.594693u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	2.01038700	0.07305900	0.18595000
C	0.23018900	0.06131300	0.56975500
H	-0.09428400	1.07638500	0.81200300
H	0.12023400	-0.55401000	1.46348700
C	-1.85899000	-0.96602200	-0.22153600
H	-2.26040000	-1.57714500	-1.03365700
H	-1.86217400	-1.59946600	0.66561600
C	-2.83310100	0.18579400	-0.01182200
O	-2.61271600	1.33600000	-0.28813800
O	-4.00641900	-0.24451100	0.50052700
H	-4.59121900	0.52383700	0.57619000
N	-0.50156000	-0.56385400	-0.54076400
H	1.49051900	-1.74756200	-0.79905000
O	2.93028300	0.52167800	1.23818200
O	2.04840800	0.97895500	-1.15574500
H	2.78231400	1.60312600	-1.12988200
O	2.27273800	-1.42194800	-0.32628500
H	-0.51680700	0.07803100	-1.32531700

NE8 structure in gas-phase at B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.70425371 ua. Zero-point correction = 0.133332 u.a.; G= -891.609954u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.99464600	-0.08515400	-0.18486900
C	0.21819000	-0.06116900	-0.57261300
H	-0.12430600	-1.07838800	-0.77674500
H	0.11420100	0.52751700	-1.48460600
C	-1.85902100	0.98598400	0.20556700
H	-2.26971200	1.60115700	1.00945400
H	-1.87862200	1.60422300	-0.69226900
C	-2.80771500	-0.18999000	0.01559800
O	-2.55336100	-1.33127000	0.29997600
O	-3.99400100	0.20811000	-0.49238300
H	-4.56288700	-0.57264800	-0.56080600
N	-0.49472900	0.60999200	0.52369000
H	1.52290000	1.79347100	0.71109800
O	2.90982600	-0.61897700	-1.20051000
O	2.00098600	-0.90552500	1.21237700
H	2.71387900	-1.55369400	1.22379600
O	2.28825400	1.43247200	0.23724500
H	-0.49441000	-0.00170400	1.33234300

NE9 structure in gas-phase at B3LYP/6-311++G (2d,2p).
E (SCF) = -891.68628826 u.a.; Zero-point correction = 0.133142 u.a.; G=-891.590957u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.78406900	-0.16360700	0.14473900
C	-0.44451100	0.93961500	0.72852900
H	0.05182700	0.41563100	1.54578500
H	-0.91551700	1.82312400	1.16591300
C	1.91280400	1.16836900	-0.00725300
H	2.49845600	1.71790400	-0.74569200
H	2.18671000	1.58607400	0.97244300
C	2.41191600	-0.26541800	-0.02992600
O	1.74364900	-1.25022800	-0.24329600
O	3.72682800	-0.33178400	0.23459800
H	3.98646400	-1.26482600	0.21704300
N	0.51113200	1.25746600	-0.33552400
H	0.29027800	2.13353600	-0.77996700
O	-1.04038500	-1.41007900	-0.52694400
O	-2.41158400	0.60634100	-1.13195300
H	-2.05975700	0.26603600	-1.96029100
O	-2.77757800	-0.45567800	1.18253300
H	-0.06403400	-1.34960900	-0.50524900

NE9 structure in gas-phase at B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.70284885 u.a.; Zero-point correction = 0.133515 u.a. ; G=-891.606785u.a.at 298,15K.

Charge = 0;Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.78059100	-0.16721200	0.13918700
C	-0.42491400	0.88681000	0.76825200
H	0.09038200	0.30360700	1.53140100
H	-0.87439600	1.74396100	1.27464900
C	1.90753100	1.17118200	-0.00427900
H	2.48166600	1.71606400	-0.75511300
H	2.20002100	1.58892100	0.97013900
C	2.40063900	-0.26372800	-0.03224200
O	1.72614500	-1.24503100	-0.24227500
O	3.71675800	-0.33270700	0.22448500
H	3.97814200	-1.26509000	0.20381400
N	0.50011300	1.25617000	-0.30699700
H	0.25981700	2.14832200	-0.70767800
O	-1.04640600	-1.40014400	-0.56684600
O	-2.37821100	0.66264000	-1.11430800
H	-1.95371900	0.40593700	-1.93880000
O	-2.79365500	-0.47783200	1.15203900
H	-0.07043500	-1.34773100	-0.53240000

2-Structures and energetics of glyphosate conformers in gas-phase, at MP2/6-311++G (2d,2p) level.

NE1 structure in gas-phase at MP2/6-311++G (2d,2p).
E (SCF) =-889.93469669 u.a.; Zero-point correction = 0.135109 u.a.; G=-889.836395u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-1.30187800	-0.25284600	-0.14165200
C	-0.86155400	1.50845300	-0.11485900
H	-1.56999700	2.03592600	0.51892100
H	-0.97639300	1.89328700	-1.12645300
C	1.56841200	1.15665700	-0.38417400
H	1.30767400	1.08334500	-1.43653000
H	2.47154200	1.76526000	-0.31900000
C	1.96094000	-0.22377800	0.10307100
O	1.60320700	-0.72465100	1.15430100
O	2.83602900	-0.81066000	-0.72552700
H	3.04122000	-1.67803900	-0.34943800
N	0.49399000	1.79202000	0.35371000
H	0.57805900	1.58948900	1.34041800
O	-2.89152700	-0.20745500	-0.34833900
H	-3.19241800	-0.97116600	-0.85187200
O	-1.18257800	-0.73373400	1.38007600
H	-0.24563800	-0.90719100	1.57522400
O	-0.53395600	-1.04979400	-1.12634800

NE2 structure in gas-phase at MP2/6-311++G (2d,2p).
E (SCF) = -889.93232888 u.a.; Zero-point correction = 0.135045 u.a.; G=-889.834036u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-1.52896700	-0.19167500	0.07342200
C	-0.87912200	1.50936600	0.11697000
H	-1.57125400	2.10737000	-0.47223600
H	-0.96038400	1.85903100	1.14440600
C	1.56317700	1.15222600	0.36773000
H	1.30876900	1.08299000	1.42221600
H	2.45229300	1.78147100	0.30019000
C	1.99810300	-0.21930800	-0.10590500
O	1.61178500	-0.77418500	-1.11846500
O	2.94334400	-0.74197800	0.69238800
H	3.19557000	-1.59384300	0.30892700
N	0.47457000	1.75387000	-0.36899100
H	0.54932200	1.55713800	-1.35672700
O	-1.14211300	-0.75381900	-1.36755800
H	-0.17563000	-0.82872200	-1.46861000
O	-0.49980600	-0.93141000	1.09406100
H	-0.96508000	-1.61711700	1.58613000
O	-2.95246300	-0.34910500	0.41764200

NE3 structure in gas-phase at MP2/6-311++G (2d,2p).
E (SCF) = -889.93218322 u.a.; Zero-point correction = 0.135102 u.a.; G=-889.833818 u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.31793000	-0.26133300	-0.13680800
C	0.88237800	1.49833400	-0.10091800
H	1.00057900	1.88917400	-1.11690500
H	1.59470100	1.99924600	0.54954700
C	-1.54131800	1.13692000	-0.35555300
H	-2.41424100	1.78334700	-0.27856100
H	-1.29619100	1.04900600	-1.41615400
C	-1.99260900	-0.23242300	0.11450500
O	-1.60819700	-0.82329600	1.10229500
O	-2.94707200	-0.71721500	-0.70207500
H	-3.17691600	-1.59490900	-0.36738200
N	-0.45933100	1.67020000	0.45067100
H	-0.62202800	2.64058200	0.66117900
O	2.91250500	-0.22623900	-0.30536400
H	3.18582100	-0.87306000	-0.96388600
O	1.16460500	-0.74934000	1.36784600
H	0.21313900	-0.77494500	1.58505400
O	0.58700900	-1.02226500	-1.17566300

NE4 structure in gas-phase at MP2/6-311++G (2d,2p).
E (SCF) = -889.93059745 u.a.; Zero-point correction = 0.134884 u.a.; G=-889.832654u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.54346600	-0.19787900	-0.06993600
C	-0.89138300	1.49655100	-0.11364700
H	-1.58619100	2.07713800	0.48878200
H	-0.96636900	1.85037300	-1.14656400
C	1.54133200	1.13333500	-0.33891100
H	1.30276900	1.05559100	-1.40186500
H	2.39711200	1.80141300	-0.25514300
C	2.02864800	-0.22747000	0.11674000
O	1.62525800	-0.85943500	1.07010100
O	3.03287000	-0.65909400	-0.67340600
H	3.30370200	-1.52177200	-0.33003900
N	0.44202500	1.62525400	0.46592900
H	0.60601900	2.57945100	0.73897200
O	-1.13983900	-0.77187000	1.35259400
H	-0.17315700	-0.72393000	1.48751900
O	-0.53670100	-0.90726100	-1.13064400
H	-0.97173400	-1.65825500	-1.54937300
O	-2.97232700	-0.33772900	-0.39737600

NE5 structure in gas-phase at MP2/6-311++G (2d,2p).
E (SCF) = -889.92902601 u.a.; Zero-point correction = 0.134688 u.a.; G=-889.831849u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.77617300	-0.18208200	0.13225000
C	-0.39095500	0.77938400	0.80257000
H	0.14619600	0.11749000	1.47942400
H	-0.76818100	1.61542100	1.39271600
C	1.89309100	1.17451700	-0.00503900
H	2.42822000	1.74428100	-0.76280400
H	2.15952400	1.60455700	0.96628400
C	2.43689300	-0.23853000	-0.05181400
O	1.80761000	-1.22580000	-0.36948000
O	3.73620000	-0.27613300	0.30662100
H	4.01766700	-1.19949100	0.24127300
N	0.48372200	1.16189100	-0.30436500
H	0.17272000	2.01448000	-0.73928900
O	-1.05432700	-1.39216600	-0.59864300
H	-0.10816800	-1.22150800	-0.75452500
O	-2.28723000	0.79341600	-1.05540300
H	-3.24147800	0.89813400	-0.97898300
O	-2.85027000	-0.55776800	1.07045500

NE6 structure in gas-phase at MP2/6-311++G (2d,2p).
E (SCF) = -889.92903597 u.a.; Zero-point correction = 0.134838 u.a.; G=-889.831688u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.76097500	-0.05755800	-0.05648900
C	-0.38754600	0.80018800	0.75941400
H	0.11228400	0.08936500	1.41402800
H	-0.74990600	1.62666100	1.37221600
C	1.92209800	1.17468300	0.01145900
H	2.48437500	1.74583900	-0.72521500
H	2.17635400	1.58326400	0.99546900
C	2.44023000	-0.24788200	-0.04606900
O	1.79949200	-1.22087700	-0.38456600
O	3.73356200	-0.31326000	0.33088500
H	3.99950300	-1.24047600	0.25650500
N	0.52049600	1.19530100	-0.31702600
H	0.23045900	2.05903800	-0.74477000
O	-2.64794100	-0.66980200	1.13953400
H	-3.54126000	-0.31654500	1.08123700
O	-1.06443900	-1.36936300	-0.62259000
H	-0.11578700	-1.22978100	-0.79143800
O	-2.52987000	0.80042300	-0.98080600

NE7 structure in gas-phase at MP2/6-311++G (2d,2p).
E (SCF) = -889.92950786 u.a.; Zero-point correction = 0.134903 u.a.; G=-889.833263u.a. at298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
C	1.42520700	-0.03605100	0.89712200
H	0.92427000	0.92736000	0.93388900
H	1.85754500	-0.20965900	1.88158400
C	2.57189900	0.03356100	-0.09254200
O	3.31738200	1.14651800	0.09424700
O	2.81723400	-0.80792500	-0.92765300
N	0.46876700	-1.08716800	0.58527100
H	-1.38662200	-0.95064900	1.59065400
C	-0.32862400	-0.80947800	-0.62233100
H	0.21628300	-0.27842100	-1.40302300
H	-0.67113600	-1.75153100	-1.04360900
P	-1.83489700	0.10235600	-0.17132600
O	-2.92376000	0.16922600	-1.16048900
O	-1.23790400	1.55610100	0.22567700
O	-2.21090400	-0.58795100	1.21893700
H	0.97963800	-1.94732900	0.43787800
H	-1.83224000	2.24820600	-0.08428500
H	4.04708400	1.10091700	-0.53934700

NE8 structure in gas-phase at MP2/6-311++G 2d, 2p).
E (SCF) = -889.92957529 u.a.; Zero-point correction = 0.134635 u.a.; G=-889.833834u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.97264400	0.08769700	0.19046000
C	0.20676300	0.02085100	0.57776400
H	-0.16112200	1.01977800	0.81329600
H	0.10561000	-0.60654300	1.46171000
C	-1.84845400	-0.99932800	-0.23384200
H	-2.26903700	-1.58523400	-1.05043100
H	-1.86701300	-1.63159100	0.65078800
C	-2.76689500	0.18884100	-0.01650500
O	-2.51000600	1.32739000	-0.33530800
O	-3.93546400	-0.18780500	0.55351800
H	-4.48074400	0.60867200	0.61980300
N	-0.48014600	-0.63007800	-0.54674700
H	1.49298100	-1.74815600	-0.74403900
O	2.90166200	0.60136300	1.20938400
O	1.92078800	0.95203500	-1.17548200
H	2.69020600	1.52724500	-1.24083000
O	2.27297300	-1.41401800	-0.27428200
H	-0.48761200	0.01702000	-1.32711200

NE9 structure in gas-phase at MP2/6-311++G (2d,2p).
E (SCF) = -889.92704437 u.a.; Zero-point correction = 0.134945 u.a.; G=-889.829329u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.77610700	-0.16861200	0.14176800
C	-0.39200900	0.81777900	0.78661900
H	0.14944000	0.18027700	1.48329200
H	-0.79273300	1.65072600	1.36421500
C	1.90173400	1.17430400	-0.00087300
H	2.46662000	1.72433000	-0.75147800
H	2.17761800	1.58915400	0.97499000
C	2.39311400	-0.25577500	-0.03886900
O	1.72019400	-1.23261600	-0.30011100
O	3.70251400	-0.33036600	0.26360600
H	3.94911400	-1.26510800	0.22039500
N	0.49184600	1.22537600	-0.31079200
H	0.23139300	2.13746700	-0.65018800
O	-1.06292400	-1.36835400	-0.63660500
O	-2.37305900	0.74076500	-1.05106700
H	-1.95903900	0.51672900	-1.88911300
O	-2.78051200	-0.52264900	1.15387400
H	-0.09047300	-1.29410500	-0.62192300

3-Structures and energetics of glyphosate conformers in gas-phase, at RHF/6-311++G (2d,2p) level.

NE1 structure in gas-phase at RHF /6-311++G (2d,2p).
E (SCF) = -888.07986980 u.a.; Zero-point correction = 0.144641 u.a.; G=-887.971677u.a. at298,15K.

Charge = 0 Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.35474000	-0.23950100	-0.13833300
C	-0.83219400	1.49180900	-0.05120100
H	-1.50899100	2.01718100	0.60793800
H	-0.96391500	1.91196300	-1.04004200
C	1.60321300	1.14623000	-0.35721000
H	1.34902800	1.09310300	-1.40495200
H	2.48743700	1.76940200	-0.28021300
C	2.03424100	-0.23344500	0.08956800
O	1.65717700	-0.77960500	1.07624600
O	2.94316700	-0.75064200	-0.70730100
H	3.17911600	-1.61023400	-0.39341800
N	0.52699300	1.72837900	0.39938900
H	0.62510900	1.53708200	1.37109500
O	-2.91101600	-0.11874700	-0.32623400
H	-3.27609300	-0.80671800	-0.85744800
O	-1.23249600	-0.80515000	1.31988800
H	-0.34912000	-1.08500400	1.51995000
O	-0.67457900	-1.01591500	-1.15392200

NE2 structure in gas-phase at RHF /6-311++G (2d,2p).
E (SCF) =-888.07663292 u.a.; Zero-point correction =0.144608 u.a.; G=-887.968467u.a. at 298,15K.

Charge = 0 Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.55900000	-0.17756000	0.06739000
C	-0.84504600	1.49028200	0.09031200
H	-1.51439400	2.09502100	-0.50666700
H	-0.93279600	1.85519600	1.10532500
C	1.60592200	1.14341600	0.34646500
H	1.37427900	1.09391200	1.40026900
H	2.47657600	1.78374300	0.25457600
C	2.06601400	-0.22796400	-0.09627300
O	1.65824000	-0.81743300	-1.04446600
O	3.03477400	-0.69374100	0.66369500
H	3.30925500	-1.53709400	0.33666500
N	0.50680600	1.69920200	-0.38895300
H	0.58738700	1.53025600	-1.36572300
O	-1.19219600	-0.79656000	-1.32123700
H	-0.26481500	-0.95109300	-1.45056000
O	-0.65873100	-0.96488600	1.11368500
H	-1.16014100	-1.57476800	1.62949100
O	-2.96700300	-0.22245500	0.37149900

NE3 structure in gas-phase at RHF /6-311++G (2d,2p).
E (SCF) = -888.07733043 u.a.; Zero-point correction = 0.144636 u.a.; G=-887.969145u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.37421100	-0.24646900	-0.13631100
C	0.85667400	1.48194500	-0.02756800
H	0.99685200	1.92118800	-1.01327900
H	1.53184500	1.97563900	0.65692200
C	-1.57311100	1.12136600	-0.33075200
H	-2.42637100	1.78294200	-0.25511000
H	-1.32408500	1.04939300	-1.38336500
C	-2.06815200	-0.24387500	0.09752800
O	-1.66690800	-0.88428300	1.00995900
O	-3.06110300	-0.64856100	-0.67213500
H	-3.32665000	-1.51362400	-0.40051700
N	-0.49347200	1.61461200	0.48437400
H	-0.66335800	2.54740700	0.77530600
O	2.93654000	-0.13492800	-0.27633500
H	3.28727300	-0.73865300	-0.90941400
O	1.20776100	-0.83383700	1.29958100
H	0.29389400	-0.96381300	1.52680700
O	0.73111900	-0.97618300	-1.20838900

NE4 structure in gas-phase at RHF /6-311++G(2d,2p).
E (SCF) =-888.07522733 u.a.; Zero-point correction = 0.144523 u.a.; G=-887.967310u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.57934800	-0.18214900	-0.06262700
C	-0.86116400	1.47927300	-0.07728400
H	-1.52626600	2.06403900	0.54295300
H	-0.94919100	1.86056200	-1.09191900
C	1.57881600	1.11567200	-0.32691000
H	1.34516300	1.04400900	-1.38365400
H	2.41507100	1.79764200	-0.24401500
C	2.10312100	-0.23786800	0.10254800
O	1.67930000	-0.91019800	0.98033500
O	3.14285600	-0.59826400	-0.62879500
H	3.44223800	-1.44694600	-0.34066000
N	0.47675400	1.57713000	0.47243800
H	0.64413100	2.49214200	0.81559800
O	-1.18875700	-0.81617900	1.30498700
H	-0.25236900	-0.84777300	1.46807200
O	-0.70264600	-0.93812300	-1.14941700
H	-1.19719400	-1.58497000	-1.62499400
O	-2.99241400	-0.21584200	-0.34450400

NE5 structure in gas-phase at RHF /6-311++G (2d,2p).
E (SCF) = -888.07543571 u.a.; Zero-point correction = 0.144202 u.a.; G=-887.968530 u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.79283300	-0.16776700	0.12747800
C	-0.42022400	0.82279500	0.75927000
H	0.07495800	0.21225800	1.50211300
H	-0.81731800	1.69063900	1.27405900
C	1.89738000	1.15206800	-0.00566000
H	2.43751800	1.72717000	-0.74614400
H	2.14643900	1.58074600	0.96249100
C	2.47373900	-0.24556100	-0.04375200
O	1.87319800	-1.23168500	-0.30568500
O	3.75991000	-0.25039000	0.25715000
H	4.08310000	-1.13783300	0.21994000
N	0.49968800	1.14912300	-0.31676100
H	0.21969900	1.96642300	-0.80463000
O	-1.11020100	-1.42404100	-0.49454700
H	-0.19066700	-1.33078200	-0.70908300
O	-2.30764300	0.68896100	-1.10143900
H	-3.24535600	0.78291900	-1.08970000
O	-2.84264800	-0.45718400	1.07414100

NE6 structure in gas-phase at RHF /6-311++G(2d,2p).
E (SCF) = -888.07568945 u.a.; Zero-point correction = 0.144251 u.a.; G=-887.968787u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.77925300	-0.06263700	-0.05923900
C	-0.41183900	0.81934200	0.72306600
H	0.05155900	0.15198700	1.43597400
H	-0.78822600	1.67687300	1.27061200
C	1.92196300	1.14976500	0.00658700
H	2.47976800	1.72456700	-0.72076800
H	2.15998800	1.56882800	0.98206900
C	2.48439500	-0.25392100	-0.03095600
O	1.87674500	-1.23427500	-0.29858300
O	3.76842900	-0.27234900	0.28044200
H	4.08308500	-1.16269700	0.24148200
N	0.53104700	1.16239400	-0.32717800
H	0.25814500	1.98221700	-0.81535300
O	-2.69180300	-0.54573000	1.13217000
H	-3.58447200	-0.26291600	1.02856900
O	-1.13441500	-1.40083400	-0.54074000
H	-0.21290200	-1.34724100	-0.75892800
O	-2.49927800	0.72569500	-1.03291400

NE7 structure in gas-phase at RHF /6-311++G (2d,2p).
E (SCF) = -888.07492113 u.a.; Zero-point correction = 0.144411 u.a.; G=-887.968412u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
C	1.49296700	0.21251000	0.82686400
H	1.05485200	1.17567400	0.61576200
H	1.88961800	0.26966800	1.83338000
C	2.67723500	0.00221000	-0.09213300
O	3.48736600	1.04904700	-0.09814100
O	2.88682800	-0.98043400	-0.71476700
N	0.49800000	-0.82714300	0.75229900
H	-1.74172500	-0.60476000	1.82055600
C	-0.32603700	-0.82586000	-0.45351600
H	0.17263700	-0.42761100	-1.32877400
H	-0.61157200	-1.84063600	-0.69314100
P	-1.87914800	0.05753400	-0.19528000
O	-2.84099900	-0.00972100	-1.26516000
O	-1.40462500	1.53442100	0.13093000
O	-2.41662900	-0.50746700	1.16725500
H	0.94245500	-1.71322300	0.84239800
H	-1.99174700	2.18482200	-0.21797700
H	4.22618300	0.86312200	-0.65733100

NE8 structure in gas-phase at RHF /6-311++G (2d,2p).
E (SCF) = -888.07631875 u.a.; Zero-point correction = 0.144265 u.a.; G=-887.970176u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.99040800	-0.08752000	-0.17638900
C	0.23296600	-0.03773800	-0.57001500
H	-0.09848200	-1.03880600	-0.81942400
H	0.14495000	0.57409500	-1.45866300
C	-1.85394300	0.96834700	0.19896600
H	-2.25879400	1.58354300	0.99368400
H	-1.86726900	1.57647400	-0.69454800
C	-2.81979600	-0.18322000	0.01429900
O	-2.59275500	-1.30940400	0.28998500
O	-3.98355200	0.22426400	-0.46811100
H	-4.56566000	-0.51727100	-0.53507800
N	-0.50619100	0.58160900	0.52103200
H	1.70863700	1.80441300	0.76048600
O	2.85550700	-0.65299300	-1.17859600
O	2.00957800	-0.86676200	1.20102400
H	2.69717400	-1.51008600	1.24641400
O	2.34667000	1.39469900	0.19816900
H	-0.51229300	-0.03359600	1.30648400

NE9 structure in gas-phase at RHF/6-311++G (2d,2p).
E (SCF) = -888.07251627 u.a.; Zero-point correction = 0.144391 u.a.; G=-887.965201u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.78713800	-0.15730000	0.13648900
C	-0.41921900	0.85760200	0.74746500
H	0.08287400	0.27025400	1.50425200
H	-0.84130900	1.71788000	1.25358600
C	1.90279400	1.15586600	-0.00789900
H	2.46777500	1.70327700	-0.75058800
H	2.16989400	1.57728100	0.95933900
C	2.42193500	-0.26262600	-0.02997700
O	1.77382900	-1.23504400	-0.23119600
O	3.71651400	-0.31075700	0.21589100
H	4.00315600	-1.21152800	0.20182700
N	0.50430400	1.21522300	-0.32084000
H	0.26527200	2.09289700	-0.71889400
O	-1.10726300	-1.38358100	-0.56598300
O	-2.38661700	0.65871000	-1.07732700
H	-2.05955500	0.38929800	-1.91696200
O	-2.75731800	-0.45479300	1.15496200
H	-0.15739700	-1.38777300	-0.56232700

4-Structures and energetics of glyphosate conformers in aqueous solution, at SMD-B3LYP-D3/6-311++G (2d,2p)and B3LYP/6-311++G (2d,2p)levels.

ZWP1 structure in aqueous solution, at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.752458365 u.a.;Zero-point correction =0.135753 u.a. ; G= -891.655650u.a. at 298,15K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	2.03619300	0.01720600	0.12548400
C	0.30238300	-0.25661500	0.66929100
H	-0.14179200	0.67019200	1.01927400
H	0.28260200	-0.99742800	1.46413500
C	-1.94853000	-1.06916200	-0.11881600
H	-2.38012500	-1.68378200	-0.90714500
H	-1.98393100	-1.61907100	0.81670100
C	-2.73488600	0.21520800	-0.02902400
O	-2.33323800	1.28283900	-0.43490600
O	-3.92998200	0.00858600	0.52497600
H	-4.43282700	0.84024800	0.52998300
N	-0.52933800	-0.77988300	-0.46517500
H	-0.09439500	-1.63414400	-0.82073200
O	2.79075700	0.57732000	1.29709400
O	1.85358900	1.14901100	-1.04191900
H	1.70510000	2.02864200	-0.67026200
O	2.49438500	-1.22328600	-0.59016200
H	-0.51004100	-0.09591100	-1.22736900

ZWP1 structure in aqueous solution, at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.736248815 u.a.;Zero-point correction= 0.136223 u.a.; G = -891.638392 u.a. at 298,15K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	2.05470700	0.00292000	0.11026600
C	0.32983800	-0.33283500	0.65525500
H	-0.10102100	0.54291700	1.13145000
H	0.33296300	-1.16196900	1.35795800
C	-1.95274500	-1.05381100	-0.13398400
H	-2.37778400	-1.67102800	-0.92390000
H	-1.96186100	-1.61605700	0.79480500
C	-2.76918600	0.21000900	-0.02292500
O	-2.39618400	1.29029800	-0.42346800
O	-3.95449100	-0.02594200	0.53905000
H	-4.47281200	0.79610000	0.55444400
N	-0.54629300	-0.72332200	-0.49788700
H	-0.12712700	-1.53079300	-0.96390000
O	2.84200400	0.35614900	1.34041700
O	1.88194900	1.31190700	-0.85267900
H	1.78880400	2.12784600	-0.34291500
O	2.48125800	-1.11376400	-0.80192800
H	-0.56145400	0.04307300	-1.17793200

ZWP2 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.752006183 u.a.;Zero-point correction= 0.135715 u.a ; G = -891.655269u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-2.04470000	0.01764900	0.14036400
C	-0.29414700	-0.21040500	0.65230900
H	-0.25089800	-0.94784300	1.44947500
H	0.13665400	0.72548500	0.99349000
C	1.94495600	-1.05267900	-0.14072800
H	1.96279100	-1.61982400	0.78488500
H	2.36652000	-1.66294400	-0.93782100
C	2.75949500	0.21189600	-0.02524800
O	2.38493400	1.29459400	-0.41686600
O	3.94552400	-0.03057400	0.53347300
H	4.46581200	0.78988400	0.55725400
N	0.53424900	-0.72622200	-0.48868500
H	0.53646700	-0.02735600	-1.23768500
O	-2.46578700	-1.22878000	-0.59332800
O	-1.94222000	1.25428100	-0.92558400
H	-1.86627500	0.93230800	-1.83326500
O	-2.79316300	0.52306500	1.33781000
H	0.08354900	-1.56443300	-0.86304800

ZWP2 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.735803244 u.a.;Zero-point correction= 0.136039 u.a ; G = -891.638448u.a. at298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-2.05630200	0.00160200	0.12092900
C	-0.32266100	-0.33881000	0.63390400
H	-0.31888800	-1.18912200	1.31071900
H	0.10668600	0.52347500	1.13464600
C	1.95538300	-1.04318200	-0.17625300
H	1.95740900	-1.64060100	0.73040200
H	2.38090000	-1.63236500	-0.98703600
C	2.77727500	0.21132200	-0.01482100
O	2.41302000	1.30730700	-0.37908200
O	3.95738800	-0.05070000	0.54637500
H	4.47785200	0.76853000	0.59713600
N	0.55146000	-0.69394500	-0.53258700
H	0.57173500	0.09194600	-1.18976500
O	-2.46601000	-1.05636700	-0.86933700
O	-1.94046700	1.44173100	-0.64378100
H	-1.80568500	1.33544600	-1.59443100
O	-2.83574500	0.24371900	1.38058500
H	0.12882900	-1.48522700	-1.02255200

ZWP3 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.752291005u.a.;Zero-point correction= 0.136017u.a. ; G = -891.654394u.a. at 298,15K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-1.98664200	-0.23073700	0.06567200
C	-0.29244200	0.18641300	0.64422500
H	0.19787000	-0.71402400	1.00253400
H	-0.32953200	0.92535900	1.43967700
C	1.94195800	1.06879500	-0.10804500
H	2.36727100	1.70644000	-0.88138600
H	1.95462600	1.60363800	0.83671400
C	2.75727000	-0.19844100	-0.03066700
O	2.39034500	-1.26580800	-0.46856200
O	3.93528300	0.02387500	0.55338800
H	4.45689900	-0.79611800	0.55208300
N	0.53367500	0.75202400	-0.47400300
H	0.08616000	1.60427900	-0.81783200
O	-1.86432600	-1.01245200	-1.21282900
O	-2.57101000	1.23417000	-0.36925700
H	-2.84586300	1.74983300	0.40063900
O	-2.73982700	-0.76777800	1.24917000
H	0.53203100	0.08082100	-1.24783900

ZWP3 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.736043366 u.a.; Zero-point correction=0.135862u.a. ; G =-891.638906u.a. at 298,15K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-2.00721000	-0.22403700	0.07333300
C	-0.31069700	0.21507900	0.63589000
H	0.16074200	-0.66437700	1.06502400
H	-0.34726200	1.00604600	1.37991700
C	1.94318000	1.05202000	-0.12566500
H	2.35557600	1.68908000	-0.90661200
H	1.93438300	1.60411800	0.80910000
C	2.79169100	-0.19099700	-0.02413300
O	2.45413400	-1.27495100	-0.44453300
O	3.96377400	0.06940300	0.55577500
H	4.50369700	-0.73864600	0.56495400
N	0.54581800	0.69476800	-0.49911900
H	0.10689700	1.51602200	-0.92034500
O	-1.89304700	-1.07017700	-1.16349400
O	-2.59963800	1.21348000	-0.43321600
H	-2.88759100	1.76379700	0.30744300
O	-2.75709600	-0.70032600	1.28491300
H	0.57091800	-0.03490500	-1.21775000

ZWP4 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.751895541 u.a.; Zero-point correction= 0.136038u.a. ; G = -891.654164u.a. at298,15K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	1.99207100	-0.22842400	-0.07687800
C	0.30539700	0.18567600	-0.67926800
H	-0.18350600	-0.71971300	-1.02724200
H	0.35662000	0.91011800	-1.48670200
C	-1.94237400	1.06781800	0.02719700
H	-2.36582100	1.76317100	0.75006100
H	-1.95423100	1.53024000	-0.95509700
C	-2.75901300	-0.19976200	0.04397800
O	-2.37737200	-1.24224300	0.52708800
O	-3.95484000	-0.00845600	-0.51379100
H	-4.47587700	-0.82644300	-0.44943000
N	-0.53495700	0.77339100	0.41593400
H	-0.09800100	1.63744900	0.74351800
O	1.85332900	-1.02736600	1.19213300
O	2.59662000	1.24898600	0.28699500
H	2.45811900	1.46812800	1.21770200
O	2.76249500	-0.74501500	-1.25591000
H	-0.53959300	0.12002900	1.20526200

ZWP4 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.735629873u.a.; Zero-point correction= 0.135620u.a. ; G = -891.639258 u.a. at 298,15K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-2.01091800	-0.22199400	0.08469700
C	-0.31816400	0.20992400	0.66281300
H	0.15317600	-0.68058000	1.06901400
H	-0.36396800	0.97756100	1.42989200
C	1.94538900	1.05568400	-0.05275800
H	2.35798800	1.74687800	-0.78608300
H	1.93897100	1.53891100	0.91930900
C	2.79174400	-0.19272000	-0.04054000
O	2.44497100	-1.24799800	-0.52209800
O	3.97201800	0.02919000	0.53846800
H	4.51054700	-0.77857400	0.49130900
N	0.54732600	0.72544400	-0.44904900
H	0.11714300	1.56389500	-0.84444200
O	-1.89180000	-1.07677100	-1.14880600
O	-2.62694400	1.23544700	-0.33178800
H	-2.52944100	1.40866200	-1.27718400
O	-2.76594600	-0.68774600	1.29501300
H	0.57587300	0.02075200	-1.19232900

ZWP5 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.751756708 u.a.; Zero-point correction= 0.136319 u.a ; G = -891.653626u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.95717300	0.04978900	0.17846000
C	0.82431900	-0.89638800	-0.92328200
H	1.19881200	-1.91464100	-0.98593200
H	0.77863700	-0.47331300	-1.92256400
C	-1.37464100	0.26170100	-0.51650100
H	-0.87794400	1.07387200	0.00597800
H	-1.44464900	0.51566100	-1.57169200
C	-2.75144700	0.04684000	0.05592900
O	-3.13310000	-1.00157900	0.52733900
O	-3.48597300	1.15738900	-0.02792200
H	-4.36791800	0.99021000	0.34528400
N	-0.57045100	-0.98272500	-0.37517900
H	-1.06827000	-1.74756200	-0.83588000
O	1.50975400	-0.21085900	1.59089400
H	-0.51229100	-1.22691000	0.61811500
O	1.59341800	1.61437100	-0.11751400
H	2.01498700	1.93032900	-0.92766900
O	3.35650300	-0.24536200	-0.28194200

ZWP5 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.735013933 u.a.; Zero-point correction= 0.136196 u.a ; G =-891.636962u.a. at 298,15K.

Charge = 0 ; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.96931300	0.04359400	0.17641700
C	0.81533700	-0.86012600	-0.94111300
H	1.18271600	-1.87856900	-1.03665100
H	0.76172300	-0.41214100	-1.92910700
C	-1.40284600	0.26830000	-0.53601900
H	-0.91021400	1.09747300	-0.03689300
H	-1.49216700	0.50010600	-1.59504800
C	-2.76937100	0.04420600	0.05839500
O	-3.13635400	-1.00354800	0.54225200
O	-3.51747400	1.14633900	-0.02174000
H	-4.39205800	0.96959300	0.36442600
N	-0.57615000	-0.95986800	-0.38406200
H	-1.06230100	-1.73852100	-0.83357300
O	1.52849600	-0.24666400	1.58509500
H	-0.50561000	-1.19130900	0.61168400
O	1.63694000	1.62287400	-0.07206200
H	2.07200300	1.96266600	-0.86543600
O	3.36096000	-0.26380200	-0.29914500

ZWP6 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.751341012 u.a.; Zero-point correction= 0.136708 u.a. ; G = -891.653550u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.98190300	0.05339200	0.16221400
C	0.80793500	-0.90548700	-0.88783600
H	1.17083600	-1.92912800	-0.92397100
H	0.75000800	-0.51421400	-1.89898700
C	-1.40087000	0.25778600	-0.50985600
H	-0.93274700	1.09565800	-0.00272700
H	-1.45979500	0.47790100	-1.57319900
C	-2.78260800	0.03973000	0.05171400
O	-3.15586800	-0.99982900	0.54819400
O	-3.52971200	1.13772200	-0.07268700
H	-4.41329900	0.97044600	0.29643000
N	-0.57908500	-0.96742800	-0.31574700
H	-1.07494000	-1.75938500	-0.73047700
O	1.49693000	-0.07183300	1.58347300
O	1.81147000	1.60014900	-0.33578100
H	1.17033400	2.08238900	0.20160400
O	3.36141100	-0.37193600	-0.24868000
H	-0.50592800	-1.15891800	0.68806200

ZWP6 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.734587158 u.a.; Zero-point correction= 0.136363u.a.; G = -891.635213 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.98969900	0.04878900	0.16254800
C	0.80265000	-0.87531100	-0.90578400
H	1.16020300	-1.89956800	-0.97093500
H	0.73948200	-0.46168400	-1.90777500
C	-1.42222300	0.26167300	-0.53037700
H	-0.95247700	1.11366500	-0.04777400
H	-1.50010400	0.46078100	-1.59689700
C	-2.79371100	0.03792800	0.05448500
O	-3.15340100	-1.00003300	0.56387100
O	-3.55331300	1.12815200	-0.06528300
H	-4.42898100	0.95238700	0.31881700
N	-0.58244100	-0.94985800	-0.32856700
H	-1.06776200	-1.75199400	-0.73577100
O	1.51437100	-0.11125200	1.58324700
O	1.83931900	1.61025600	-0.29235600
H	1.17384600	2.07928900	0.22739400
O	3.36400200	-0.37577000	-0.26593700
H	-0.50072600	-1.13226700	0.67640000

ZWP7 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.750505257 u.a.; Zero-point correction=0.135978u.a ; G = -891.652959 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	2.00671700	0.08478000	-0.06075900
C	0.29263900	-0.19003100	0.55917600
H	-0.14385400	0.74225300	0.90330800
H	0.30752700	-0.91373700	1.36959900
C	-1.97389000	-1.05752500	-0.09832400
H	-2.42750200	-1.71262100	-0.84032500
H	-1.94816500	-1.57245900	0.85715200
C	-2.78948700	0.20923600	-0.01568300
O	-2.43193300	1.27315900	-0.46945400
O	-3.95648500	-0.01015700	0.59063400
H	-4.47884200	0.80935800	0.59267800
N	-0.58155900	-0.74607300	-0.52554500
H	-0.15309800	-1.60008100	-0.88981400
O	2.75199900	0.54709700	1.31186500
H	2.99381300	-0.21031300	1.86162300
O	2.01052500	1.27398700	-0.97911300
O	2.53400800	-1.24485900	-0.53343600
H	-0.62020900	-0.07548700	-1.29901000

ZWP7 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.734673403 u.a.; Zero-point correction= 0.135879 u.a. ; G = -891.637863 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	2.01905100	0.08693100	-0.05938500
C	0.31173900	-0.23641600	0.56081100
H	-0.11303300	0.66749800	0.98605900
H	0.33393100	-1.02080900	1.31274300
C	-1.97426800	-1.04652000	-0.11858900
H	-2.41629900	-1.69487600	-0.87355100
H	-1.93617600	-1.58180700	0.82509500
C	-2.81244800	0.20314900	-0.01051100
O	-2.47765300	1.27995700	-0.45138000
O	-3.97232100	-0.04293700	0.59861000
H	-4.50652400	0.76889800	0.61140600
N	-0.58844800	-0.70297100	-0.54459200
H	-0.17131100	-1.52761200	-0.98189900
O	2.76950700	0.48760400	1.32989400
H	3.02799500	-0.28932300	1.84388300
O	2.00420400	1.32378500	-0.91228300
O	2.56454400	-1.20502200	-0.60847700
H	-0.64159400	0.02649500	-1.26198900

ZWC1 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.749842390 u.a.; Zero-point correction= 0.134594 u.a ; G = -891.651753 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.50141800	-0.20631300	-0.07887700
C	-0.84257300	1.49266600	-0.09593900
H	-1.48172500	2.08551000	0.55390300
H	-0.90116900	1.88897600	-1.10597300
C	1.66691100	1.04553300	-0.43000900
H	1.35058300	1.01835700	-1.46676300
H	2.52869100	1.70173400	-0.34201700
C	2.08633200	-0.34870900	0.04630800
O	1.57118400	-0.80270500	1.11555700
O	2.95129200	-0.90800600	-0.65087100
N	0.56594900	1.65737000	0.39534500
H	0.73784800	2.66193400	0.45781600
O	-1.00722000	-0.90153400	1.25040300
H	0.00286000	-0.93661800	1.28587000
O	-0.68273900	-0.87068400	-1.28027000
H	-0.63022500	-1.83708900	-1.23524100
O	-2.97670500	-0.20648000	-0.21017700
H	0.64225000	1.28864100	1.34885300

ZWC1 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.730634092 u.a.; Zero-point correction= 0.134120 u.a ; G = -891.633558u.a. at298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.53444300	-0.19450100	-0.06890000
C	-0.82469800	1.48747700	-0.06957800
H	-1.44248700	2.08549200	0.59615700
H	-0.88305600	1.90534600	-1.07078600
C	1.68505500	1.03088600	-0.43674800
H	1.34226700	0.98646500	-1.46519600
H	2.52844900	1.71349100	-0.38021700
C	2.14937600	-0.34909500	0.04013300
O	1.59852000	-0.84883000	1.07034100
O	3.07265700	-0.85720300	-0.62082500
N	0.58997000	1.61688200	0.41610300
H	0.66868200	1.20473800	1.35153600
O	-0.97873300	-0.95064000	1.20104000
H	0.03378000	-0.98394200	1.20826800
O	-0.82767900	-0.83301100	-1.35187500
H	-0.98266600	-1.78389400	-1.45763500
O	-3.01555300	-0.15534400	-0.09694900
H	0.76978200	2.61625900	0.52194600

ZWC2 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.748271703 u.a. ; Zero-point correction= 0.134740 u.a ; G = -891.650934 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.64242800	-0.17596400	-0.14703400
C	0.52815000	1.20551900	-0.57716200
H	0.12682000	1.03811000	-1.57221000
H	1.14183100	2.10188800	-0.59999200
C	-1.99002800	1.10636200	-0.11412000
H	-2.69161900	1.67012100	0.49665400
H	-2.07659500	1.44114500	-1.14279500
C	-2.34670800	-0.37475800	0.00912500
O	-1.53965000	-1.14325500	0.62013100
O	-3.44946900	-0.69488000	-0.46818800
N	-0.61373900	1.45210900	0.37978000
H	-0.61166100	2.44678300	0.60811800
O	0.83145300	-1.51502100	-0.22599700
H	-0.12218400	-1.41512300	0.11990900
O	1.89920300	-0.01675400	1.42772800
H	2.45126700	0.74624900	1.65355900
O	2.85239200	-0.14679600	-1.00189100
H	-0.45802100	0.95643600	1.26248600

ZWC2 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.730538989 u.a.; Zero-point correction= 0.134410 u.a ; G = -891.634293u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.65562800	-0.17229800	-0.14792800
C	0.52982100	1.20967400	-0.55105200
H	0.13534900	1.05689700	-1.55152300
H	1.13501400	2.11233600	-0.55683700
C	-1.99712400	1.10395400	-0.11512500
H	-2.69884200	1.68345800	0.48010600
H	-2.06145800	1.43548400	-1.14675300
C	-2.37640900	-0.37198100	0.00611500
O	-1.56412200	-1.16640800	0.57517200
O	-3.50094200	-0.66692200	-0.43621300
N	-0.62350200	1.43634800	0.39911300
H	-0.62419200	2.42694200	0.64502600
O	0.83302100	-1.50524400	-0.19416500
H	-0.13297900	-1.39870800	0.12065800
O	1.98281800	-0.01667100	1.41341500
H	2.62633300	0.67989700	1.61016200
O	2.83582900	-0.14996800	-1.04450300
H	-0.47969100	0.92555000	1.27499800

ZWC3 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E (SCF) = -891.747840563 u.a.; Zero-point correction= 0.135093 u.a ; G = -891.649445 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.35192600	-0.25446700	-0.14749700
C	-0.78643200	1.48454000	-0.04100900
H	-1.40344500	1.99668900	0.69261400
H	-0.91882000	1.95116200	-1.01351300
C	1.69360900	1.01260800	-0.48394600
H	1.32951300	0.95633700	-1.50417000
H	2.57105200	1.65308900	-0.45699800
C	2.09807700	-0.37399400	0.03179100
O	1.61098300	-0.76207500	1.13832600
O	2.91692000	-0.98832800	-0.67583100
N	0.64260000	1.66351900	0.37417600
H	0.76345100	1.30849600	1.32867700
O	-2.93459400	-0.14290400	-0.03479100
H	-3.37701300	-0.14836200	-0.89581600
O	-1.01458300	-0.90753000	1.25305300
H	-0.01993700	-0.95701900	1.35349900
O	-0.83089400	-0.94856600	-1.35022400
H	0.82171000	2.66827800	0.40363300

ZWC3 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.729275997 u.a.; Zero-point correction= 0.134387u.a.; G = -891.632006 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.41067500	-0.24365500	-0.16043800
C	-0.78340900	1.47492400	-0.01208500
H	-1.39003900	1.99080000	0.72754000
H	-0.88657500	1.97564800	-0.97069900
C	1.70910600	1.01407300	-0.45832100
H	1.32781200	0.95533700	-1.47296900
H	2.55235100	1.69857200	-0.44249000
C	2.18835200	-0.36186200	0.01949800
O	1.64716800	-0.85780700	1.05632900
O	3.10545100	-0.86975700	-0.65020100
N	0.64436000	1.60086700	0.43157700
H	0.74850200	1.17267700	1.35742300
O	-2.97217100	-0.10303900	0.11876500
H	-3.50437600	-0.12104200	-0.68951800
O	-0.95155000	-0.98472300	1.15594600
H	0.05455800	-1.02427100	1.20265000
O	-1.04971300	-0.87969200	-1.45148900
H	0.82960400	2.59836400	0.54423500

ZWC4 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.747513032u.a.; Zero-point correction= 0.135224u.a; G = -891.649372u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.58114300	-0.14760700	0.05072800
C	0.48196700	1.15956200	-0.59707100
H	0.08181800	0.87304500	-1.56402000
H	1.08897800	2.05272300	-0.71779200
C	-2.02893500	1.09876600	-0.13626500
H	-2.74106200	1.65173900	0.47233100
H	-2.13412600	1.41218000	-1.17009400
C	-2.33264600	-0.39289900	0.01462300
O	-1.50528200	-1.11118900	0.65635200
O	-3.41295200	-0.76730100	-0.47668300
N	-0.65799500	1.49472000	0.33278400
H	-0.65965500	2.50516900	0.47444500
O	2.76446800	-0.23089100	-1.01150500
H	3.47884500	0.39815200	-0.83591800
O	0.87882600	-1.53178100	-0.21843400
H	-0.07621400	-1.48451100	0.10644900
O	1.97824100	0.15032800	1.45065200
H	-0.49849400	1.07666700	1.25341800

ZWC4 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.729914629 u.a.; Zero-point correction= 0.135224 u.a ; G = -891.649372 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.60099400	-0.14654700	0.05218200
C	0.49442100	1.16840500	-0.57358800
H	0.10471400	0.90059500	-1.55053100
H	1.09517300	2.06868700	-0.67284600
C	-2.02880500	1.09530400	-0.13892400
H	-2.74026500	1.66329900	0.45618800
H	-2.11558100	1.40680300	-1.17523300
C	-2.36152600	-0.39073300	0.00981400
O	-1.53440200	-1.14369200	0.61008000
O	-3.46882100	-0.73010200	-0.44680300
N	-0.66027300	1.48479600	0.34625900
H	-0.66857200	2.49431200	0.49623700
O	2.75469200	-0.23995400	-1.04210300
H	3.50086600	0.35068400	-0.86409500
O	0.87525700	-1.52196800	-0.19177100
H	-0.08878500	-1.46083700	0.11334800
O	2.04907800	0.14557400	1.43801800
H	-0.51152100	1.06436000	1.26720600

NE2 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.744837025u.a. ; Zero-point correction= 0.133402 u.a; G = -891.647979u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.51810600	-0.17823700	0.09837000
C	-0.84859600	1.51695900	0.13293600
H	-1.57269100	2.11258700	-0.42158400
H	-0.89446600	1.84957900	1.16947800
C	1.60340300	1.17471600	0.30537900
H	1.41456300	1.17737400	1.37686900
H	2.50058100	1.77959200	0.15102900
C	2.00551100	-0.22353800	-0.11003700
O	1.58526300	-0.81897000	-1.08835400
O	2.94818500	-0.73102900	0.68937300
H	3.20876500	-1.60834900	0.36340200
N	0.48502000	1.76438700	-0.40991700
H	0.51885200	1.50219900	-1.38848400
O	-1.14442700	-0.82423600	-1.31620500
H	-0.17047600	-0.85503500	-1.44484400
O	-0.59330800	-0.92031000	1.18342900
H	-0.68984300	-1.88394300	1.18737700
O	-2.98330600	-0.27545200	0.33562600

NE2 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.726209895u.a.; Zero-point correction= 0.132807u.a; G = -891.630630u.a. at 298,15K
.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.55869300	-0.16030200	0.09115100
C	-0.81224500	1.50728100	0.14066100
H	-1.53057200	2.13594100	-0.38503700
H	-0.82103400	1.82723500	1.18197900
C	1.65157000	1.17029500	0.26855600
H	1.48784700	1.21033400	1.34416300
H	2.53673800	1.78213400	0.07632800
C	2.06624500	-0.23817800	-0.10026600
O	1.58802300	-0.91285600	-0.99680800
O	3.09010700	-0.66600200	0.64531200
H	3.34557600	-1.55775300	0.35645900
N	0.51102800	1.72688300	-0.43520300
H	0.52286400	1.45247300	-1.41029600
O	-1.13092000	-0.85081600	-1.28627500
H	-0.15195600	-0.91634900	-1.36661700
O	-0.76191400	-0.93851000	1.24999700
H	-0.97842700	-1.88143800	1.30518600
O	-3.04045300	-0.17839300	0.22818400

NE1 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.742787953 u.a.; Zero-point correction= 0.133148 u.a; G = -891.646821 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.37680700	-0.23007700	-0.15468600
C	-0.78757200	1.49711400	-0.14336200
H	-1.52096600	2.05992000	0.43221800
H	-0.83952100	1.85329200	-1.17149500
C	1.66118300	1.16494600	-0.31106600
H	1.47729300	1.17969500	-1.38367400
H	2.56228800	1.76088900	-0.14667600
C	2.04592600	-0.24229500	0.09341100
O	1.60434000	-0.84556200	1.05589900
O	2.99495400	-0.74784000	-0.70183900
H	3.24267400	-1.63209400	-0.38485700
N	0.54269000	1.75614500	0.40392500
H	0.57429200	1.48414800	1.38017700
O	-2.96501500	-0.05955500	-0.23128800
H	-3.40944700	-0.82323700	-0.62710000
O	-1.16765800	-0.78247100	1.33749400
H	-0.21237400	-0.90911500	1.51011700
O	-0.78389300	-1.10631500	-1.20399000

NE1 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.724785415u.a.; Zero-point correction= 0.132890 u.a ; G =-891.629206u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.40497200	-0.22544600	-0.15847000
C	-0.77055900	1.48901600	-0.13115300
H	-1.49923800	2.06297600	0.43989900
H	-0.80946900	1.85219500	-1.15756800
C	1.68584400	1.16485300	-0.28617800
H	1.50957700	1.20120600	-1.36010200
H	2.57857800	1.76845900	-0.10451800
C	2.08269000	-0.24800900	0.08669900
O	1.60438200	-0.90493800	0.99481900
O	3.08600500	-0.70048700	-0.67426500
H	3.32943600	-1.59455400	-0.38243800
N	0.55622500	1.73217400	0.42834300
H	0.58036100	1.45234900	1.40210100
O	-2.99023000	-0.00599700	-0.16983700
H	-3.47292400	-0.72295600	-0.60617600
O	-1.16328100	-0.82218300	1.31085700
H	-0.20514900	-0.96160200	1.46048100
O	-0.88912800	-1.09598900	-1.25273000

NE4 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.742095886 u.a.; Zero-point correction=0.133047 u.a ; G = -891.645979u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.54455300	-0.17671700	-0.08967200
C	-0.85749600	1.50098000	-0.11143300
H	-1.57557800	2.10515700	0.44030200
H	-0.87945600	1.83615800	-1.15470100
C	1.58394400	1.15387300	-0.25850800
H	1.40165200	1.15664300	-1.33783100
H	2.44177300	1.80553300	-0.09072900
C	2.04964300	-0.23503000	0.11243300
O	1.58985700	-0.94660600	0.98874000
O	3.08589700	-0.61424800	-0.64402200
H	3.36704700	-1.50525700	-0.37944400
N	0.45483000	1.63208500	0.52647800
H	0.59924300	2.61296200	0.71990300
O	-1.12170600	-0.87640800	1.27948500
H	-0.13969200	-0.89762600	1.36975600
O	-0.67724300	-0.89439400	-1.23607800
H	-0.76025800	-1.85919600	-1.23861100
O	-3.01765400	-0.23673800	-0.27860800

NE4 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.724453599u.a.; Zero-point correction= 0.132725 u.a ; G = -891.628964u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.58144100	-0.15902500	0.07590900
C	0.81390900	1.48904700	0.13240000
H	1.51606900	2.13505000	-0.39188600
H	0.80561300	1.80216500	1.18218300
C	-1.63439400	1.14264000	0.24895200
H	-1.46635500	1.16452800	1.33080400
H	-2.48218900	1.80127200	0.05941500
C	-2.10600600	-0.24927200	-0.10277300
O	-1.60932800	-0.99817400	-0.92650200
O	-3.18758200	-0.58955600	0.60715900
H	-3.46160700	-1.48828000	0.36161300
N	-0.48986600	1.59851700	-0.52643400
H	-0.63109400	2.57403500	-0.74781300
O	1.09706500	-0.89243700	-1.25449000
H	0.11141300	-0.92888100	-1.30425700
O	0.85378600	-0.90891500	1.29686400
H	1.10930600	-1.83919200	1.38584300
O	3.06671400	-0.15084700	0.15184800

NE5 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.742133943u.a. ; Zero-point correction= 0.133114 u.a ; G= -891.645583 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.71753200	-0.16714900	0.13735400
C	-0.45172100	1.01377400	0.68205200
H	0.03527400	0.56484900	1.54835200
H	-0.97823300	1.89946900	1.04042900
C	1.90340600	1.16819500	-0.00822800
H	2.52809200	1.71658200	-0.71371000
H	2.14602600	1.55487200	0.98887600
C	2.37307200	-0.26300700	-0.04636700
O	1.69768500	-1.23652300	-0.33680900
O	3.66272400	-0.36690500	0.28658700
H	3.92895600	-1.30047400	0.25591300
N	0.50996200	1.32397300	-0.38166200
H	0.36375100	2.27249500	-0.69338000
O	-0.95897500	-1.41539600	-0.48138400
H	0.02776500	-1.31100800	-0.49639200
O	-2.41075900	0.43966600	-1.18298600
H	-3.11704900	1.06663900	-0.97435500
O	-2.70191000	-0.51306400	1.20094800

NE5 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.726031277u.a.; Zero-point correction= 0.132966u.a ; G=-891.629783 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.72205600	-0.16553500	0.13813300
C	-0.46148800	1.03135500	0.66647000
H	0.01645100	0.61002900	1.55161400
H	-0.99408800	1.92524000	0.99479200
C	1.90438300	1.16599900	-0.00224700
H	2.53341600	1.72422200	-0.69606200
H	2.13324100	1.54687200	1.00020900
C	2.38043600	-0.26333600	-0.04518800
O	1.70904600	-1.23986700	-0.33485900
O	3.67152300	-0.36456900	0.28406000
H	3.93684600	-1.29843400	0.25244000
N	0.51423800	1.32357400	-0.39000000
H	0.37809100	2.27064800	-0.71115300
O	-0.95803700	-1.42085200	-0.46018700
H	0.02856300	-1.31706900	-0.47869000
O	-2.41886400	0.41580100	-1.19161800
H	-3.12945400	1.04264200	-0.99647900
O	-2.70515500	-0.50179400	1.20599400

NE6 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.741652314 u.a.; Zero-point correction= 0.132937u.a ; G= -891.645694 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.71978500	-0.07499700	-0.05050100
C	-0.43833400	1.00225500	0.64618600
H	0.01833100	0.45977100	1.47337500
H	-0.93442600	1.87657700	1.06925600
C	1.93229100	1.16361100	0.03126000
H	2.58790300	1.72830200	-0.63176100
H	2.14423400	1.51133800	1.04959900
C	2.38057700	-0.27313500	-0.03895800
O	1.69391800	-1.22753200	-0.36414400
O	3.66281100	-0.40639900	0.31211700
H	3.91359400	-1.34362800	0.26527900
N	0.55296600	1.35101200	-0.38226900
H	0.42647600	2.31696800	-0.64662000
O	-2.56120800	-0.63551200	1.20089700
H	-3.38747000	-0.15082400	1.33467700
O	-0.97357300	-1.39010100	-0.53796000
H	0.01398000	-1.30337600	-0.53376700
O	-2.58492400	0.56158700	-1.08310600

NE6 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.725840778 u.a.; Zero-point correction= 0.132800u.a ; G= -891.629905 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.72762000	-0.15608300	0.14227400
C	-0.45818200	1.03239200	0.66805900
H	0.02099800	0.60258500	1.54842300
H	-0.98610900	1.92620600	1.00287700
C	1.90664900	1.16198100	-0.00150200
H	2.53923500	1.71823000	-0.69356700
H	2.13462600	1.54135000	1.00173000
C	2.37661600	-0.26923700	-0.04300700
O	1.70096100	-1.24383500	-0.32936000
O	3.66756100	-0.37478900	0.28480000
H	3.92907000	-1.30984900	0.25602800
N	0.51681200	1.32717800	-0.39020600
H	0.38619100	2.27959100	-0.69828100
O	-0.96605800	-1.41698000	-0.45931000
O	-2.52539800	0.47850700	-1.10083300
H	-2.05412500	0.42763300	-1.94360800
O	-2.70773700	-0.48857700	1.21125900
H	0.02160100	-1.32017200	-0.47001700

NE7 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.739240248 u.a.; Zero-point correction=0.132349 u.a; G= -891.646135 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
C	1.52354500	0.24982300	0.89854300
H	1.06895100	1.20912900	0.66242000
H	1.99651900	0.36441200	1.87538000
C	2.64318400	-0.00778100	-0.09046500
O	3.43544400	1.06976700	-0.24180300
O	2.83666900	-1.05747600	-0.66798300
N	0.51519800	-0.79384200	0.96218300
H	-2.25749600	-0.17254200	1.89964500
C	-0.29940300	-0.92154500	-0.24973900
H	0.22238300	-0.66980900	-1.17736900
H	-0.63951300	-1.95127400	-0.34986500
P	-1.82366900	0.05467800	-0.22836300
O	-2.65865500	-0.10922100	-1.44707000
O	-1.29363600	1.54003600	0.05643000
O	-2.69184300	-0.36000700	1.05555100
H	0.97568300	-1.68148200	1.11825000
H	-1.99907400	2.20010600	0.12856100
H	4.15340900	0.85040200	-0.85789900

NE7 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.723172397 u.a.; Zero-point correction= 0.132163 u.a; G= -891.630636u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
C	1.55056200	0.27964500	0.88534700
H	1.11038300	1.23972300	0.62562300
H	2.01655100	0.40984700	1.86397300
C	2.67789700	-0.01134300	-0.08667400
O	3.47203300	1.05998700	-0.27096800
O	2.87992600	-1.07941700	-0.62626100
N	0.52744400	-0.74798500	0.96645300
H	-2.32333500	-0.18336800	1.89612200
C	-0.29229000	-0.88957100	-0.24048200
H	0.22126400	-0.62769000	-1.16990200
H	-0.60838300	-1.92717200	-0.34092800
P	-1.84410500	0.04846400	-0.22708600
O	-2.65917200	-0.13580100	-1.45671200
O	-1.36559000	1.54883200	0.06784600
O	-2.72014000	-0.39883200	1.04043200
H	0.97325900	-1.63886100	1.14447700
H	-2.08941700	2.19207700	0.10828400
H	4.19566800	0.81382800	-0.87037700

NE8 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.739696603 u.a.; Zero-point correction= 0.132706u.a; G= -891.645286 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.94570500	-0.13177200	-0.17308000
C	0.20333300	0.10739700	-0.57886000
H	-0.19911700	-0.87926400	-0.83263100
H	0.18057000	0.71139600	-1.48623200
C	-1.90266800	1.05880100	0.15729800
H	-2.36026100	1.67846200	0.93095000
H	-1.96493800	1.62267200	-0.77203400
C	-2.77459300	-0.17520000	0.03855800
O	-2.47859900	-1.27715100	0.45188000
O	-3.95131700	0.09505400	-0.55519200
H	-4.49359500	-0.71049100	-0.56381000
N	-0.51303500	0.79829100	0.49639400
O	2.70550100	-0.84598100	-1.22891100
O	1.97905900	-0.80179400	1.28645800
H	1.53797900	-1.66276800	1.32661300
O	2.60454700	1.29012400	0.12842000
H	-0.48812100	0.21137100	1.32397400
H	2.16319800	1.78915400	0.83140800

NE8 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.724118289 u.a.; Zero-point correction= 0.132400 u.a ; G= -891.630405 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.96248400	-0.11881400	-0.17822300
C	0.20662800	0.09858500	-0.54997800
H	-0.17452600	-0.88767900	-0.83717300
H	0.16311600	0.73140400	-1.43696400
C	-1.90446900	1.03783200	0.19601000
H	-2.35655900	1.64876400	0.98022300
H	-1.93903900	1.62858000	-0.71772400
C	-2.80759000	-0.16918400	0.03519000
O	-2.55932600	-1.28492300	0.44302700
O	-3.96006200	0.14024200	-0.58667600
H	-4.52190800	-0.65150900	-0.61588800
N	-0.52459700	0.73917800	0.54549000
O	2.71547100	-0.76007000	-1.28518500
O	2.05005700	-0.86739400	1.23954100
H	1.69217500	-1.76710100	1.22338400
O	2.59948200	1.29951600	0.17977100
H	-0.51982500	0.11437300	1.34454600
H	2.15908000	1.76875400	0.90333900

NE9 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.742117984 u.a.; Zero-point correction=0.134208 u.a; G= -889.867310 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.72319800	-0.15823900	0.14251500
C	-0.44628100	1.01062100	0.68730100
H	0.04356800	0.54921200	1.54529100
H	-0.96629600	1.89499900	1.05713700
C	1.90601500	1.16430200	-0.00814200
H	2.53267700	1.70990400	-0.71402200
H	2.15032300	1.55038800	0.98876800
C	2.36885000	-0.26895600	-0.04528500
O	1.68956100	-1.23908600	-0.33814200
O	3.65662500	-0.37875600	0.29202800
H	3.91878300	-1.31354700	0.26303400
N	0.51217500	1.32732100	-0.37929400
H	0.37003900	2.28156600	-0.67573300
O	-0.96854500	-1.40546100	-0.49475000
O	-2.51970000	0.51112400	-1.08336500
H	-2.04663500	0.47170400	-1.92560000
O	-2.69926000	-0.51136300	1.20860600
H	0.01932100	-1.30934200	-0.49980000

NE9 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.725840778u.a.; Zero-point correction= 0.132888u.a.; G= -891.629760u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.72762000	-0.15608300	0.14227400
C	-0.45818200	1.03239200	0.66805900
H	0.02099800	0.60258500	1.54842300
H	-0.98610900	1.92620600	1.00287700
C	1.90664900	1.16198100	-0.00150200
H	2.53923500	1.71823000	-0.69356700
H	2.13462600	1.54135000	1.00173000
C	2.37661600	-0.26923700	-0.04300700
O	1.70096100	-1.24383500	-0.32936000
O	3.66756100	-0.37478900	0.28480000
H	3.92907000	-1.30984900	0.25602800
N	0.51681200	1.32717800	-0.39020600
H	0.38619100	2.27959100	-0.69828100
O	-0.96605800	-1.41698000	-0.45931000
O	-2.52539800	0.47850700	-1.10083300
H	-2.05412500	0.42763300	-1.94360800
O	-2.70773700	-0.48857700	1.21125900
H	0.02160100	-1.32017200	-0.47001700

NE10 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.744598549 u.a.; Zero-point correction= 0.133307u.a ; G= -891.647862 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.51928400	-0.19083500	0.09068700
C	-0.86848600	1.51603700	0.07702800
H	-0.94828700	1.88348800	1.10044600
H	-1.57916900	2.08770000	-0.51843600
C	1.57859300	1.17234900	0.31624400
H	2.47311800	1.79034900	0.20578700
H	1.35050800	1.15428100	1.38035600
C	2.01098300	-0.21474100	-0.10519100
O	1.60513500	-0.81336600	-1.08755900
O	2.95966400	-0.70743400	0.69603500
H	3.23666700	-1.57924100	0.36893900
N	0.47883200	1.75621800	-0.43293300
H	-0.15347700	-0.89221500	-1.42491800
O	-2.98289700	-0.26534600	0.34154300
O	-0.60440800	-1.02769300	1.11946700
H	-0.60444700	-0.65827000	2.01421500
O	-1.12756700	-0.87845300	-1.29177200
H	0.53657100	1.47936800	-1.40634400

NE10 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.725919911 u.a.; Zero-point correction= 0.132880 u.a ; G= -891.630099 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.55615100	-0.17679200	0.08419300
C	-0.85036600	1.51179400	0.05219300
H	-0.92218500	1.89713100	1.06955600
H	-1.54538500	2.09406900	-0.55205200
C	1.60481200	1.16349700	0.29956700
H	2.48706900	1.79904200	0.19032700
H	1.36954700	1.15668700	1.36288900
C	2.06750000	-0.22228800	-0.09372300
O	1.61615700	-0.89269200	-1.00751400
O	3.09648300	-0.63396500	0.65303500
H	3.37816700	-1.51404700	0.35309900
N	0.49952900	1.71744800	-0.46256800
H	-0.12691900	-0.95830100	-1.33958100
O	-3.03497200	-0.19049200	0.24351000
O	-0.74928900	-1.02122100	1.19368600
H	-0.85180500	-0.67435200	2.09157400
O	-1.10697800	-0.92526000	-1.24762600
H	0.55418700	1.42053600	-1.42967800

NE11 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.742732034u.a. ; Zero-point correction= 0.133036 u.a ; G= -891.647534 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.37520800	-0.22882900	-0.14800700
C	-0.78289100	1.49942600	-0.13891800
H	-1.50857700	2.05894500	0.44942700
H	-0.85384900	1.85705900	-1.16574200
C	1.66288700	1.15711100	-0.33018600
H	1.46897400	1.15691300	-1.40110200
H	2.56915900	1.74968600	-0.18302600
C	2.04199400	-0.24595600	0.09337800
O	1.60247600	-0.82988600	1.06893800
O	2.98184100	-0.77100900	-0.69958600
H	3.22556100	-1.65193600	-0.37039200
N	0.55483400	1.76468600	0.38716500
H	0.59758300	1.50798000	1.36715000
O	-2.97143800	-0.10990600	-0.19389500
H	-3.35671000	-0.60120400	-0.93295200
O	-1.16565300	-0.77293800	1.34436000
H	-0.20815600	-0.85923700	1.53071300
O	-0.78743100	-1.09151800	-1.21103800

NE11 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.724662337 u.a.; Zero-point correction= 0.132436 u.a. ; G= -891.629089 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.39675000	-0.22362700	-0.15200200
C	-0.77033300	1.49542800	-0.12740100
H	-1.49159000	2.06338900	0.45873900
H	-0.83009500	1.86179900	-1.15196900
C	1.68302400	1.15865800	-0.30682800
H	1.49796200	1.17924900	-1.37952000
H	2.58248900	1.75718900	-0.14208000
C	2.07041300	-0.25084400	0.08842200
O	1.60160700	-0.88016600	1.02092100
O	3.05296500	-0.73346100	-0.68084500
H	3.29154800	-1.62341800	-0.37278600
N	0.56491800	1.74600300	0.40974600
H	0.60071800	1.48210000	1.38766900
O	-2.99157900	-0.07061200	-0.15581000
H	-3.40597300	-0.54292300	-0.89166000
O	-1.16721600	-0.80371600	1.32355400
H	-0.20817800	-0.90810000	1.49487900
O	-0.86311200	-1.08158800	-1.24739900

NE12 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.742936479u.a. ; Zero-point correction=0.133134 u.a ; G= -891.647176 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.36614700	-0.24049100	0.16890600
C	-0.79005800	1.49467300	0.14896400
H	-1.52625100	2.05056300	-0.43068300
H	-0.84963500	1.85307200	1.17605200
C	1.65855100	1.16724700	0.31321200
H	1.47811700	1.17421800	1.38631800
H	2.56116300	1.76129000	0.15002200
C	2.03591700	-0.23749200	-0.10653900
O	1.59738300	-0.82159500	-1.08240800
O	2.97337800	-0.76284200	0.68907100
H	3.21656100	-1.64454900	0.36154200
N	0.53986500	1.76742900	-0.39423900
H	0.57242600	1.50519300	-1.37321600
O	-2.95635300	-0.21457300	0.33628500
H	-3.42484800	0.27502000	-0.35478400
O	-1.18013200	-0.78777600	-1.32681500
H	-0.22656200	-0.87432100	-1.53149000
O	-0.74856100	-1.08967600	1.22242800

NE12 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.724787036u.a.; Zero-point correction= 0.132896u.a ; G= -891.629245u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.40824800	-0.23220800	0.17693700
C	-0.77010400	1.48609700	0.13648600
H	-1.50104100	2.06073300	-0.43192000
H	-0.80355000	1.85217400	1.16201200
C	1.68892500	1.16680900	0.27634300
H	1.52020300	1.20427000	1.35141600
H	2.57916300	1.77191100	0.08747300
C	2.08679000	-0.24538800	-0.09728400
O	1.60048600	-0.90650500	-0.99853500
O	3.10036600	-0.69266700	0.65221000
H	3.34202100	-1.58749700	0.36110000
N	0.55343700	1.73040400	-0.43150100
H	0.57153700	1.44909600	-1.40493900
O	-3.00507400	-0.14262900	0.23724800
H	-3.40827300	0.34227400	-0.49740200
O	-1.15293700	-0.84514300	-1.28160700
H	-0.19007600	-0.94411100	-1.44156800
O	-0.90459000	-1.06601500	1.30156000

NE13 structure in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.742209821 u.a.; Zero-point correction=0.133509u.a ; G= -891.645658u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.71082600	-0.16449000	-0.14385900
C	0.41064000	0.94995300	-0.73303700
H	-0.11235500	0.39532600	-1.51360800
H	0.92802500	1.77257900	-1.22893400
C	-1.91249300	1.18875300	0.02907200
H	-2.52998600	1.69214000	0.77468600
H	-2.19436000	1.61268700	-0.93424700
C	-2.35108100	-0.26147300	0.03808700
O	-1.65785400	-1.21912700	0.34214100
O	-3.63378200	-0.39466400	-0.30676700
H	-3.88466000	-1.33258900	-0.26709800
N	-0.51224300	1.44669900	0.30284200
H	-0.28234200	1.06949900	1.21375400
O	2.63715300	-0.60316200	-1.21940800
O	0.98244000	-1.33497600	0.64940200
H	-0.00693200	-1.30520200	0.56623100
O	2.55166100	0.61049800	0.98400200
H	2.08658500	0.70406500	1.82752400

NE13 structure in aqueous solution at SMD-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.725064966u.a.; Zero-point correction=0.133174u.a.; G= -891.629022u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.71406800	-0.16400800	-0.14452500
C	0.44095800	1.00480000	-0.69889300
H	-0.06140600	0.52052200	-1.53674000
H	0.99180600	1.85051600	-1.11559000
C	-1.91241200	1.18339800	0.02320800
H	-2.54333700	1.69502500	0.75210300
H	-2.17499500	1.60220200	-0.94799800
C	-2.36082100	-0.26440700	0.03300700
O	-1.67621100	-1.23126700	0.32762100
O	-3.64819300	-0.38663800	-0.30026900
H	-3.90314800	-1.32349400	-0.26107500
N	-0.52008500	1.45080600	0.32281700
H	-0.29674200	1.08122000	1.23806500
O	2.64636300	-0.57116900	-1.22780500
O	0.96968000	-1.36143600	0.59026200
H	-0.02078400	-1.31737300	0.52287600
O	2.56393400	0.54975300	1.01764200
H	2.08724900	0.65917100	1.85298000

5-Structures and energetics of glyphosate conformers in aqueous solution, at SMD-MP2/6-311++G(2d,2p) level.

ZWP1structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88997673668179D+03u.a.;Zero-point correction= 0.137079 u.a.; G= -889.878131u.a. at 29,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	2.01325800	0.01550100	0.12425700
C	0.28899600	-0.25730100	0.66785800
H	-0.16594700	0.66080200	1.02253400
H	0.26622100	-1.00692300	1.45230100
C	-1.93232400	-1.07744800	-0.12209800
H	-2.36635700	-1.68642300	-0.91006800
H	-1.95896900	-1.62235800	0.81421000
C	-2.70234200	0.21350800	-0.03100300
O	-2.29512300	1.27110500	-0.46915300
O	-3.88848300	0.02734200	0.55665000
H	-4.37031800	0.87060200	0.55066600
N	-0.52386100	-0.77646200	-0.47046000
H	-0.07328200	-1.61945100	-0.82930900
O	2.79457300	0.51234800	1.30863100
O	1.83585100	1.19329400	-0.99161800
H	1.75523000	2.06144400	-0.57676500
O	2.42465800	-1.20932300	-0.64927400
H	-0.51621000	-0.08566800	-1.22463300

ZWP2structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88997611871157D+03u.a.; Zero-point correction= 0.137014u.a.; G= -889.877933 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.97121900	-0.22884400	-0.08167200
C	0.29562500	0.20403500	-0.67361500
H	-0.20327600	-0.68947900	-1.03408500
H	0.34534100	0.94152400	-1.46719300
C	-1.92870700	1.07881600	0.03066800
H	-2.35921700	1.76733200	0.75211000
H	-1.93052400	1.53551300	-0.95219300
C	-2.72642300	-0.19798000	0.04399300
O	-2.33290300	-1.23144400	0.54728500
O	-3.91911000	-0.02765600	-0.53506000
H	-4.41712100	-0.85833200	-0.46082500
N	-0.53231200	0.77764100	0.42676800
H	-0.09015900	1.63212400	0.76736500
O	1.82034900	-1.04883200	1.17443700
O	2.57409000	1.23880200	0.30707100
H	2.46983200	1.41526600	1.25037600
O	2.73875700	-0.72787700	-1.27220900
H	-0.54942000	0.11204700	1.20367600

ZWP3 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88997655984675D+03 u.a. ; Zero-point correction= 0.137098 u.a.; G= -889.877818 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.95777000	-0.23339300	0.06635000
C	-0.28716100	0.21883900	0.65700900
H	0.21760900	-0.66537700	1.03136200
H	-0.33326800	0.97273500	1.43549800
C	1.92694400	1.08323400	-0.10232000
H	2.35780200	1.71489700	-0.87397800
H	1.93945700	1.60891400	0.84529500
C	2.71530800	-0.19800500	-0.03147200
O	2.32658300	-1.25321400	-0.49121800
O	3.89541600	-0.00486300	0.56652900
H	4.38934900	-0.84091200	0.54865800
N	0.52540600	0.76940100	-0.46702500
H	0.07567100	1.61525100	-0.81917500
O	-1.78303600	-0.99787900	-1.21895800
O	-2.56708300	1.21728900	-0.36754300
H	-2.87247300	1.71221000	0.40341300
O	-2.71419600	-0.80061400	1.23533800
H	0.52254700	0.08721600	-1.22962900

ZWP4structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88997606675038D+03u.a.; Zero-point correction= 0.137315u.a ; G=-889.876823u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.97121900	-0.22884400	-0.08167200
C	0.29562500	0.20403500	-0.67361500
H	-0.20327600	-0.68947900	-1.03408500
H	0.34534100	0.94152400	-1.46719300
C	-1.92870700	1.07881600	0.03066800
H	-2.35921700	1.76733200	0.75211000
H	-1.93052400	1.53551300	-0.95219300
C	-2.72642300	-0.19798000	0.04399300
O	-2.33290300	-1.23144400	0.54728500
O	-3.91911000	-0.02765600	-0.53506000
H	-4.41712100	-0.85833200	-0.46082500
N	-0.53231200	0.77764100	0.42676800
H	-0.09015900	1.63212400	0.76736500
O	1.82034900	-1.04883200	1.17443700
O	2.57409000	1.23880200	0.30707100
H	2.46983200	1.41526600	1.25037600
O	2.73875700	-0.72787700	-1.27220900
H	-0.54942000	0.11204700	1.20367600

ZWP5 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) = -0.88997562329473D+03 u.a.; Zero-point correction= 0.137459 u.a; G= -889.876048 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.93022100	0.05426300	0.18075100
C	0.82473000	-0.92293900	-0.90798700
H	1.20105000	-1.93987000	-0.94400200
H	0.77661800	-0.52473800	-1.91568700
C	-1.32855000	0.26530100	-0.48494400
H	-0.83004100	1.04498400	0.07972500
H	-1.36677400	0.54851200	-1.53214900
C	-2.71831100	0.05108000	0.04930900
O	-3.11827400	-1.00803200	0.49073500
O	-3.44192200	1.17369100	-0.02972600
H	-4.32896600	0.99127700	0.32160000
N	-0.56156700	-0.99554400	-0.36050400
H	-1.07847300	-1.74097600	-0.82832000
O	1.41260400	-0.14128200	1.58205800
H	-0.50328600	-1.24842700	0.62851000
O	1.59823800	1.60375000	-0.20115500
H	2.08867100	1.87970800	-0.98576700
O	3.34330900	-0.28015900	-0.21065200

ZWP6 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88997502631493D+03u.a. ; Zero-point correction=0.138013u.a ; G= -889.874659u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.98925200	0.05841400	0.11977800
C	0.76273100	-1.02094600	-0.71063900
H	1.10984700	-2.04483900	-0.61776900
H	0.64136200	-0.77940400	-1.76081100
C	-1.32952900	0.29264000	-0.27957100
H	-0.94260000	1.06780600	0.37155700
H	-1.21279900	0.59501900	-1.31611300
C	-2.78724400	0.04871800	0.00734800
O	-3.25902000	-1.05048400	0.22173000
O	-3.48071700	1.19104500	-0.02560900
H	-4.41655900	0.98743600	0.13655800
N	-0.57878600	-0.96652700	-0.05911700
H	-1.15358800	-1.74277500	-0.39184000
O	1.61395200	0.08307900	1.58066500
O	1.73531400	1.53219400	-0.53055600
H	1.15541100	2.06578400	0.02650600
O	3.34180000	-0.39066400	-0.35626200
H	-0.45474100	-1.10337700	0.94649700

ZWP7 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) = -0.88997482978727D+03 u.a.; Zero-point correction= 0.137213 u.a ; G= -889.875999 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.97420600	0.09149500	-0.05788100
C	0.28404800	-0.24045800	0.56992400
H	-0.17760700	0.66770200	0.94112200
H	0.31537300	-0.98770800	1.35611800
C	-1.96337600	-1.07809900	-0.09123200
H	-2.43096600	-1.72604700	-0.82709900
H	-1.93815000	-1.57859000	0.86961900
C	-2.73877900	0.21108800	-0.02025000
O	-2.35613200	1.25370200	-0.51270000
O	-3.90140500	0.03851500	0.61633900
H	-4.38884300	0.87833400	0.59927300
N	-0.57624500	-0.78277500	-0.52152600
H	-0.15002500	-1.63459600	-0.88859100
O	2.71662300	0.56679200	1.30741100
H	2.99210100	-0.18987700	1.84042900
O	1.92297400	1.28953100	-0.96614500
O	2.53307400	-1.22004600	-0.54934300
H	-0.61369000	-0.10535700	-1.28710700

ZWC1 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) = -0.88997260362580D+03 u.a.; Zero-point correction= 0.136413 u.a; G= -889.872343u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.47035200	-0.20775500	-0.07998700
C	-0.82189300	1.48609400	-0.11544300
H	-1.45980800	2.08113900	0.53126200
H	-0.88927600	1.87210600	-1.12747500
C	1.65584700	1.03339600	-0.47041700
H	1.32674900	0.99464900	-1.50100000
H	2.53121500	1.67040200	-0.39670400
C	2.03027000	-0.35371800	0.04948600
O	1.55622000	-0.70025900	1.18302500
O	2.81788700	-1.00741200	-0.66442600
N	0.58199900	1.66360400	0.35762300
H	0.75313000	2.66759200	0.40592300
O	-1.03929400	-0.85545500	1.29616400
H	-0.04092600	-0.88310400	1.36296900
O	-0.58043500	-0.88265000	-1.21834900
H	-0.62230700	-1.85054200	-1.22345300
O	-2.93976000	-0.22558300	-0.27709400
H	0.68022400	1.29510400	1.30859800

ZWC2 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88996992345502D+03u.a.; Zero-point correction= 0.136143u.a; G= -889.871626u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.62649500	-0.17298200	-0.15008500
C	0.49894300	1.18780800	-0.58276700
H	0.08535300	1.00600000	-1.56927400
H	1.10585100	2.08628700	-0.62893100
C	-1.99426700	1.11229800	-0.12205500
H	-2.69991700	1.66796800	0.48812800
H	-2.07311200	1.44452400	-1.15003900
C	-2.31530300	-0.37283900	0.01316000
O	-1.51532500	-1.07916800	0.71449200
O	-3.36957000	-0.75486500	-0.53256700
N	-0.62656700	1.44332900	0.37853800
H	-0.61108600	2.43349500	0.61941300
O	0.82849200	-1.52288200	-0.21744400
H	-0.10326000	-1.42265200	0.15407600
O	1.87769100	-0.00118500	1.42033200
H	2.42249100	0.76962200	1.63465400
O	2.83023900	-0.13974300	-1.01558700
H	-0.48623200	0.92534200	1.24964200

ZWC3 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) = -0.88997132192472D+03u.a.; Zero-point correction= 0.136888u.a; G= -889.870472 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.31672500	-0.25881300	-0.14336400
C	-0.77120400	1.47855100	-0.08027300
H	-1.39428600	2.00473800	0.63568700
H	-0.89601800	1.92275000	-1.06272500
C	1.68126900	1.00413900	-0.51284000
H	1.31633700	0.94253200	-1.53054800
H	2.57008800	1.62579700	-0.48664100
C	2.04304100	-0.37585700	0.03828600
O	1.57780600	-0.68124000	1.18642400
O	2.80899100	-1.06118400	-0.67033800
N	0.64723700	1.66826200	0.33647700
H	0.77500400	1.30965500	1.28802900
O	-2.90056700	-0.15479200	-0.09586000
H	-3.30232100	-0.13788800	-0.97584300
O	-1.04759200	-0.83998500	1.30301000
H	-0.06137600	-0.88766800	1.42741500
O	-0.73000300	-0.99884500	-1.28951300
H	0.82506400	2.67181600	0.35893100

ZWC4 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88997009635384D+03u.a.; Zero-point correction= 0.136557u.a; G= -889.870888 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.51063000	-0.14001000	0.05354100
C	0.40117300	1.10984900	-0.66679000
H	-0.04195300	0.75531000	-1.59062400
H	1.00963400	1.98223600	-0.88304400
C	-2.05366300	1.09287900	-0.13617400
H	-2.76608400	1.60663500	0.50202800
H	-2.20933100	1.39279400	-1.16579500
C	-2.22695900	-0.41266500	0.03571400
O	-1.34391000	-1.01084200	0.73194800
O	-3.24299300	-0.91446300	-0.49152700
N	-0.68812500	1.53209500	0.27155100
H	-0.68309300	2.54861100	0.33652600
O	2.79484100	-0.12338700	-0.88340400
H	3.40666100	0.59183500	-0.66004100
O	0.96422400	-1.57160600	-0.33424700
H	0.03088900	-1.62351900	-0.00145700
O	1.72602400	0.14705300	1.49651800
H	-0.49809500	1.16716000	1.20762800

N1 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) = -0.88996554090085D+03u.a.; Zero-point correction= 0.134646u.a; G=-889.867503u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.31811200	-0.24096300	-0.14631500
C	-0.81985600	1.49795600	-0.14483800
H	-1.55329600	2.03567400	0.45018100
H	-0.90104600	1.85609300	-1.16854400
C	1.60550900	1.16028800	-0.36124300
H	1.37746200	1.12982800	-1.42294000
H	2.51822100	1.74575200	-0.25200300
C	1.97431800	-0.22796600	0.10208500
O	1.59752800	-0.74371000	1.14369700
O	2.84248900	-0.81804200	-0.73299300
H	3.08795600	-1.67858700	-0.35637700
N	0.51897500	1.79729900	0.36765200
H	0.57089800	1.52985500	1.34412500
O	-2.89861900	-0.13819000	-0.33379300
H	-3.28761400	-0.95020200	-0.68844700
O	-1.19102700	-0.74323600	1.37049300
H	-0.24896300	-0.85955900	1.59496000
O	-0.59844400	-1.10146900	-1.12938000

NE2 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88996704711425D+03 u.a.; Zero-point correction= 0.134864 u.a; G= -889.868441u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.49299500	-0.18676200	0.10077600
C	-0.85764400	1.50644900	0.15050200
H	-1.58992700	2.10190000	-0.38976800
H	-0.89344100	1.82919000	1.18874700
C	1.58212600	1.17465000	0.31814500
H	1.38198700	1.16974700	1.38553100
H	2.48167900	1.77242200	0.17040700
C	1.96934400	-0.21798400	-0.11371100
O	1.57947700	-0.77699300	-1.12931100
O	2.87171700	-0.76305500	0.71349700
H	3.12711300	-1.62914800	0.35652300
N	0.47077900	1.77858400	-0.39763000
H	0.50202400	1.50302600	-1.37236500
O	-1.14864200	-0.78969600	-1.33745800
H	-0.18016800	-0.80551000	-1.48432500
O	-0.51458900	-0.91425000	1.14235000
H	-0.60164000	-1.87861200	1.14161800
O	-2.94935100	-0.31730200	0.37914600

NE4 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) = -0.88996526352071D+03u.a.; Zero-point correction= 0.134438u.a; G=-889.867196 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.50325900	-0.19161700	-0.09567800
C	-0.86732000	1.49257700	-0.16001200
H	-1.60314200	2.09864600	0.36244700
H	-0.87128900	1.79893300	-1.20962700
C	1.55866700	1.16245600	-0.27828400
H	1.38217100	1.16304600	-1.35522300
H	2.42480500	1.79683400	-0.09755400
C	1.99001100	-0.22456500	0.12259100
O	1.59549000	-0.85424300	1.09233600
O	2.93009800	-0.69679100	-0.71084400
H	3.20426800	-1.57123200	-0.39115100
N	0.43199900	1.66145400	0.49783900
H	0.56616200	2.65482100	0.62281700
O	-1.13679600	-0.79501700	1.33283900
H	-0.16505100	-0.78415700	1.46918900
O	-0.53818100	-0.91394000	-1.15265600
H	-0.61836300	-1.87875800	-1.14792100
O	-2.96096400	-0.31711700	-0.36273100

NE5 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) = -0.88996473439816D+03u.a.; Zero-point correction= 0.134058 u.a.; G= -889.868144 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.71199800	-0.16833800	0.13779900
C	-0.41691500	0.95838800	0.69182500
H	0.10114800	0.45136100	1.50472400
H	-0.90241300	1.83107400	1.12543200
C	1.90593700	1.17302600	-0.00925500
H	2.52929100	1.72089100	-0.71247800
H	2.13070300	1.55636900	0.98961000
C	2.36494300	-0.25799500	-0.04888300
O	1.68422600	-1.22256700	-0.36735400
O	3.64982900	-0.37298100	0.31174700
H	3.89515200	-1.31116600	0.26712800
N	0.51107100	1.30593800	-0.39357700
H	0.35159900	2.26910400	-0.65060500
O	-0.97183000	-1.36559900	-0.59161300
H	0.01124200	-1.26902500	-0.56945900
O	-2.45621200	0.51810000	-1.10767600
H	-3.20612200	1.05815600	-0.82416100
O	-2.64750200	-0.57742400	1.22436300

NE6 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) = -0.88996452833315D+03u.a.; Zero-point correction= 0.134623u.a; G= -889.866662 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.71864200	-0.06414500	-0.04333000
C	-0.39317300	0.92188700	0.67530400
H	0.10352300	0.29562500	1.41425100
H	-0.83063100	1.76342800	1.20965400
C	1.93386200	1.17152400	0.02882000
H	2.57994700	1.73291300	-0.64224400
H	2.14017100	1.51894100	1.04477800
C	2.36735600	-0.26609900	-0.04528100
O	1.67313200	-1.20773700	-0.40068300
O	3.64356900	-0.41606800	0.33418600
H	3.87057500	-1.35782900	0.27055100
N	0.54841800	1.33250500	-0.37951300
H	0.39478800	2.31072400	-0.57898000
O	-2.52109300	-0.70458200	1.18938200
H	-3.31030600	-0.19347600	1.41302000
O	-1.00153700	-1.34926400	-0.64014700
H	-0.01863900	-1.26712900	-0.61625100
O	-2.59869600	0.66110000	-1.00290100

NE7 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) = -0.88996247531577D+03 u.a.; Zero-point correction= 0.134021u.a; G= -889.867279 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
C	1.52362900	0.30670900	0.87789000
H	1.09022300	1.26178500	0.59764400
H	1.97904900	0.43738500	1.85803700
C	2.64501500	-0.01926000	-0.08217000
O	3.45287100	1.04203500	-0.28927900
O	2.82939400	-1.10809900	-0.59355400
N	0.49626000	-0.71845000	0.93880700
H	-2.12427100	-0.39078900	1.87041700
C	-0.26451500	-0.82245800	-0.31319300
H	0.27354300	-0.46904700	-1.19427700
H	-0.52840500	-1.86129300	-0.49725400
P	-1.83100600	0.05373100	-0.23016600
O	-2.69165200	-0.08337100	-1.43580700
O	-1.36223400	1.54017800	0.12846700
O	-2.62244200	-0.49636800	1.04820300
H	0.95541500	-1.60799300	1.08488500
H	-2.10012300	2.14963300	0.27642700
H	4.17355800	0.75856800	-0.87443500

NE8 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) = -0.88996323476214D+03 u.a.; Zero-point correction= 0.133708u.a; G=-889.868296 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.92365400	-0.13394700	0.17608400
C	-0.18933000	0.12328800	0.56595100
H	0.23281100	-0.85385700	0.81429100
H	-0.16193700	0.73034100	1.46898600
C	1.89678700	1.07261500	-0.15959000
H	2.36866500	1.68997600	-0.92237300
H	1.94872000	1.62122700	0.77678400
C	2.73911600	-0.17644800	-0.04332300
O	2.43829000	-1.26388800	-0.49952200
O	3.90196100	0.06260900	0.59853300
H	4.42179600	-0.75672300	0.59117300
N	0.50794100	0.82669400	-0.51271100
H	-2.15326100	1.76591500	-0.85181900
O	-2.67030900	-0.84158200	1.24792800
O	-1.95598300	-0.81585200	-1.27398600
H	-1.56625100	-1.70135500	-1.28120500
O	-2.58472400	1.28119400	-0.13461900
H	0.49536100	0.23025000	-1.33301200

NE9 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88996456684391D+03u.a.; Zero-point correction= 0.134208u.a; G= -889.867310 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.72542200	-0.16104000	-0.13679600
C	0.40292800	0.89846000	-0.74949200
H	-0.13043100	0.31979000	-1.50251700
H	0.85155700	1.74858000	-1.26006100
C	-1.89907200	1.17054800	-0.00495300
H	-2.50204100	1.72498200	0.71085900
H	-2.14305000	1.55212200	-0.99996600
C	-2.36215400	-0.25864300	0.05036800
O	-1.67945000	-1.22256900	0.36613500
O	-3.65200100	-0.37098700	-0.29383800
H	-3.90118900	-1.30758500	-0.23948000
N	-0.49523500	1.29191100	0.34650600
H	-0.31100000	2.25791700	0.57655400
O	0.99279400	-1.38134500	0.57329400
O	2.47660200	0.63055000	1.03725700
H	1.92828400	0.76116900	1.82230800
O	2.72866500	-0.56341100	-1.15993600
H	0.01008800	-1.28486700	0.55988200

NE10 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88996664048242D+03 u.a.; Zero-point correction= 0.134730u.a; G= -889.868173 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.48849800	-0.19847100	0.09263700
C	-0.87139000	1.50483300	0.13169700
H	-0.92496800	1.83745200	1.16660000
H	-1.59911300	2.09065500	-0.42502700
C	1.56393900	1.17571400	0.33555700
H	2.46298100	1.78080900	0.21785500
H	1.33966100	1.15215100	1.39829300
C	1.96758400	-0.20787800	-0.10978700
O	1.59486400	-0.75438100	-1.13834600
O	2.86097900	-0.75814700	0.72340400
H	3.12611800	-1.61874500	0.36037000
N	0.46390000	1.78171800	-0.39651700
H	-0.16975400	-0.80950000	-1.48918900
O	-2.93997900	-0.30800800	0.39946400
O	-0.51156600	-1.06340000	1.03117100
H	-0.55834500	-0.80080300	1.96127600
O	-1.13767200	-0.79941700	-1.33803900
H	0.50980000	1.50383600	-1.37013300

NE11 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88996554109434D+03 u.a.; Zero-point correction=0.134644 u.a; G=-889.867508 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.31811800	-0.24093900	-0.14637100
C	-0.81998000	1.49796400	-0.14504900
H	-1.55350100	2.03592600	0.44961600
H	-0.90062500	1.85597100	-1.16883500
C	1.60543300	1.16033600	-0.36101100
H	1.37745200	1.13006200	-1.42272100
H	2.51804300	1.74588200	-0.25151700
C	1.97433900	-0.22795800	0.10207800
O	1.59760400	-0.74392100	1.14361900
O	2.84254200	-0.81776200	-0.73309600
H	3.08805700	-1.67837200	-0.35666400
N	0.51876200	1.79712000	0.36791000
H	0.57047800	1.52921900	1.34426500
O	-2.89864500	-0.13847500	-0.33388000
H	-3.28762500	-0.95057900	-0.68833900
O	-1.19106600	-0.74292500	1.37053600
H	-0.24904100	-0.86035800	1.59463800
O	-0.59813000	-1.10136200	-1.12922200

NE12 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) =-0.88996550327588D+03u.a.; Zero-point correction= 0.134733u.a; G= -889.867188 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.31476000	-0.24847000	0.16186300
C	-0.81332400	1.49341300	0.15218100
H	-1.55069100	2.02927700	-0.44077200
H	-0.89593700	1.85152700	1.17603400
C	1.61341700	1.16172700	0.35416700
H	1.39581700	1.13157700	1.41802500
H	2.52683400	1.74421200	0.23535900
C	1.97234600	-0.22737700	-0.11415500
O	1.58343400	-0.73991600	-1.15313700
O	2.84595900	-0.82199300	0.71111200
H	3.08391700	-1.68360700	0.33213000
N	0.52210300	1.80290900	-0.36309200
H	0.56984800	1.54367300	-1.34204900
O	-2.88996600	-0.28295600	0.41152600
H	-3.40277600	0.19966700	-0.25197900
O	-1.19630100	-0.75228300	-1.35343700
H	-0.25506400	-0.82032800	-1.60194900
O	-0.59811300	-1.08483800	1.16340400

NE13 structure in aqueous solution at SMD-MP2/6-311++G (2d,2p).
E (MP2) = -0.88996449123926D+03 u.a.; Zero-point correction= 0.135174u.a; G= -889.865888u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.70638000	-0.16531500	-0.14568800
C	0.36596700	0.87629100	-0.74599400
H	-0.18119900	0.25170500	-1.45337300
H	0.82606700	1.67379100	-1.32559700
C	-1.91529400	1.19519500	0.02223800
H	-2.53089700	1.70688000	0.75957300
H	-2.17446800	1.60956700	-0.94865400
C	-2.34368900	-0.25333200	0.04453600
O	-1.64466200	-1.19606800	0.39064900
O	-3.61879100	-0.40367800	-0.33438200
H	-3.84710800	-1.34553300	-0.27234300
N	-0.50984000	1.42602900	0.30433000
H	-0.30164100	0.99773600	1.19825600
O	2.57987100	-0.67753500	-1.23377600
O	1.01182100	-1.26675200	0.76889800
H	0.03130100	-1.27883400	0.65354800
O	2.59002400	0.68730500	0.88128800
H	2.16310700	0.82711700	1.73751200

6-Structures and energetics of glyphosate conformers in aqueous solution, at IEFPCM-B3LYP-D3/6-311++G(2d,2p) and IEFPCM-B3LYP/6-311++G(2d,2p) levels.

ZWP1structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6888315u.a; Zero-point correction=0.136543 u.a ; G= -891.5906631u.a. at 298,15K.
E_{gas} = -891,66701836u.a

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	2.05702000	-0.01394100	0.12028600
C	0.29931500	-0.11594500	0.68903100
H	-0.11573500	0.84318100	0.97870900
H	0.22487800	-0.82065000	1.51225500
C	-1.91937600	-1.03887200	-0.12808300
H	-2.31346200	-1.66132700	-0.92936600
H	-1.93458800	-1.60928200	0.79539800
C	-2.76677700	0.21146700	-0.01646900
O	-2.38725500	1.30418000	-0.35892300
O	-3.96932500	-0.07165100	0.47723100
H	-4.50461400	0.73731100	0.50451800
N	-0.51643100	-0.66197500	-0.45364400
H	0.00367200	-1.46385900	-0.82619300
O	2.90545100	0.42230700	1.26924600
O	1.95224400	1.17818400	-1.00453900
H	2.06395700	2.04672300	-0.60119700
O	2.27213400	-1.28423100	-0.64951600
H	-0.52934800	0.04064100	-1.19776000

ZWP1structure in aqueous solution at IEF-PCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6724431 u.a.; Zero-point correction=0.136022u.a. ; G=-891.5754672 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	2.08300600	-0.04833900	0.09814800
C	0.32380200	-0.10496900	0.68304100
H	-0.03827400	0.83366500	1.08858400
H	0.23156900	-0.88929500	1.42888100
C	-1.90400400	-0.98887200	-0.17956800
H	-2.25873600	-1.59279500	-1.01315100
H	-1.87387000	-1.61050100	0.70960900
C	-2.83356700	0.19336100	-0.00268800
O	-2.53136700	1.32207700	-0.30427200
O	-4.00952800	-0.18464100	0.49021900
H	-4.59337200	0.58812500	0.55240500
N	-0.53437300	-0.49513300	-0.49253400
H	0.01369200	-1.19486900	-1.01061700
O	2.97754800	0.01840000	1.29213900
O	2.13928700	1.36268000	-0.73278000
H	2.37707600	2.09880500	-0.15719400
O	2.14261400	-1.13799100	-0.93512100
H	-0.62839500	0.31655800	-1.10918800

ZWP2 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.6879974u.a.; Zero-point correction= 0.136619 u.a; G= -891.5895743u.a. at 298,15K.
E_{gas} = -891,66351458u.a

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	2.06619800	0.02539800	0.14537600
C	0.27448100	-0.02699600	0.61138900
H	0.12639300	0.61959000	1.47145000
H	-0.09089200	-1.02353100	0.83080900
C	-1.90383400	1.00495300	-0.18905400
H	-1.86764400	1.61575900	0.70752300
H	-2.28458800	1.61201800	-1.00855800
C	-2.80923600	-0.19528800	-0.00821300
O	-2.49826100	-1.31550300	-0.33031800
O	-3.97807400	0.16299600	0.51711100
H	-4.55178900	-0.61665300	0.58560800
N	-0.52980200	0.54457800	-0.52895900
H	-0.60018900	-0.16015000	-1.26604900
O	2.18755100	1.24968500	-0.72429100
O	2.22016000	-1.30318900	-0.80433600
H	2.23501400	-1.05165400	-1.73441800
O	2.86182700	-0.19362500	1.38746400
H	0.03523800	1.31268800	-0.91407500

ZWP2 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6715645 u.a.; Zero-point correction= 0.135952u.a. ; G= -891.5728427 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-2.09309100	-0.05946600	0.10848000
C	-0.32316200	-0.11452800	0.66449200
H	-0.20759400	-0.95923000	1.33721200
H	0.01465200	0.79288900	1.15288400
C	1.89239600	-0.94656600	-0.28377700
H	1.84029600	-1.65657500	0.53548000
H	2.23033900	-1.47078300	-1.17573800
C	2.85819000	0.18088000	0.01518000
O	2.59197300	1.34354400	-0.16885200
O	4.01957600	-0.28268700	0.46727800
H	4.62636700	0.46074500	0.61198700
N	0.54008200	-0.37857500	-0.54311900
H	0.67031500	0.50040800	-1.05068200
O	-2.12040200	-0.97805600	-1.08599100
O	-2.27664000	1.48295900	-0.41269000
H	-2.20150600	1.53275000	-1.37236100
O	-2.95188800	-0.23883600	1.31400200
H	-0.02258500	-0.99229800	-1.14949100

ZWP3 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.688421u.a.; Zero-point correction= 0.136427 u.a; G= -891.5908425u.a. at 298,15K.
E_{gas} = -891,66418995u.a

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.94868500	-0.25335700	0.04418500
C	-0.32453700	0.28144500	0.75322700
H	0.19734100	-0.58043600	1.15679800
H	-0.42112200	1.05060600	1.51295300
C	1.93706900	1.09340100	-0.05728100
H	2.36166000	1.73188900	-0.82961500
H	2.00317000	1.60895000	0.89600300
C	2.69866900	-0.21496000	-0.02888300
O	2.23987500	-1.26191600	-0.41314300
O	3.92803200	-0.03643800	0.44920600
H	4.40662500	-0.88013200	0.42676700
N	0.50607000	0.83105200	-0.37640500
H	0.06945100	1.69082800	-0.71149700
O	-1.59033400	-0.93731400	-1.24198600
O	-2.58674900	1.19931200	-0.38433600
H	-3.07574200	1.59246100	0.34770100
O	-2.75965000	-0.88142400	1.12963700
H	0.42980500	0.15173900	-1.14445600

ZWP3 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.6718282 u.a.; Zero-point correction= 0.136235 u.a ; G= -891.5740612 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.93555800	-0.25453500	-0.05139200
C	0.35030300	0.36368100	-0.78594800
H	-0.17258900	-0.47612100	-1.23338100
H	0.49343500	1.14507700	-1.52499900
C	-1.95679500	1.10307300	-0.01904800
H	-2.39601300	1.78777300	0.70391300
H	-2.03510500	1.54714900	-1.00678600
C	-2.68786300	-0.22078400	0.05403700
O	-2.20743800	-1.22209800	0.52375300
O	-3.91998500	-0.11360700	-0.43814100
H	-4.37550900	-0.96526600	-0.34412300
N	-0.51971400	0.90116500	0.32062200
H	-0.13214100	1.78512900	0.64840600
O	1.54782000	-0.78150200	1.30370100
O	2.78212100	1.13616800	0.15522900
H	2.81045800	1.38105700	1.08689200
O	2.62278800	-1.06970800	-1.09431300
H	-0.42422900	0.23523300	1.10053200

ZWP4 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6876569 u.a.; Zero-point correction= 0.136445 u.a. ; G= -891.5896856 u.a. at 298,15K.
E_{gas} =-891,66035261u.a

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.93396300	-0.25556600	0.04577700
C	-0.32695200	0.29051100	0.78162200
H	0.20357900	-0.58268600	1.14728500
H	-0.44788400	1.01509000	1.57985700
C	1.95275900	1.10436700	0.02769700
H	2.39310100	1.79107700	-0.69237700
H	2.03711000	1.53864500	1.01934400
C	2.67649500	-0.22329900	-0.05497800
O	2.18362200	-1.22404300	-0.51296700
O	3.91581300	-0.11672500	0.41866100
H	4.36950900	-0.96919700	0.32411900
N	0.51345100	0.91012500	-0.30437300
H	0.10814800	1.80885800	-0.56526200
O	-1.58235500	-0.75859000	-1.32804000
O	-2.71115200	1.18313300	-0.11605100
H	-2.76899800	1.42904800	-1.04597400
O	-2.64429200	-1.07090700	1.07306300
H	0.41382000	0.29936300	-1.12639300

ZWP4 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.6709794u.a.; Zero-point correction=0.136115 u.a. ; G= -891.5736043u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.93555800	-0.25453500	-0.05139200
C	0.35030300	0.36368100	-0.78594800
H	-0.17258900	-0.47612100	-1.23338100
H	0.49343500	1.14507700	-1.52499900
C	-1.95679500	1.10307300	-0.01904800
H	-2.39601300	1.78777300	0.70391300
H	-2.03510500	1.54714900	-1.00678600
C	-2.68786300	-0.22078400	0.05403700
O	-2.20743800	-1.22209800	0.52375300
O	-3.91998500	-0.11360700	-0.43814100
H	-4.37550900	-0.96526600	-0.34412300
N	-0.51971400	0.90116500	0.32062200
H	-0.13214100	1.78512900	0.64840600
O	1.54782000	-0.78150200	1.30370100
O	2.78212100	1.13616800	0.15522900
H	2.81045800	1.38105700	1.08689200
O	2.62278800	-1.06970800	-1.09431300
H	-0.42422900	0.23523300	1.10053200

ZWP5 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6897488u.a.; Zero-point correction=0.136425 u.a ; G= -891.5917392u.a. at 298,15K.
E_{gas} =-891,67260982u.a

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.91358600	0.03869300	0.20673500
C	0.87342600	-0.73840100	-1.12017700
H	1.27678900	-1.72336300	-1.33521900
H	0.82114100	-0.16165100	-2.03773300
C	-1.39403900	0.26448400	-0.67904200
H	-0.86237400	1.12104000	-0.27139200
H	-1.60985700	0.45543100	-1.72668200
C	-2.67127800	0.02818300	0.09391100
O	-2.88838200	-0.96705200	0.74021500
O	-3.50096200	1.06285500	-0.03446800
H	-4.30624500	0.89292300	0.47913700
N	-0.51806600	-0.93568500	-0.57293200
H	-0.97617200	-1.73169400	-1.01503500
O	1.29841900	-0.47525400	1.47846400
H	-0.39078000	-1.16535800	0.42406500
O	1.49823100	1.62343100	0.11765500
H	2.05949700	2.09387100	-0.50937900
O	3.35044600	-0.13615600	-0.16016900

ZWP5 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.6729355 u.a.; Zero-point correction= 0.136149u.a ; G=-891.5757336u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.93305600	0.02988100	0.19921600
C	0.85716200	-0.70374100	-1.12556200
H	1.24542300	-1.68708900	-1.37336300
H	0.78853100	-0.10734600	-2.02932200
C	-1.41445300	0.28264500	-0.66167100
H	-0.89842000	1.14560900	-0.24764900
H	-1.62021700	0.47191900	-1.71205900
C	-2.70245600	0.02681500	0.08874700
O	-2.93491600	-0.98970800	0.69492200
O	-3.52798700	1.06789400	-0.01359900
H	-4.34172400	0.87773700	0.47938500
N	-0.52263100	-0.90387600	-0.54784100
H	-0.97999900	-1.71474400	-0.96250000
O	1.31047600	-0.48723200	1.46699900
H	-0.36234600	-1.10966400	0.45149600
O	1.57003000	1.62720800	0.14121000
H	2.15355000	2.09710000	-0.46583900
O	3.36192900	-0.18427500	-0.17735600

ZWP6 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.6878556u.a.; Zero-point correction=0.136402u.a ; G= -891.5897796u.a. at 298,15K.
E_{gas} =-891,66695638u.a

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.93448100	0.06564100	0.17826900
C	0.87191500	-0.78818200	-1.07610000
H	1.28185000	-1.77969800	-1.24085200
H	0.80124600	-0.26568600	-2.02412300
C	-1.42765100	0.18322800	-0.73709700
H	-0.91487700	1.10368200	-0.46965800
H	-1.67686900	0.22219300	-1.79370500
C	-2.67496300	0.02062500	0.10239900
O	-2.82865200	-0.86630600	0.90529900
O	-3.55464900	0.98479400	-0.16385500
H	-4.33859300	0.86623900	0.39540000
N	-0.50993500	-0.96485100	-0.49602100
H	-0.94237400	-1.82005400	-0.84294200
O	1.36810200	-0.36655000	1.50639800
O	1.52781100	1.64164500	-0.05590800
H	1.14870700	2.00654400	0.75185200
O	3.35644200	-0.14035700	-0.22100600
H	-0.37500000	-1.08370800	0.51952100

ZWP6 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.6710289u.a.; Zero-point correction=0.136060 u.a ; G=-891.5738259u.a. at 298,15K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	1.97009000	0.04238300	0.17097100
C	0.84211900	-0.71242600	-1.09259700
H	1.21856900	-1.70279000	-1.32872800
H	0.75020200	-0.13748500	-2.00775300
C	-1.45367000	0.24957600	-0.68088900
H	-0.97196200	1.16424600	-0.34637000
H	-1.66427800	0.33997300	-1.74344200
C	-2.73494700	0.01416400	0.08841200
O	-2.93876900	-0.96164800	0.76706800
O	-3.58955900	1.02036500	-0.09126800
H	-4.40050800	0.84251700	0.41088300
N	-0.52158700	-0.89111700	-0.46775100
H	-0.96174900	-1.75052200	-0.79408100
O	1.38161000	-0.39481600	1.48899200
O	1.67955100	1.64784200	-0.01096200
H	1.29579700	2.01289700	0.79437900
O	3.37345800	-0.24563900	-0.24231100
H	-0.33766500	-1.00347400	0.54308800

ZWP7structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.6862811u.a.; Zero-point correction=0.136373u.a ; G= -891.5883328 u.a. at 298,15K.
E_{gas} =-891,66345707u.a

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-2.04714600	-0.09711300	-0.04407700
C	-0.26161200	-0.16520500	0.49390600
H	0.09607400	-1.16805600	0.69353400
H	-0.11853800	0.46026900	1.36988300
C	1.88896400	0.97023800	-0.24093300
H	2.27383600	1.57104100	-1.06324800
H	1.78226100	1.60670500	0.63208100
C	2.84709900	-0.17286400	0.01998300
O	2.61163300	-1.31817100	-0.27628900
O	3.97058400	0.26540500	0.58367600
H	4.58048400	-0.47947000	0.70491500
N	0.55725600	0.43082600	-0.62344600
H	-0.04188400	1.16273700	-1.03545100
O	-2.81719400	0.19099800	1.36670600
H	-2.80962400	1.13114500	1.58067000
O	-2.49035000	-1.43907200	-0.52298000
O	-2.08648800	1.13084200	-0.91940700
H	0.69160500	-0.27650000	-1.34850500

ZWP7 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6705783u.a.; Zero-point correction= 0.136156 u.a. ; G=-891.5730937 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	2.06631000	0.10447800	-0.03443100
C	0.28924800	0.15033300	0.54382700
H	-0.03366100	1.13213500	0.87017200
H	0.14115400	-0.56990300	1.34272500
C	-1.86502300	-0.92014500	-0.29213800
H	-2.21090700	-1.48240000	-1.15794600
H	-1.73395400	-1.60897200	0.53642900
C	-2.88364000	0.15266300	0.03121000
O	-2.70321700	1.32541900	-0.18713300
O	-3.99132200	-0.37386400	0.54764300
H	-4.63678100	0.33307100	0.70692500
N	-0.56049300	-0.28774600	-0.62342000
H	0.04997200	-0.92395800	-1.16472600
O	2.84929800	-0.48114700	1.27267700
H	2.80236600	-1.44347600	1.31284600
O	2.57386700	1.48880500	-0.26065600
O	2.02792800	-0.93514000	-1.12786300
H	-0.74533600	0.52085900	-1.22075300

ZWC1 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.692131 u.a.; Zero-point correction=0.135001 u.a ; G= -891.593588u.a. at 298,15K.
E_{gas} =-891,6813855u.a

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.51654700	-0.21275400	0.06442500
C	0.84509600	1.49325600	0.03943000
H	1.45276900	2.05747000	-0.66294200
H	0.94813900	1.93536100	1.02617500
C	-1.64579700	1.01848800	0.49602700
H	-1.24939000	0.91796900	1.49952400
H	-2.49323400	1.69659800	0.51070300
C	-2.10907600	-0.35137200	-0.04412700
O	-1.58047400	-0.73832300	-1.13727200
O	-2.97273200	-0.92111700	0.62387300
N	-0.58838200	1.63013500	-0.39446300
H	-0.78116600	2.62292400	-0.51747600
O	0.96703200	-0.94909500	-1.21451900
H	-0.05014200	-0.95855900	-1.23624600
O	0.71101200	-0.79584700	1.32420100
H	0.82192800	-1.74583200	1.46187800
O	2.98696100	-0.20695200	0.16333800
H	-0.71415900	1.18287700	-1.31169500

ZWC1 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.6728121 u.a. ; Zero-point correction= 0.134927u.a. ; G= -891.5745276 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.53777700	-0.20508200	-0.05924000
C	-0.83005100	1.48844600	-0.02272400
H	-1.42265700	2.05420300	0.69146100
H	-0.93446200	1.94801800	-1.00134600
C	1.66230500	1.01234900	-0.50084600
H	1.25579400	0.90776300	-1.50038400
H	2.49715300	1.70560000	-0.52691200
C	2.14914100	-0.35042800	0.03888100
O	1.60049500	-0.75663700	1.11535500
O	3.04068400	-0.89782800	-0.61085400
N	0.60715300	1.60211300	0.40617600
H	0.80557700	2.58899400	0.56315500
O	-0.95518100	-0.98293700	1.18056200
H	0.06072400	-0.99214800	1.19396300
O	-0.80836300	-0.77693000	-1.36870700
H	-1.00238300	-1.70404500	-1.56142300
O	-3.01100300	-0.16917000	-0.09269200
H	0.73540800	1.11886100	1.30566900

ZWC2 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.6894794u.a.; Zero-point correction= 0.134824 u.a ; G= -891.5923614u.a. at 298,15K.
E_{gas} =-891,6751412u.a

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.63759500	-0.17900600	-0.14887100
C	0.48928200	1.17004600	-0.64143100
H	0.04691100	0.93316900	-1.60397300
H	1.08249900	2.07258200	-0.74937900
C	-2.01509300	1.11781200	-0.10410100
H	-2.70064500	1.66112300	0.54147500
H	-2.13735400	1.47088200	-1.12236000
C	-2.32136100	-0.38763100	0.01383200
O	-1.46610300	-1.08814200	0.64562400
O	-3.39099000	-0.75297000	-0.47566400
N	-0.61815200	1.44987800	0.35338500
H	-0.57998900	2.43436000	0.61168000
O	0.85148700	-1.52639000	-0.26296200
H	-0.10003100	-1.44228100	0.09927000
O	1.76980500	0.01992100	1.44392000
H	2.42711300	0.68183000	1.69499300
O	2.89264500	-0.10180700	-0.91775500
H	-0.44709000	0.91802700	1.21255800

ZWC2 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6714170u.a.; Zero-point correction=0.134718 u.a. ; G= -891.5739669 u.a. at 298,15K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	1.64043800	-0.17973400	-0.15698800
C	0.55094100	1.25527200	-0.52673000
H	0.18086000	1.17883700	-1.54418800
H	1.16993300	2.14499900	-0.45648200
C	-1.99204400	1.11220300	-0.15174300
H	-2.71412000	1.70226000	0.40644900
H	-2.02130600	1.41838200	-1.19202300
C	-2.34208100	-0.38010800	0.00671500
O	-1.50119300	-1.08965600	0.64956500
O	-3.42200100	-0.72935200	-0.47071900
N	-0.62762300	1.43587600	0.40761000
H	-0.62766500	2.39910200	0.73742400
O	0.79595900	-1.48371500	-0.33613900
H	-0.14320800	-1.40828400	0.06190700
O	1.83113400	-0.10241400	1.43874100
H	2.52640700	0.50663600	1.71952000
O	2.87373100	-0.10255600	-0.96072000
H	-0.50604200	0.84029200	1.23367600

ZWC3 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6905917u.a.; Zero-point correction=0.135047 u.a. ; G= -891.5923762u.a. at 298,15K.
E_{gas} =-891,6780758u.a

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	1.36676800	-0.26283900	0.15273800
C	0.80728600	1.48383900	-0.01397300
H	1.39211200	1.96519700	-0.79262300
H	0.96848700	1.99903400	0.92850700
C	-1.65356900	0.99059000	0.54022900
H	-1.20458400	0.85393300	1.51764600
H	-2.49986600	1.66501800	0.62188000
C	-2.13576600	-0.36370100	-0.02721500
O	-1.63203100	-0.71637600	-1.14332600
O	-2.97976500	-0.95466300	0.64768800
N	-0.64144600	1.62645400	-0.38485600
H	-0.80453600	1.18126300	-1.29836200
O	2.94399400	-0.14757600	-0.05370900
H	3.43251000	-0.21949000	0.77578700
O	0.94200900	-0.95989800	-1.19545800
H	-0.06601900	-0.98160200	-1.26049000
O	0.91402900	-0.87018200	1.42065900
H	-0.84309000	2.61923800	-0.49049500

ZWC3 structure in aqueous solution atIEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.6719282 u.a. ; Zero-point correction=0.135122u.a ; G= -891.5735448u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.39327300	-0.25646800	-0.15968600
C	-0.79819200	1.47817200	0.03399000
H	-1.37259600	1.95663100	0.82230400
H	-0.95333100	2.01545900	-0.89719600
C	1.66785900	0.99207900	-0.53245600
H	1.21431300	0.85966500	-1.50886300
H	2.49886700	1.68513400	-0.61488600
C	2.17603100	-0.35929600	0.02065600
O	1.64732900	-0.74920600	1.11302400
O	3.05590600	-0.91432900	-0.63845100
N	0.65185600	1.59560800	0.40921300
H	0.81122800	1.10923800	1.30285300
O	-2.95878400	-0.12372000	0.11866300
H	-3.48675000	-0.16764500	-0.68846300
O	-0.92750800	-1.00142700	1.14861300
H	0.08182000	-1.01988900	1.20321000
O	-1.01567400	-0.83739700	-1.46415500
H	0.85820900	2.58207400	0.55715100

ZWC4 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.6895668u.a.; Zero-point correction=0.135342u.a ; G=-891.5912324u.a. at 298,15K.
E_{gas} =-891,6795819u.a

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.55121300	-0.14399000	0.05794700
C	0.41578600	1.08120200	-0.71149700
H	-0.04882800	0.68384100	-1.60735500
H	0.99614800	1.95857700	-0.97891300
C	-2.06204100	1.10322500	-0.11188200
H	-2.73489600	1.62682700	0.56289300
H	-2.24868100	1.43966600	-1.12636000
C	-2.29477100	-0.41485100	0.02549300
O	-1.38902000	-1.06689200	0.63066100
O	-3.36179200	-0.83136400	-0.43422600
N	-0.65943400	1.50171700	0.26426800
H	-0.62271300	2.51253300	0.38311000
O	2.83480900	-0.16102300	-0.88683500
H	3.51125000	0.47125200	-0.61301500
O	0.96787300	-1.57192600	-0.25529200
H	0.01049900	-1.57625300	0.05452600
O	1.76979100	0.23378000	1.47242300
H	-0.44207300	1.09332600	1.17950200

ZWC4 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.6714576u.a.; Zero-point correction= 0.135184 u.a ; G= -891.5736188u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.56184000	-0.14412300	0.05776500
C	0.43054400	1.10100700	-0.68916300
H	-0.01904700	0.73437100	-1.60584600
H	1.01021400	1.98990300	-0.91885200
C	-2.06176700	1.10267000	-0.12574200
H	-2.74249900	1.64107700	0.52919800
H	-2.22224100	1.43328800	-1.14667000
C	-2.31117400	-0.41180300	0.02176400
O	-1.40660000	-1.07144700	0.62114400
O	-3.38660200	-0.82023700	-0.42536600
N	-0.66390400	1.49098800	0.27928200
H	-0.63072700	2.49826700	0.42680000
O	2.83139900	-0.17127400	-0.90562300
H	3.52673200	0.44228800	-0.63613300
O	0.95711400	-1.56283900	-0.25577900
H	-0.00132600	-1.56202200	0.05338900
O	1.80685300	0.21812100	1.47169000
H	-0.46431300	1.05792900	1.18697300

NE1 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6899646 u.a.; Zero-point correction= 0.133003u.a ; G= -891.5947832 u.a. at298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.38519600	-0.23313100	-0.15434100
C	-0.81404500	1.50753200	-0.09960000
H	-1.51804700	2.05641800	0.52442800
H	-0.90282100	1.90018000	-1.11309400
C	1.64425100	1.15727500	-0.32239100
H	1.43671400	1.15201700	-1.39172400
H	2.53852500	1.77189900	-0.18804100
C	2.05629400	-0.24732500	0.08987400
O	1.60562100	-0.86649400	1.03423800
O	3.03856600	-0.71890900	-0.67981300
H	3.29612800	-1.59874300	-0.36285900
N	0.53451100	1.73662700	0.40291100
H	0.60159100	1.55591100	1.39511300
O	-2.98607900	-0.11860600	-0.16371000
H	-3.38525000	-0.68479600	-0.83571600
O	-1.12644300	-0.80972800	1.31729400
H	-0.16065900	-0.90519200	1.45505700
O	-0.80526800	-1.03776300	-1.25747400

NE1 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.6768142u.a.; Zero-point correction= 0.132712 u.a ; G= -891.5822882u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.43145600	-0.22452500	-0.16158500
C	-0.78897000	1.49658600	-0.09277200
H	-1.48716600	2.06600800	0.51990400
H	-0.85008300	1.89637300	-1.10560800
C	1.68437000	1.15740400	-0.28289500
H	1.50111900	1.19364600	-1.35677500
H	2.56529900	1.78112100	-0.10779400
C	2.11344200	-0.25756100	0.07745900
O	1.61096400	-0.95722500	0.93561600
O	3.17233100	-0.64748500	-0.63485200
H	3.42951300	-1.54006400	-0.35507600
N	0.55216700	1.69486200	0.43546000
H	0.60371700	1.51026100	1.42707000
O	-3.02424700	-0.04224700	-0.05634900
H	-3.49418100	-0.57185800	-0.71229700
O	-1.10386300	-0.86036600	1.27017000
H	-0.13268600	-0.97450300	1.35951200
O	-0.97792300	-1.02214200	-1.32760300

NE2 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.6922871 u.a. ; Zero-point correction= 0.133371u.a ; G= -891.5957533u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.55618400	-0.17530000	0.09041200
C	-0.86257900	1.52038400	0.07923700
H	-1.55802900	2.11374900	-0.51355400
H	-0.92302000	1.89195000	1.10272100
C	1.60325100	1.16769900	0.28894700
H	1.39831600	1.17182600	1.35868100
H	2.48547800	1.79762100	0.14574800
C	2.04289200	-0.23389600	-0.10070600
O	1.58038200	-0.89455200	-1.01158500
O	3.06398100	-0.65518500	0.64591800
H	3.33575700	-1.53653500	0.34537900
N	0.48232400	1.71590300	-0.44050100
H	0.54153500	1.52520300	-1.43080800
O	-1.11522000	-0.87402300	-1.27729700
H	-0.13443900	-0.91289900	-1.35135700
O	-0.64441500	-0.85412000	1.23775700
H	-0.80555400	-1.79960400	1.35267900
O	-3.01909600	-0.26690100	0.29432900

NE2 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.6735269u.a.; Zero-point correction= 0.133011u.a ; G= -891.5777117u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.58517400	-0.16402700	0.08162300
C	-0.84104700	1.51439600	0.06683400
H	-1.52425400	2.12118000	-0.52723900
H	-0.89530300	1.89259400	1.08839000
C	1.63394000	1.16146700	0.27302800
H	1.43664400	1.18529600	1.34460900
H	2.50872800	1.79831300	0.11527900
C	2.08700600	-0.24411000	-0.09121500
O	1.59079800	-0.95562100	-0.94411200
O	3.16077000	-0.61205400	0.60926200
H	3.43201000	-1.50025200	0.32877000
N	0.50434600	1.68977100	-0.45523200
H	0.56155300	1.50866100	-1.44682000
O	-1.10271500	-0.91198400	-1.24483300
H	-0.12003800	-0.96620000	-1.28860700
O	-0.76714200	-0.84642300	1.29510100
H	-1.00809200	-1.76785100	1.45782300
O	-3.05964300	-0.20270200	0.20935700

NE4 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6910561 u.a.; Zero-point correction= 0.133243u.a ; G=-891.5945924u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.56800100	-0.17927900	-0.08236200
C	-0.87778500	1.50652300	-0.08591100
H	-1.57117000	2.09862100	0.50888000
H	-0.92713600	1.87633700	-1.11722600
C	1.57346800	1.14628100	-0.27556700
H	1.36886800	1.12693700	-1.35090700
H	2.41867900	1.82124300	-0.13897100
C	2.07178000	-0.23589400	0.10728400
O	1.60542700	-0.95842600	0.96509300
O	3.13584800	-0.58246900	-0.62246200
H	3.42814200	-1.46738900	-0.35492400
N	0.44674400	1.59185600	0.51937300
H	0.60508800	2.52437800	0.86589800
O	-1.09785800	-0.88148200	1.26810300
H	-0.11435500	-0.86677700	1.34385400
O	-0.68337100	-0.84825300	-1.25562700
H	-0.83205400	-1.79694200	-1.35847900
O	-3.03354800	-0.26332900	-0.26425000

NE4 structure in aqueous solution atIEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) = -891.6731142u.a.; Zero-point correction= 0.132962u.a ; G= -891.57728884u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.59956400	-0.16680000	-0.07170100
C	-0.85472600	1.50038200	-0.07124900
H	-1.52965600	2.10898300	0.52831400
H	-0.89907500	1.87892000	-1.09946400
C	1.60159000	1.13498200	-0.27259300
H	1.38965300	1.12283900	-1.34706700
H	2.43636500	1.82297700	-0.13815000
C	2.12006900	-0.24474200	0.09537200
O	1.62469500	-1.00885600	0.89945300
O	3.23235800	-0.54224600	-0.58190400
H	3.52605000	-1.43104300	-0.32851900
N	0.47252700	1.55841500	0.53087400
H	0.63457900	2.47673300	0.91203800
O	-1.08051500	-0.92133200	1.23142800
H	-0.09428800	-0.92003600	1.27586300
O	-0.81639400	-0.83453500	-1.31522100
H	-1.05455400	-1.75723100	-1.47351800
O	-3.07575700	-0.19962800	-0.16866500

NE5 structure in aqueous solution atIEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6903619u.a.; Zero-point correction= 0.133041u.a. ; G=-891.594696u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.73880600	-0.17320700	0.13442200
C	-0.45302200	0.97431100	0.72896500
H	0.04043200	0.47985200	1.56628100
H	-0.94817800	1.85986600	1.13244600
C	1.90174200	1.17328000	-0.00113900
H	2.49221800	1.72965000	-0.72948700
H	2.16603500	1.57789000	0.98414600
C	2.39722200	-0.25772100	-0.04262400
O	1.72492600	-1.23619600	-0.30555700
O	3.69452600	-0.33815400	0.25571600
H	3.97188100	-1.26686600	0.22323100
N	0.50037300	1.27393700	-0.33841100
H	0.29473100	2.15758900	-0.77576500
O	-0.95695200	-1.39875500	-0.50067600
H	0.02458600	-1.27973900	-0.51685400
O	-2.37342800	0.51517900	-1.18094000
H	-3.17553500	1.00865000	-0.97183500
O	-2.75936400	-0.53276800	1.14760500

NE5 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6739950u.a.; Zero-point correction= 0.132883 u.a. ; G= -891.5786099u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.74560600	-0.16763900	0.13808600
C	-0.49046800	1.04456900	0.67676900
H	-0.03152500	0.64069100	1.58001400
H	-1.01475600	1.95513000	0.97321600
C	1.89951700	1.16665300	0.01534100
H	2.51029300	1.74432600	-0.67863100
H	2.12690600	1.55206600	1.01717300
C	2.40852400	-0.26011300	-0.03841600
O	1.74521100	-1.24391900	-0.30420100
O	3.70801200	-0.33291600	0.25262400
H	3.98821300	-1.26074000	0.21623500
N	0.50895300	1.27546100	-0.36513100
H	0.33650000	2.14092800	-0.85000000
O	-0.93762500	-1.42305400	-0.39680200
H	0.04136100	-1.28807300	-0.44725100
O	-2.37331900	0.41161200	-1.23229600
H	-3.17943300	0.91784400	-1.07471500
O	-2.77497600	-0.47703300	1.15897800

NE6 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6895183u.a.; Zero-point correction= 0.133098u.a ; G= -891.593831u.a. at298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.73279000	-0.06898600	-0.05960300
C	-0.43780900	0.96489100	0.69615100
H	0.02413900	0.37799600	1.48986800
H	-0.90515600	1.83267300	1.16585400
C	1.93373400	1.16994100	0.03037400
H	2.55229400	1.73242300	-0.66936500
H	2.18275100	1.54260500	1.03231100
C	2.39867600	-0.26992400	-0.03574500
O	1.70941100	-1.22924100	-0.32409000
O	3.69060300	-0.38328100	0.27509000
H	3.94833900	-1.31710700	0.22982500
N	0.54238300	1.31030200	-0.33606700
H	0.36236700	2.22530600	-0.71743700
O	-2.59106100	-0.66471200	1.16927600
H	-3.44345500	-0.22138900	1.25464100
O	-0.97347700	-1.36926500	-0.56702200
H	0.01010700	-1.27497600	-0.56031900
O	-2.57345200	0.61846000	-1.06869700

NE6 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6732889u.a.; Zero-point correction= 0.132860u.a. ; G=-891.5781534 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.73756200	-0.07543000	-0.06146600
C	-0.46985200	1.01958200	0.66150300
H	-0.03343800	0.50316300	1.51636700
H	-0.96142400	1.91584900	1.04495200
C	1.92939300	1.16432400	0.04543800
H	2.56018800	1.74546500	-0.62748700
H	2.14989500	1.52276900	1.05902100
C	2.41060200	-0.27064400	-0.03319700
O	1.73288100	-1.23604000	-0.32846800
O	3.70429300	-0.37449700	0.27425600
H	3.96692200	-1.30675200	0.22308100
N	0.54659700	1.30806500	-0.35304600
H	0.38985700	2.20766000	-0.77817900
O	-2.61638000	-0.61299100	1.17919300
H	-3.48137400	-0.18766600	1.21714500
O	-0.95641100	-1.39599800	-0.47409200
H	0.02554300	-1.28534400	-0.50230000
O	-2.56435600	0.54206200	-1.12610800

NE7 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6860328u.a; Zero-point correction= 0.132736u.a; G= -891.5922312 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
C	1.46658900	0.11622400	0.87772500
H	1.00967600	1.09818200	0.76531600
H	1.89080300	0.08577700	1.88243800
C	2.62541500	0.00499800	-0.10115300
O	3.43297200	1.07727100	-0.02659200
O	2.81970200	-0.92821800	-0.84305000
N	0.46369400	-0.92481500	0.74328900
H	-1.41695700	-0.54887500	1.78455700
C	-0.33295900	-0.88140600	-0.49151000
H	0.19378100	-0.47604700	-1.35727700
H	-0.65936300	-1.88766000	-0.74672900
P	-1.85651400	0.07149700	-0.19359200
O	-2.99307800	-0.11167000	-1.12139300
O	-1.27672200	1.57406600	-0.13577500
O	-2.24190200	-0.32072800	1.31406400
H	0.89284300	-1.83477300	0.83738100
H	-1.96253300	2.24612000	-0.03092400
H	4.17155700	0.95386100	-0.64231400

NE7 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6693999u.a.; Zero-point correction= 0.132716u.a. ; G=-891.575636u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
C	1.49186300	0.17588800	0.84782200
H	1.05059700	1.15686700	0.67751800
H	1.89699500	0.19343800	1.86124100
C	2.67131400	-0.00096000	-0.09756400
O	3.48460100	1.06945900	-0.07152800
O	2.88185500	-0.97937000	-0.77377300
N	0.47639500	-0.85723400	0.75305700
H	-1.42075400	-0.50365900	1.80140900
C	-0.33100500	-0.85338100	-0.47509000
H	0.17833600	-0.44857400	-1.35156600
H	-0.62843200	-1.87283900	-0.71412500
P	-1.88587100	0.05655200	-0.19157700
O	-3.01966400	-0.19088000	-1.10816500
O	-1.36588600	1.58126200	-0.17516300
O	-2.25219000	-0.31371600	1.32602400
H	0.89485800	-1.76822900	0.88052500
H	-2.07763800	2.23241700	-0.12338600
H	4.23656400	0.89962700	-0.65952300

NE8 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.685460u.a.; Zero-point correction= 0.132943 u.a. ; G= -891.5913178 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.99613200	-0.07942800	-0.18320700
C	0.21563500	-0.15634900	-0.53847800
H	-0.09456800	-1.19580800	-0.66647500
H	0.06891000	0.36004000	-1.48696500
C	-1.84442300	0.97095600	0.18671500
H	-2.24177800	1.61195000	0.97582100
H	-1.84157300	1.56796200	-0.72488800
C	-2.82122500	-0.18210400	0.01543500
O	-2.58907000	-1.33157600	0.30565900
O	-3.99712700	0.23786400	-0.48188400
H	-4.59794700	-0.52054600	-0.54404600
N	-0.49079900	0.56959800	0.52461200
O	2.90151500	-0.50568100	-1.26972400
O	2.19519000	-0.87624300	1.20427800
H	2.34533300	-1.82070000	1.07330800
O	2.20220700	1.43101500	0.29639000
H	-0.50394800	0.00698100	1.36728100
H	1.35753600	1.75630700	0.66199200

NE8 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6696922 u.a.; Zero-point correction= 0.132572 u.a. ; G= -891.5762519u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	2.00519500	-0.08090600	-0.18770900
C	0.22621300	-0.13548400	-0.54109700
H	-0.07451900	-1.16552000	-0.74717800
H	0.08769300	0.44306100	-1.45451800
C	-1.84231800	0.94991900	0.23213600
H	-2.23121400	1.56127600	1.04903300
H	-1.82358500	1.59044200	-0.64917300
C	-2.84590400	-0.17076500	0.00359000
O	-2.64944900	-1.33821600	0.24375800
O	-4.00920500	0.29973600	-0.47931500
H	-4.62599300	-0.44231900	-0.57477700
N	-0.49654700	0.51340000	0.55789700
H	1.47580100	1.72419700	0.82549000
O	2.94113000	-0.43362600	-1.27541000
O	2.07471600	-1.03167500	1.10857100
H	2.96475900	-1.14393900	1.46668700
O	2.25768900	1.41553800	0.33567900
H	-0.52203900	-0.10349400	1.36073700

NE9 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6915451 u.a.; Zero-point correction=0.133492u.a; G= -891.5953034 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.75342300	-0.15559200	0.12429600
C	-0.483 90700	0.97910700	0.77763900
H	0.00350300	0.48187800	1.61596000
H	-0.98413600	1.86429100	1.17225800
C	1.87839200	1.16163200	0.03642600
H	2.46891400	1.73173900	-0.68083800
H	2.14600400	1.54403800	1.02925500
C	2.37082900	-0.26767500	-0.03467000
O	1.69323000	-1.24792100	-0.27569400
O	3.67889700	-0.34463900	0.21109700
H	3.95725600	-1.27264400	0.16769600
N	0.47343400	1.28867200	-0.29260700
H	0.29276200	2.20570400	-0.67073000
O	-0.97421400	-1.48954000	-0.25991100
O	-2.21682500	0.50481700	-1.27195300
H	-1.47366900	0.62305900	-1.87888800
O	-2.93338600	-0.38962400	0.98423300
H	0.00316800	-1.36800800	-0.34945000

NE9 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6747846 u.a.; Zero-point correction=0.133066 u.a. ; G= -891.5794918 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.75589800	-0.15505400	-0.12832000
C	0.50828900	1.03299200	-0.73165500
H	0.04583800	0.60714500	-1.62216500
H	1.03205300	1.93710300	-1.04472300
C	-1.87997700	1.15838100	-0.04527800
H	-2.48706400	1.74299300	0.64587700
H	-2.11809400	1.52794400	-1.05037300
C	-2.38267700	-0.26819600	0.03207900
O	-1.71287300	-1.25267400	0.27811100
O	-3.69089800	-0.34041800	-0.21510500
H	-3.96994300	-1.26827400	-0.17044900
N	-0.48363800	1.29096600	0.31946400
H	-0.32549200	2.19485300	0.73665900
O	0.95635400	-1.48598900	0.22094000
O	2.26243400	0.44090600	1.28183300
H	1.54939600	0.52714000	1.92820400
O	2.91829600	-0.38173200	-1.01406600
H	-0.01999900	-1.35966200	0.32094400

NE10 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.6917206u.a.; Zero-point correction=0.133358 u.a. ; G= -891.5950935u.a. at 298,15K.
E_{gas} =-891,7056879u.a

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-1.55110800	-0.18769500	0.07850100
C	-0.87259100	1.51809600	0.07368100
H	-0.95259300	1.89358400	1.09489700
H	-1.56130800	2.10737200	-0.53120200
C	1.59316500	1.16903700	0.31130800
H	2.47532800	1.80325300	0.18689700
H	1.37782700	1.15884800	1.37910900
C	2.04191700	-0.22498200	-0.09517500
O	1.59148700	-0.87061700	-1.02290500
O	3.05507800	-0.65630700	0.65575200
H	3.33236300	-1.53212800	0.34414900
N	0.47936300	1.72378000	-0.42401300
H	-0.11631600	-0.89138300	-1.36730300
O	-3.01077600	-0.25329600	0.30984700
O	-0.64747300	-1.01617600	1.13538800
H	-0.89399600	-0.84991600	2.05350100
O	-1.09795100	-0.86093300	-1.28967300
H	0.55191900	1.54506800	-1.41563100

NE10 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6729445 u.a.; Zero-point correction= 0.133148u.a. ; G= -891.5767811u.a. at 298,15K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-1.58184600	-0.17557900	0.07113500
C	-0.85173300	1.51345600	0.05671700
H	-0.92531200	1.90039200	1.07438700
H	-1.52728400	2.11370100	-0.55269500
C	1.62266300	1.16288300	0.29502900
H	2.49649000	1.80650500	0.16086900
H	1.40942500	1.16938500	1.36392900
C	2.08833800	-0.23437900	-0.08461300
O	1.60090500	-0.93764900	-0.94967100
O	3.16044300	-0.60472600	0.61621700
H	3.43813600	-1.48803400	0.32663400
N	0.50140100	1.69476900	-0.44321100
H	-0.09909700	-0.94784000	-1.29736300
O	-3.05408600	-0.18435900	0.22185600
O	-0.77648000	-1.01014800	1.19986100
H	-1.08282600	-0.82838600	2.09705800
O	-1.08327400	-0.90423300	-1.25137600
H	0.57267500	1.52174100	-1.43525300

NE11 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.6899646 u.a.; Zero-point correction=0.133002 u.a. ; G= -891.5947882 u.a. at 298,15K.
E_{gas} =-891,7101419u.a

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-1.38513700	-0.23313900	-0.15432700
C	-0.81403500	1.50753700	-0.09992700
H	-1.51814800	2.05669400	0.52374100
H	-0.90251200	1.89987100	-1.11356700
C	1.64433200	1.15735600	-0.32221900
H	1.43718800	1.15238700	-1.39162700
H	2.53862800	1.77186600	-0.18740900
C	2.05616800	-0.24733400	0.08990100
O	1.60556100	-0.86645000	1.03432900
O	3.03827800	-0.71905200	-0.67993900
H	3.29578100	-1.59889600	-0.36297100
N	0.53442400	1.73668900	0.40283100
H	0.60132600	1.55610000	1.39506800
O	-2.98595200	-0.11850900	-0.16397200
H	-3.38527700	-0.68592400	-0.83484300
O	-1.12650400	-0.80949400	1.31741100
H	-0.16075000	-0.90517500	1.45519300
O	-0.80499900	-1.03799900	-1.25720700

NE11 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6716836u.a.; Zero-point correction= 0.132724u.a. ; G=-891.5771108 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.43152900	-0.22480300	-0.16175200
C	-0.78859900	1.49601600	-0.09569200
H	-1.48799000	2.06740800	0.51379000
H	-0.84691200	1.89324800	-1.10967900
C	1.68518500	1.15802000	-0.28134600
H	1.50446400	1.19627500	-1.35559000
H	2.56577700	1.78133100	-0.10310800
C	2.11349300	-0.25747000	0.07762100
O	1.61077400	-0.95785100	0.93503900
O	3.17230700	-0.64701200	-0.63504600
H	3.42949400	-1.53975500	-0.35578100
N	0.55146600	1.69497700	0.43518200
H	0.60117900	1.50959600	1.42678600
O	-3.02369300	-0.03752600	-0.05841200
H	-3.49677100	-0.58856800	-0.69417300
O	-1.10389200	-0.85890600	1.27096000
H	-0.13301200	-0.97555600	1.35936700
O	-0.97850000	-1.02572600	-1.32568100

NE12 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6894317u.a.; Zero-point correction=0.133385u.a. ; G= -891.5931163 u.a. at 298,15K.
E_{gas} =-891,70465757u.a

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-1.38298800	-0.23616200	0.18470900
C	-0.81944500	1.50918200	0.08669100
H	-1.52290300	2.05044400	-0.54492600
H	-0.90338100	1.92101500	1.09292200
C	1.64127600	1.16095600	0.29994000
H	1.43740300	1.16224500	1.36986000
H	2.53322200	1.77712300	0.15749900
C	2.05482900	-0.24542000	-0.10364700
O	1.59571800	-0.87546500	-1.03702200
O	3.04810300	-0.70564400	0.65822500
H	3.30516200	-1.58761600	0.34682400
N	0.52719900	1.73089200	-0.42622400
H	0.58823500	1.53512900	-1.41600700
O	-2.98409400	-0.22431300	0.27729600
H	-3.42869600	0.06944600	-0.52762400
O	-1.13446600	-0.84893100	-1.27499400
H	-0.16929600	-0.92559300	-1.43197500
O	-0.78092000	-0.98618600	1.31005200

NE12 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6709983 u.a.; Zero-point correction= 0.133138u.a. ; G= -891.5753359 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.42408700	-0.22701200	0.18939600
C	-0.79538000	1.50153500	0.08631900
H	-1.49400000	2.06779000	-0.52895100
H	-0.85069300	1.91302100	1.09475500
C	1.67872400	1.16089000	0.26418900
H	1.50148600	1.20247700	1.33872000
H	2.55965500	1.78219900	0.08038000
C	2.10318800	-0.25591300	-0.09297600
O	1.60024000	-0.95408400	-0.95234900
O	3.15943100	-0.64893500	0.62111900
H	3.41468400	-1.54219500	0.34170500
N	0.54357100	1.69666500	-0.45114500
H	0.58896800	1.50230400	-1.44131700
O	-3.02782600	-0.15860400	0.18498800
H	-3.41813500	0.11839700	-0.65340000
O	-1.11577300	-0.88720300	-1.23676600
H	-0.14489400	-0.98215400	-1.35261400
O	-0.93106500	-0.97272200	1.36958400

NE13 structure in aqueous solution at IEFPCM-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.6888136 u.a.; Zero-point correction=0.132626u.a. ; G= -891.5945363 u.a. at 298,15K.
E_{gas} =-891,7038467u.a

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	1.72008200	-0.13395300	-0.13382900
C	0.62078900	1.27164900	-0.52017500
H	0.29247000	1.13946800	-1.55038000
H	1.27403600	2.14802700	-0.51013300
C	-1.85428600	1.16382200	-0.08056100
H	-2.57551300	1.74911700	0.49408000
H	-1.98856900	1.47262800	-1.11859400
C	-2.32352900	-0.28194900	0.01746400
O	-1.64319600	-1.24287000	0.32453800
O	-3.62425000	-0.38936500	-0.25565100
H	-3.88914500	-1.32029500	-0.19101700
N	-0.52136900	1.47148700	0.36126600
H	-0.34264800	1.21682600	1.32032100
O	2.99563100	-0.16177700	-0.88521500
O	0.91453500	-1.49325900	-0.31533900
H	-0.01795000	-1.42877000	0.00843700
O	1.86669500	0.08957700	1.45911400
H	2.36249900	-0.60769300	1.90591600

NE13 structure in aqueous solution at IEFPCM-B3LYP/6-311++G (2d,2p).
E (SCF) =-891.6720898 u.a. ; Zero-point correction= 0.132521u.a. ; G= -891.5777309 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.72748000	-0.13575100	-0.13227300
C	0.62168100	1.26596600	-0.52303800
H	0.29519400	1.13231900	-1.55371200
H	1.27162200	2.14536400	-0.51499900
C	-1.85901600	1.16047200	-0.08807100
H	-2.57654600	1.75540000	0.48104100
H	-1.98942100	1.46346000	-1.12863300
C	-2.33970400	-0.28256000	0.01663600
O	-1.66419500	-1.25320400	0.30313800
O	-3.64693300	-0.37818500	-0.23003000
H	-3.91450100	-1.30846100	-0.16568400
N	-0.52500500	1.46669500	0.35066800
H	-0.34836900	1.24744600	1.31845600
O	2.98866900	-0.18265200	-0.90720300
O	0.91613300	-1.49657500	-0.27558800
H	-0.02292200	-1.42638100	0.02823900
O	1.91283700	0.11617400	1.45199200
H	2.45791400	-0.54749200	1.89309400

7-Structures and energetics of glyphosate conformers in aqueous solution, atIEFPCM-MP2/6-311++G(2d,2p) level.

ZWP1structure in aqueous solution atIEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.914673 u.a.; Zero-point correction= 0.137632u.a ; G=-889.8155938 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	2.03840000	-0.01804400	0.11658600
C	0.29323400	-0.12722500	0.69441600
H	-0.12370500	0.81974600	1.01441200
H	0.21662900	-0.85927100	1.49118000
C	-1.89853500	-1.04177800	-0.14030300
H	-2.28885400	-1.65210700	-0.94936300
H	-1.90334300	-1.61865500	0.77677100
C	-2.74062300	0.20658400	-0.01470700
O	-2.36165400	1.30047200	-0.37434400
O	-3.93675800	-0.07319800	0.50399500
H	-4.45840800	0.74382700	0.52555200
N	-0.50966800	-0.63920900	-0.46073700
H	0.03250000	-1.41226900	-0.86056500
O	2.91695500	0.33271100	1.27510100
O	1.93677700	1.23292600	-0.93670100
H	2.07310700	2.07060600	-0.48099200
O	2.20220500	-1.25067800	-0.73063000
H	-0.54090500	0.08989400	-1.17641700

ZWP2 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =E= -889.9136011 u.a.; Zero-point correction=0.137723u.a ; G= -889.8140542 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-2.04638100	-0.02694600	0.14654900
C	-0.26510500	0.01732600	0.61651200
H	-0.11202500	-0.65731600	1.45210800
H	0.10388700	1.00431700	0.86399700
C	1.88133200	-1.00683400	-0.21091300
H	1.83613900	-1.62973400	0.67429400
H	2.25986800	-1.59452800	-1.04210700
C	2.77937100	0.19073800	-0.00618500
O	2.46943900	1.31529400	-0.33568300
O	3.94099000	-0.16888200	0.54184900
H	4.50115100	0.61944700	0.61161800
N	0.52033800	-0.52381200	-0.53915500
H	0.60267000	0.20292400	-1.25131200
O	-2.14358000	-1.23504900	-0.75443700
O	-2.18875400	1.31843500	-0.77505200
H	-2.23080000	1.07270100	-1.70506000
O	-2.85529300	0.15939400	1.38804600
H	-0.06354300	-1.26784700	-0.94195500

ZWP3 structure in aqueous solution atIEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9161416u.a.; Zero-point correction= 0.137652u.a. ; G=-889.8166473u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.90356300	-0.25855800	0.04257700
C	-0.32405800	0.35065200	0.77086600
H	0.21928900	-0.48098500	1.20518300
H	-0.45149100	1.13736400	1.50504900
C	1.92828300	1.11479300	-0.04616100
H	2.36662900	1.74224400	-0.81637000
H	2.00875300	1.61610700	0.91136300
C	2.63881600	-0.21862800	-0.03405600
O	2.14359200	-1.24133300	-0.45474600
O	3.86921700	-0.09650000	0.46781300
H	4.30393000	-0.96171600	0.42009200
N	0.49916200	0.88281900	-0.36055500
H	0.07586600	1.74599700	-0.69807700
O	-1.47184800	-0.88340000	-1.25593800
O	-2.62586200	1.15485100	-0.36389900
H	-3.15158900	1.48941500	0.37070300
O	-2.68655300	-0.96694000	1.10216500
H	0.40131200	0.19588000	-1.11977700

ZWP4 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9135500u.a.; Zero-point correction= 0.137682u.a. ; G= -889.8140620 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.90121300	-0.25852500	-0.05195700
C	0.32226100	0.32719500	-0.79461600
H	-0.22432000	-0.52391700	-1.18468500
H	0.45555900	1.07115100	-1.57056900
C	-1.93481000	1.11795600	-0.02440500
H	-2.37965900	1.79189500	0.70130700
H	-2.02168300	1.55108200	-1.01411000
C	-2.62833200	-0.22201700	0.05759200
O	-2.11699800	-1.20668200	0.54469500
O	-3.86251500	-0.15062400	-0.44404900
H	-4.28547100	-1.01615900	-0.33449600
N	-0.50253600	0.92338800	0.30314000
H	-0.09247100	1.81259400	0.58282400
O	1.50339300	-0.77544900	1.30795200
O	2.68516200	1.16785100	0.15137200
H	2.74313800	1.37274300	1.09044400
O	2.62212700	-1.06920900	-1.07879500
H	-0.39960800	0.28886200	1.10582000

ZWP5 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =E= -889.9153533 u.a.; Zero-point correction=0.137733u.a. ; G= -889.8157269 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.85706800	0.05585700	0.21953500
C	0.89330000	-0.80334500	-1.10499200
H	1.31683800	-1.79015500	-1.25449600
H	0.85935300	-0.27643900	-2.05117000
C	-1.34627700	0.22107800	-0.72254000
H	-0.78184600	1.07284600	-0.35530000
H	-1.58609700	0.37776400	-1.76828100
C	-2.59843900	0.03562300	0.09745200
O	-2.79421700	-0.92055300	0.81587300
O	-3.43348400	1.06442300	-0.07298600
H	-4.21397500	0.91587800	0.48233100
N	-0.50166400	-0.99043100	-0.59137900
H	-0.96002000	-1.78254500	-1.03592000
O	1.13177800	-0.35536400	1.47485600
H	-0.39654600	-1.19903500	0.41120500
O	1.48172800	1.63199100	-0.01536100
H	2.11898800	2.04501000	-0.60824300
O	3.31512300	-0.16903500	-0.02650900

ZWP6 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9133500u.a.; Zero-point correction=0.137537u.a ; G= -889.8141568 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.85643000	0.11308100	0.18411400
C	0.90721400	-0.96610100	-0.97365300
H	1.35590600	-1.95280600	-0.95975400
H	0.86256700	-0.60298800	-1.99339900
C	-1.38839100	0.00436800	-0.82924100
H	-0.83833800	0.93776100	-0.76687600
H	-1.71151800	-0.14700900	-1.85279200
C	-2.56520900	0.03995100	0.11490800
O	-2.63846900	-0.63337700	1.11978600
O	-3.48162800	0.91717200	-0.30266500
H	-4.20551100	0.92910500	0.34198100
N	-0.48308800	-1.09982300	-0.42944200
H	-0.89573800	-1.99313700	-0.68748600
O	1.16112000	-0.08619700	1.51097700
O	1.46650900	1.60750600	-0.37144000
H	1.07433300	2.12016500	0.34390000
O	3.31174700	-0.13988100	-0.03783700
H	-0.38244100	-1.07964100	0.59615900

ZWP7 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) = -889.9118892 u.a.; Zero-point correction= 0.137591u.a. ; G= -889.8125847 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	2.02102400	0.10279900	-0.04316500
C	0.25837300	0.08809600	0.53565800
H	-0.12782400	1.06052300	0.81187200
H	0.14402500	-0.60783000	1.35978200
C	-1.88176300	-0.98591900	-0.24505800
H	-2.26781900	-1.56650000	-1.07787400
H	-1.78696500	-1.62801300	0.62250000
C	-2.81236200	0.17499600	0.01717800
O	-2.55278000	1.31650300	-0.29693100
O	-3.94182000	-0.23667700	0.59564600
H	-4.52584800	0.52988600	0.70198700
N	-0.54996200	-0.45066400	-0.60581200
H	0.04926400	-1.16386900	-1.04444700
O	2.83950900	-0.16676400	1.33854400
H	2.87638700	-1.10915300	1.53417200
O	2.39176900	1.46968700	-0.52141900
O	2.07178400	-1.11457400	-0.93707500
H	-0.68002300	0.28917000	-1.29663300

ZWC1structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).

E (MP2) =-889.9161084 u.a. ; Zero-point correction=0.136655 u.a. ; G=-889.8155142u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.49300600	-0.21188800	-0.06762100
C	-0.82300300	1.48551700	-0.07455800
H	-1.43599500	2.06429900	0.60894500
H	-0.91760900	1.90718100	-1.06957100
C	1.64450900	1.01611700	-0.51816500
H	1.25563800	0.92464900	-1.52373900
H	2.50441200	1.67608000	-0.51889700
C	2.06262600	-0.35394800	0.04584500
O	1.56016000	-0.65900200	1.18456300
O	2.86889200	-0.99983300	-0.63377000
N	0.59858900	1.63076000	0.36414100
H	0.73407800	1.16961700	1.27410300
O	-0.99525600	-0.89902400	1.26139300
H	0.01175600	-0.91367200	1.29624900
O	-0.63244000	-0.82958600	-1.26853600
H	-0.76017600	-1.77916100	-1.39149900
O	-2.96130600	-0.21184000	-0.22097100
H	0.78766700	2.62219000	0.48956400

ZWC2 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9128642 u.a.; Zero-point correction=0.136605u.a. ; G=-889.8133780 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.62029900	-0.17183900	-0.14877300
C	0.41689300	1.09960300	-0.69026500
H	-0.07243200	0.77229000	-1.60100400
H	0.97734500	2.00059400	-0.91123000
C	-2.03473600	1.12419400	-0.09792600
H	-2.70879900	1.64919300	0.57135000
H	-2.17909800	1.48187400	-1.10961600
C	-2.28192200	-0.38809200	0.02232900
O	-1.42203600	-1.01948500	0.73020000
O	-3.29922800	-0.82728600	-0.52735000
N	-0.63694600	1.44027600	0.32817400
H	-0.56236700	2.42558200	0.56841900
O	0.88307800	-1.55397400	-0.19131000
H	-0.05712300	-1.46835700	0.16710000
O	1.74950200	0.10894400	1.42818400
H	2.40665600	0.78443200	1.63743800
O	2.86610000	-0.09183200	-0.93693300
H	-0.47080400	0.90486800	1.18476000

ZWC3 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9151878 u.a.; Zero-point correction= 0.136846 u.a. ; G=-889.8145718 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.32490400	-0.26684500	-0.14509000
C	-0.78632100	1.48048100	-0.03016600
H	-1.37633900	1.97934000	0.73109600
H	-0.94804000	1.96679600	-0.98639000
C	1.64794100	0.98355300	-0.57125000
H	1.20755300	0.85117700	-1.55119900
H	2.51596200	1.62869800	-0.64155800
C	2.06784800	-0.36964700	0.03533900
O	1.59333300	-0.61970900	1.19922300
O	2.84349800	-1.05453700	-0.64210500
N	0.65248800	1.64361600	0.33512200
H	0.82700000	1.20563600	1.25065000
O	-2.90831800	-0.14987000	-0.02443900
H	-3.34229200	-0.20758800	-0.88405300
O	-0.98753600	-0.89300500	1.26319600
H	0.00941200	-0.92236600	1.35442800
O	-0.79264900	-0.93391500	-1.35397300
H	0.84947000	2.63763300	0.41877400

ZWC4 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9140256 u.a.; Zero-point correction=0.137058u.a. ; G=-889.8136349 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.51679900	-0.13392100	0.05875100
C	0.35377700	1.02417800	-0.75444200
H	-0.14874200	0.56633400	-1.59834500
H	0.91683800	1.88080700	-1.10713900
C	-2.07509800	1.09912800	-0.10853600
H	-2.73963500	1.60537900	0.58430300
H	-2.28933100	1.42836800	-1.11816800
C	-2.23763200	-0.42141800	0.03715000
O	-1.30463900	-1.00247600	0.68475000
O	-3.26650600	-0.91182600	-0.45124200
N	-0.67677300	1.50601900	0.22714500
H	-0.62723700	2.51896100	0.30185100
O	2.81759900	-0.12844000	-0.85917300
H	3.44601300	0.55785500	-0.60508400
O	1.01552400	-1.59710900	-0.24383300
H	0.07034100	-1.63383900	0.07104000
O	1.68188300	0.29058700	1.47034200
H	-0.43998700	1.12560200	1.14847400

NE1 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9115197 u.a. ; Zero-point correction= 0.134352 u.a; G=-889.8144310 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.32728200	-0.24528400	-0.14959500
C	-0.83912100	1.50308100	-0.12957400
H	-1.55558700	2.04304500	0.48426600
H	-0.92973200	1.87825100	-1.14712000
C	1.60261700	1.16142500	-0.35144700
H	1.38020500	1.13280300	-1.41498600
H	2.50486600	1.76247700	-0.23423500
C	1.98616300	-0.23301800	0.10124700
O	1.58938200	-0.77712700	1.11841200
O	2.89070600	-0.78437600	-0.71586100
H	3.13495700	-1.64832800	-0.35089800
N	0.50620000	1.77837900	0.36767400
H	0.57318600	1.59125600	1.35860400
O	-2.91826500	-0.16046100	-0.28932600
H	-3.28404400	-0.91625700	-0.76442500
O	-1.15886800	-0.75087100	1.36093900
H	-0.20703000	-0.86225900	1.54440800
O	-0.62157100	-1.06957800	-1.16501000

NE2 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =E= -889.9147572u.a.; Zero-point correction= 0.134833u.a ; G= -889.8164582u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.52415200	-0.18573100	0.09538500
C	-0.87300700	1.51152400	0.10607100
H	-1.57970300	2.10363100	-0.47115500
H	-0.92655900	1.86912300	1.13284700
C	1.58067400	1.16990200	0.30582500
H	1.36809200	1.16380900	1.37173700
H	2.46796800	1.78874000	0.16768600
C	1.99794100	-0.22582700	-0.10834100
O	1.57663100	-0.83239300	-1.08041800
O	2.95876000	-0.70741500	0.68650900
H	3.21906500	-1.57783400	0.34870800
N	0.46679500	1.74235600	-0.41865300
H	0.52073500	1.53797500	-1.40631300
O	-1.12438000	-0.82665700	-1.31135900
H	-0.14978200	-0.85046800	-1.41288800
O	-0.54238500	-0.86044900	1.18103400
H	-0.69375800	-1.80768000	1.29259900
O	-2.97674900	-0.31951300	0.35614000

NE4 structure in aqueous solution atIEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9146846 u.a.; Zero-point correction=0.134897 u.a; G= -889.8162124u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.53604600	-0.19035900	-0.08978300
C	-0.88444500	1.49759100	-0.12689100
H	-1.59437200	2.09492700	0.43961500
H	-0.91193200	1.84310900	-1.16451000
C	1.55349600	1.15247100	-0.28566800
H	1.35466100	1.13569500	-1.35913800
H	2.40445500	1.81380700	-0.13393900
C	2.02491700	-0.22791500	0.11621000
O	1.60019800	-0.89466900	1.04346100
O	3.02632400	-0.63910200	-0.67357500
H	3.30652300	-1.51412200	-0.36620000
N	0.42746800	1.61307100	0.50528900
H	0.57537600	2.57266400	0.77419500
O	-1.11127200	-0.81626400	1.31107200
H	-0.13570600	-0.77095500	1.41810100
O	-0.57462200	-0.86916100	-1.19039900
H	-0.71003800	-1.82134200	-1.27549600
O	-2.99117400	-0.32115100	-0.33366100

NE5 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9138434 u.a.; Zero-point correction= 0.134556u.a ; G= -889.8163911 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.73621700	-0.17474200	0.13354000
C	-0.41266000	0.88982900	0.76054000
H	0.11629100	0.31613200	1.52013700
H	-0.85204500	1.75113600	1.26260600
C	1.89867600	1.17790700	-0.00239500
H	2.47362100	1.73397100	-0.73982700
H	2.15483200	1.58638500	0.97953800
C	2.39014700	-0.24946400	-0.04592900
O	1.71494400	-1.22240700	-0.33827900
O	3.68413300	-0.33535500	0.28018300
H	3.94458600	-1.26744700	0.23177400
N	0.49221900	1.24185100	-0.33598900
H	0.25976600	2.15089000	-0.70332500
O	-0.97902200	-1.35832000	-0.60233600
H	-0.00297600	-1.23190200	-0.60694600
O	-2.37735400	0.61925900	-1.11177700
H	-3.17908800	1.08582000	-0.84929300
O	-2.73948100	-0.59148200	1.14481700

NE6 structure in aqueous solutionat IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) = -889.9130287u.a.; Zero-point correction= 0.134493u.a ; G= -889.8157982u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.73101200	-0.06045700	-0.05239500
C	-0.40588300	0.89518800	0.72379400
H	0.08694400	0.24867600	1.44723000
H	-0.82320300	1.73878000	1.27212700
C	1.92844400	1.17431900	0.02986500
H	2.53393400	1.73860400	-0.67606200
H	2.16676800	1.54881100	1.02973200
C	2.39116400	-0.26148100	-0.04095500
O	1.70200600	-1.21502700	-0.36300800
O	3.67889000	-0.37955900	0.29965700
H	3.92137800	-1.31559000	0.23621400
N	0.53226000	1.28033400	-0.33676200
H	0.32787600	2.21246700	-0.66115000
O	-2.57621500	-0.71251300	1.15063300
H	-3.40692200	-0.24299500	1.28600700
O	-0.99197500	-1.34338200	-0.62761800
H	-0.01438900	-1.23435700	-0.63335600
O	-2.56712700	0.70072600	-1.01387700

NE7 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9103943 u.a.; Zero-point correction=0.134250 u.a ; G=-889.8146344u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
C	1.45213100	0.09364300	0.89189600
H	0.98865100	1.07264700	0.81009700
H	1.88073700	0.02513100	1.89008600
C	2.59856400	0.00756300	-0.09623700
O	3.38498600	1.10010300	-0.02847700
O	2.80640600	-0.92861700	-0.83905600
N	0.45381600	-0.94758800	0.71655400
H	-1.41103800	-0.70014400	1.70522400
C	-0.31516700	-0.83054300	-0.53247500
H	0.23087200	-0.36888900	-1.35448100
H	-0.62544100	-1.82005700	-0.85778400
P	-1.84082800	0.08426600	-0.19506700
O	-2.95873000	-0.01979300	-1.16100000
O	-1.25473100	1.56886600	0.00420300
O	-2.24384100	-0.44742400	1.26119400
H	0.91026100	-1.84904800	0.73439700
H	-1.94296600	2.22856700	0.15635900
H	4.11874100	0.97186200	-0.64777800

NE8 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) = -889.9102341 u.a.; Zero-point correction=0.134371 u.a; G= -889.8144862u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.97353200	-0.08218200	0.18808800
C	-0.20189500	-0.10941300	0.54597300
H	0.13763000	-1.13317900	0.70350900
H	-0.05872400	0.44561400	1.47113700
C	1.83896700	0.98960900	-0.20993400
H	2.25002700	1.60408600	-1.00924500
H	1.83790200	1.59576200	0.69237800
C	2.77993700	-0.18349200	-0.01925100
O	2.53788000	-1.32447300	-0.35281600
O	3.94146100	0.20359300	0.54346400
H	4.51480100	-0.57532700	0.59875200
N	0.47890200	0.60321600	-0.54322100
H	-1.33730900	1.71760200	-0.69038200
O	-2.87879700	-0.49682400	1.28254900
O	-2.13760400	-0.91435900	-1.17947900
H	-2.26331500	-1.85711100	-1.01955200
O	-2.19174400	1.41016900	-0.33163100
H	0.49803800	0.00769900	-1.36278500

NE9 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) = -889.9145083 u.a.; Zero-point correction= 0.134859 u.a; G= -889.8167354 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
C	1.45213100	0.09364300	0.89189600
H	0.98865100	1.07264700	0.81009700
H	1.88073700	0.02513100	1.89008600
C	2.59856400	0.00756300	-0.09623700
O	3.38498600	1.10010300	-0.02847700
O	2.80640600	-0.92861700	-0.83905600
N	0.45381600	-0.94758800	0.71655400
H	-1.41103800	-0.70014400	1.70522400
C	-0.31516700	-0.83054300	-0.53247500
H	0.23087200	-0.36888900	-1.35448100
H	-0.62544100	-1.82005700	-0.85778400
P	-1.84082800	0.08426600	-0.19506700
O	-2.95873000	-0.01979300	-1.16100000
O	-1.25473100	1.56886600	0.00420300
O	-2.24384100	-0.44742400	1.26119400
H	0.91026100	-1.84904800	0.73439700
H	-1.94296600	2.22856700	0.15635900
H	4.11874100	0.97186200	-0.64777800

NE10 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9140843u.a.; Zero-point correction=0.134676u.a ; G= -889.8159753u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.51873300	-0.19753800	-0.08291200
C	-0.88608200	1.50972100	-0.10290100
H	-0.95806800	1.86779000	-1.12876000
H	-1.58602000	2.09965500	0.48473900
C	1.56718000	1.17065900	-0.33166800
H	2.45381300	1.79542600	-0.21739500
H	1.34090000	1.14562300	-1.39464900
C	1.99673900	-0.21555400	0.10213200
O	1.58616200	-0.80741600	1.08793200
O	2.95374600	-0.70527300	-0.69149300
H	3.22020100	-1.56927700	-0.34212300
N	0.46104100	1.75071800	0.39873500
H	-0.12950000	-0.82869200	1.42515500
O	-2.96702100	-0.30954000	-0.37268700
O	-0.54195500	-1.02217000	-1.07003300
H	-0.79023800	-0.92448700	-1.99717400
O	-1.10509400	-0.80890900	1.32493500
H	0.52889100	1.55952300	1.38812400

NE11 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.913193 u.a.; Zero-point correction=0.134353u.a ; G= -889.8161023u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.32745000	-0.24526300	-0.14962600
C	-0.83899300	1.50304500	-0.12975400
H	-1.55565700	2.04323300	0.48366000
H	-0.92914700	1.87803500	-1.14740600
C	1.60269600	1.16144300	-0.35123500
H	1.38032200	1.13291200	-1.41478900
H	2.50490500	1.76254900	-0.23398300
C	1.98636200	-0.23303900	0.10123100
O	1.58937900	-0.77756600	1.11808800
O	2.89127500	-0.78399400	-0.71577200
H	3.13555500	-1.64801500	-0.35099400
N	0.50618100	1.77818800	0.36788400
H	0.57299000	1.59086700	1.35878400
O	-2.91849400	-0.16024400	-0.28890700
H	-3.28433500	-0.91600100	-0.76403200
O	-1.15864500	-0.75077000	1.36088800
H	-0.20673200	-0.86216200	1.54408100
O	-0.62224200	-1.06973800	-1.16524300

NE12 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) =-889.9124446 u.a.; Zero-point correction= 0.134644 u.a ; G= -889.8146115u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.32427700	-0.24550400	0.17417300
C	-0.83228700	1.50591000	0.11868600
H	-1.54586700	2.04147900	-0.50263200
H	-0.92433400	1.89561300	1.13092900
C	1.61040500	1.16139900	0.33431200
H	1.39447300	1.13861600	1.39920300
H	2.51454700	1.75750600	0.20732400
C	1.98226400	-0.23698400	-0.11492100
O	1.56958800	-0.78446100	-1.12433100
O	2.89454600	-0.78857800	0.69265500
H	3.12944800	-1.65594900	0.32962800
N	0.51274500	1.77918300	-0.38147600
H	0.57680800	1.59013600	-1.37224200
O	-2.90896600	-0.29017000	0.38608200
H	-3.41675600	0.02030400	-0.37262200
O	-1.17324800	-0.78038300	-1.32749600
H	-0.22291800	-0.85305600	-1.53925200
O	-0.60601400	-1.01744800	1.21670600

NE13 structure in aqueous solution at IEFPCM-MP2/6-311++G (2d,2p).
E (MP2) = -889.9101740u.a.; Zero-point correction= 0.134583u.a ; G= -889.8128880u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

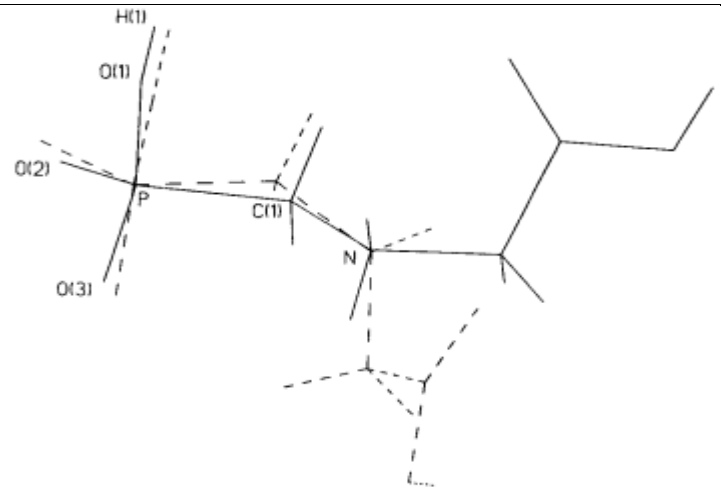
	X	Y	Z
P	1.70866200	-0.17661000	-0.14672700
C	0.37834600	0.88627700	-0.75918800
H	-0.16635700	0.27545000	-1.48040200
H	0.85438800	1.68552000	-1.32549000
C	-1.91780800	1.19491300	0.02422000
H	-2.51587400	1.70818100	0.77520700
H	-2.20105200	1.61295500	-0.93964500
C	-2.34505800	-0.26117700	0.04265100
O	-1.63067600	-1.20591100	0.34224500
O	-3.62871000	-0.40606500	-0.29460900
H	-3.85075700	-1.34845900	-0.24582900
N	-0.51289900	1.42709000	0.27334100
H	-0.27250100	1.09996000	1.19752100
O	2.52910900	-0.74494900	-1.23922500
O	1.00314600	-1.19635000	0.85342800
H	0.03251500	-1.25293400	0.69277600
O	2.61068800	0.71213100	0.83946600
H	2.31867000	0.68792400	1.75684000

8-Table S89 The electronic energies in gas phase (E), the thermal correction to Gibbs free energies ($\delta G_{cor.}$), the Gibbs free energies (G)(u.a) and the solvation free energies ($\Delta G_{solv.}$[b])(kcal.mol^{-1}) values for the most stable ZWP1 and NE2 glyphosate conformers (conf.) in aqueous solution at DFT-D3 and MP2 levels using the 6-311++G(2d,2p) basis set and IEFPCM and SMD continuum solvation models.

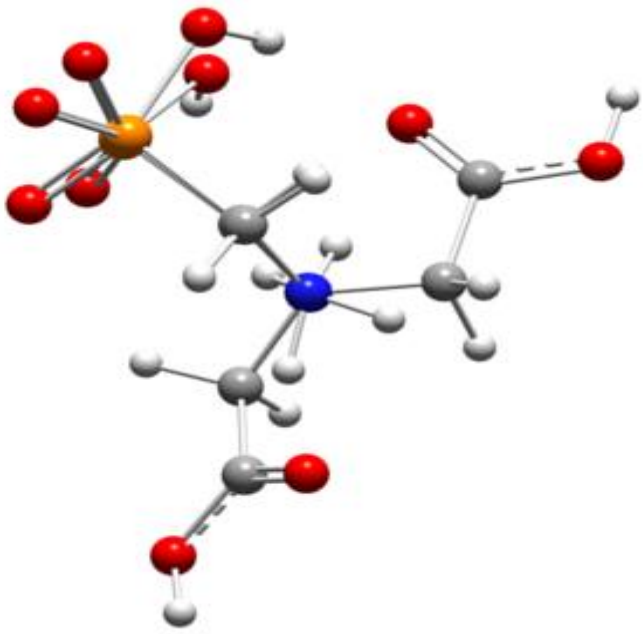
Level	Conf.	E	ΔE[a]	$\delta G_{cor.}$	$\Delta G_{solv.tot}$	$\delta\Delta G_{solv.tot}$[a,b]	G	ΔG[a]
IEFPCM-DFT-D3		-891.675571			-8.3		-891.590663	
	ZWP1			0.098169		-19.0		3.2
	NE2	-891.709380	21.2	0.096534	10.7		-891.595753	
SMD-DFT-D3		-891.667018			-53.6			
	ZWP1		26.6	0.096809		-31.4	-891.655650	-4.8
	NE2	-891.709380		0.096858	-22.2		-891.647979	
IEFPCM-MP2					-7.3		-889.815594	
	ZWP1	-889.902964		0.099080		-18.4		0.5
	NE2	-889.932329	18.4		11.1			
				0.098299			-889.816458	
SMD-MP2	ZWP1	-889.892498	25.0		-52.9	-31.1		
				0.098605			-889.878131	-6.1
	NE2	-889.932329		0.098606	-21.8			
							-889.868441	

[a]Differences in energies between ZWP1and NE2 conformers at different levels of calculation are in kcal.mol^{-1}.
[b]$\delta\Delta G_{solv.}$stands for the difference in solvation energies defined as: $\delta\Delta G_{solv.tot}=\Delta G_{solv.}(ZWP1)-\Delta G_{solv.}(NE2)$ where $\Delta G_{solv.tot}= E_s- E_g$ with E_s is the total electronic enery in aqueous solution (the energy sommation of the electrostatic and nonelectrostatic terms) and E_g is the electronic energy in the gas phase.

9-



a)



b)

Fig.S90 a) The fitting of the two molecules showing the different conformations of the first polymorphic form 1 (chain ----)[22] and the second polymorphic form 2 (chain —)[23], of the molecule of glyphosate. b) Superposition of the calculated ZWP1 and ZWP5 conformers of glyphosate at C1-N bond in agreement with the observations in crystal phase. [23]

10- Structures and energetics for the interconversion transition states (TS) at SMD-B3LYP-D3/6-311++G(2d,2p)

Structure of $TS_{2\text{-}10}$ at SMD-B3LYP-D3/6-311++G (2d, 2p)
E=-891.74322824u.a ; Zero-point correction=0.132612u.a. ; G= -891.647058u.a. at 298, 15 K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-1.52045500	-0.17735600	0.07873700
C	-0.83865700	1.51506200	0.15043900
N	0.50580800	1.76828900	-0.36141000
C	1.60984700	1.15372700	0.35496200
C	2.02118100	-0.22798600	-0.10496200
O	-2.98281900	-0.26697200	0.33321400
O	-0.62157700	-1.02830800	1.10767300
O	-1.14239000	-0.75752500	-1.36024200
O	1.58702100	-0.80329700	-1.08898200
O	2.98207000	-0.74607800	0.66521700
H	-1.54809200	2.12241900	-0.41079800
H	-0.90350300	1.82919700	1.19167300
H	1.39765500	1.11330500	1.42170100
H	2.50923000	1.76457500	0.24501600
H	3.24178400	-1.61470600	0.31610100
H	0.55547200	1.53554100	-1.34666800
H	-0.16823200	-0.78986500	-1.48754900
H	-1.15081900	-1.50552900	1.76166000

Structure of $TS_{10\text{-}12}$ at SMD-B3LYP-D3/6-311++G (2d,2p)
E=-891.73519291u.a ; Zero-point correction=0.132894u.a. ; G= -891.638912u.a. at 298, 15 K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-1.88542300	0.17872900	0.05099600
C	-0.72004000	-0.47084500	-1.21793100
H	-0.68226800	0.28057200	-2.00489100
H	-1.21907200	-1.34469000	-1.63440200
C	1.48536600	0.34137200	-0.59635100
H	1.72586300	0.80198600	-1.55454300
H	1.03281600	1.12661800	0.02130700
C	2.76839700	-0.02799100	0.08999900
O	3.00444300	-1.09717400	0.61410200
O	3.63795600	0.99903100	0.09425100
H	4.43311400	0.73564800	0.58480800
N	0.63140700	-0.82213500	-0.80435000
H	-2.53910000	-1.81676300	0.64470800
O	-2.63763900	1.40881900	-0.31454500
O	-0.96155200	0.29459100	1.35569100
H	-1.43515600	0.63028800	2.13117500
O	-2.95085000	-0.98388200	0.37207100
H	0.60410600	-1.36593100	0.05047500

Structure of $TS_{12\text{-}13}$ at SMD-B3LYP-D3/6-311++G (2d,2p)
E=-891.73972238u.a ; Zero-point correction=0.133228u.a. ; G= −891.642340u.a. at 298, 15 K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	1.59778400	-0.20621600	-0.17025700
C	0.55809400	1.27741300	-0.49796700
H	1.26351400	2.10968700	-0.50481600
H	0.19099000	1.17093900	-1.51640100
C	-1.87799700	1.17916900	-0.03673200
H	-2.03409200	1.49373700	-1.06787100
H	-2.62688900	1.71109300	0.55465200
C	-2.26991800	-0.28048300	0.06103200
O	-1.62565300	-1.16784700	0.59847000
O	-3.46807900	-0.50601500	-0.48297800
H	-3.70477100	-1.44156000	-0.37015400
N	-0.55559600	1.56758300	0.40457500
H	-0.37643300	1.24227900	1.34535900
O	3.00431800	0.29964900	0.41462500
H	2.92474300	0.81853200	1.22768800
O	0.96329700	-0.95553300	1.08306700
H	-0.02027200	-1.06471600	0.98431400
O	1.85668500	-1.04230800	-1.37430300

Structure of $TS_{13\text{-}9}$ at SMD-B3LYP-D3/6-311++G (2d,2p)
E=-891.73790469u.a ; Zero-point correction=0.131759u.a. ; G= -891.642996u.a. at 298, 15 K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-1.74160400	-0.14172200	0.12911900
C	-0.59765500	1.19287900	0.60590200
H	-0.22147800	0.94732200	1.59838100
H	-1.20700300	2.09535800	0.70913300
C	1.86023300	1.15717400	0.05598800
H	2.51428300	1.75947600	-0.57558400
H	2.05293700	1.48571200	1.08219900
C	2.37663300	-0.26816100	-0.02606900
O	1.71445600	-1.26375700	-0.27024600
O	3.68881200	-0.33162400	0.21702400
H	3.97947400	-1.25783900	0.18533800
N	0.49765400	1.35795400	-0.31378900
H	0.29640400	1.71161400	-1.23032300
O	-0.89979000	-1.48791000	0.06286100
O	-2.19543600	0.18264700	-1.38324700
H	-1.48230900	0.09884200	-2.03204500
O	-2.95773700	-0.26942000	0.97608100
H	0.07047200	-1.35118600	-0.11205700

Structure of $TS_{9\text{-}5}$ at SMD-B3LYP-D3/6-311++G (2d,2p)
E=-891.73917852u.a ; Zero-point correction=0.132415u.a. ; G= −891.643180u.a. at 298, 15 K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-1.72990100	-0.16253500	0.13326800
C	-0.46905600	1.01069900	0.70819100
H	0.00366200	0.54006000	1.57065100
H	-0.98981900	1.89678300	1.07376700
C	1.89519200	1.16066400	0.03704000
H	2.52338700	1.74156800	-0.63869100
H	2.12339600	1.50914000	1.05105000
C	2.37268400	-0.26592500	-0.05667300
O	1.70701700	-1.22581700	-0.40606700
O	3.65670800	-0.37931200	0.29664400
H	3.92842100	-1.30919100	0.22706200
N	0.50497400	1.32288000	-0.34345900
H	0.35819300	2.26986100	-0.65956000
O	-0.96381900	-1.44757300	-0.41026400
H	0.00947900	-1.30726300	-0.52787600
O	-2.41837400	0.46766400	-1.17968900
H	-2.13876700	1.36735700	-1.39306400
O	-2.75617800	-0.53534700	1.14568900

Structure of $TS_{1\text{-}4}$ at SMD-B3LYP-D3/6-311++G (2d,2p)
E=-891.74727748u.a ; Zero-point correction=0.135936u.a. ; G= -891.648127u.a. at 298, 15 K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	-2.04296400	0.13017000	-0.17461900
C	-0.27297700	-0.20412000	-0.64676600
H	0.19662800	0.71306600	-0.98607100
H	-0.24413500	-0.94417100	-1.44030600
C	1.95699200	-1.05881800	0.13966000
H	2.38232600	-1.67097100	0.93343800
H	1.97559300	-1.62183700	-0.78840900
C	2.76724200	0.20907900	0.02890300
O	2.39712200	1.28577400	0.44065200
O	3.94503800	-0.02363300	-0.55132600
H	4.46363600	0.79795900	-0.57213800
N	0.54561700	-0.74078400	0.49264500
H	0.10070400	-1.58477700	0.85692300
O	-2.28865100	1.61193200	-0.25683200
O	-2.07309700	-0.34366700	1.39327900
H	-1.85235000	0.38383000	1.99011000
O	-2.91111400	-0.83744000	-0.92716300
H	0.54081100	-0.06074300	1.25756100

Structure of $TS_{4\text{-}3}$at SMD-B3LYP-D3/6-311++G (2d,2p)
E=-891.74716903u.a ; Zero-point correction=0.135139u.a. ; G= −891.650173u.a. at 298, 15 K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	1.97853900	-0.22594700	-0.04460200
C	0.29859600	0.22455000	-0.65378800
H	-0.18443000	-0.68464500	-0.99947000
H	0.33875200	0.94563100	-1.46518400
C	-1.95712400	1.07437700	0.07989900
H	-2.39438700	1.71986200	0.83994200
H	-1.98451300	1.58844700	-0.87612100
C	-2.74514300	-0.21071900	0.03211500
O	-2.34573000	-1.26640000	0.46946100
O	-3.94139400	-0.01712900	-0.52482800
H	-4.44711600	-0.84674700	-0.50175300
N	-0.54082400	0.80018200	0.44953800
H	-0.11833200	1.67234000	0.77430400
O	1.81913900	-0.75488600	1.35721700
O	2.77559400	1.20405200	0.03494900
H	2.24348300	1.97798900	-0.18496500
O	2.64113600	-1.07349700	-1.09354100
H	-0.51371200	0.14868000	1.24010200

11-Structures and energetics of transition states (TS) and non-ionized (NE) conformers involved in the intramolecular concerted ZWP ⇋ NE tautomerzation process of glyphosate at SMD-B3LYP-D3/6-311++G(2d,2p) (Path A).

Structure of TS1 at SMD-B3LYP-D3/6-311++G (2d,2p)
E= -891.73207256 u.a ; Zero-point correction= 0.129937 u.a ; G=-891.639765 u.a. at 298,15 K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	1.93237200	-0.09906600	0.18825700
C	0.26718300	0.70384600	0.26040000
H	0.35478800	1.77797100	0.13576100
H	-0.20148100	0.49485400	1.21753100
C	-1.64073700	-0.71783700	-0.48260700
H	-2.01535700	-1.26067200	-1.35022700
H	-1.33379100	-1.45617800	0.25605700
C	-2.77914000	0.10523500	0.07396400
O	-2.80853800	1.31676700	0.09348100
O	-3.77058400	-0.67449400	0.52919700
H	-4.49560900	-0.11556800	0.85400000
N	-0.48806400	0.09244900	-0.87457000
H	0.58026600	-0.66722200	-1.26415000
O	2.38718800	-0.72493800	1.46395500
O	2.98416200	1.00253400	-0.34345900
H	3.48448800	1.40877100	0.37768100
O	1.67671000	-1.00817200	-1.05756100
H	-0.77777800	0.81583700	-1.52397300

Structure of NE14 at SMD-B3LYP-D3/6-311++G (2d,2p)
E=-891.73913051 u.a ; Zero-point correction= 0.133070u.a ; G= -891.644856u.a. at 298,15 K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.82477400	0.06752900	0.23865800
C	-0.28943100	-0.90042900	0.22438500
H	-0.61412300	-1.93780000	0.30224700
H	0.23471900	-0.66506300	1.15446700
C	1.53343600	0.30397700	-0.87682400
H	1.99741100	0.47247800	-1.84992800
H	1.09007900	1.25219700	-0.57903800
C	2.66030300	-0.01489100	0.08639200
O	2.84745400	-1.09483100	0.60715000
O	3.46447100	1.04566200	0.28604400
H	4.18792900	0.78682800	0.88015100
N	0.51684400	-0.72781800	-0.98637400
H	-1.22146500	1.68564600	-1.09765500
O	-2.50351400	0.02409500	1.55990500
O	-2.71282500	-0.41355700	-1.01047100
H	-2.93678500	-1.35477700	-0.98288800
O	-1.51807300	1.57862000	-0.18227600
H	0.96999000	-1.60957300	-1.18914100

Structure of TS2 at SMD-B3LYP-D3/6-311++G (2d,2p)
E=-891.73034437u.a ; Zero-point correction=0.129760 u.a. ; G= -891.637729 u.a. at 298, 15 K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.71178400	-0.24517100	0.03920500
C	0.39404100	0.71293300	0.90642700
H	0.80417700	1.51254400	1.51592500
H	-0.16900800	0.03337300	1.53843800
C	-1.91266800	1.14121400	0.02639500
H	-2.20176900	1.56844700	0.98731500
H	-2.42385800	1.70812900	-0.75147400
C	-2.40826500	-0.27985000	-0.04556300
O	-1.73519200	-1.24125100	-0.34374100
O	-3.71323800	-0.34805300	0.26185400
H	-4.00623100	-1.27101200	0.19068300
N	-0.46592000	1.23127600	-0.19919700
H	0.16248200	0.46070000	-1.13522100
O	2.05137100	-1.55469400	0.66698100
O	3.00445000	0.71396300	-0.08347600
H	3.63458300	0.57354700	0.63663400
O	1.08992700	-0.21711500	-1.39292000
H	-0.23288800	2.20432400	-0.36914600

Structure of TS3 at SMD-B3LYP-D3/6-311++G (2d,2p)
E= -891.73031391 u.a ; Zero-point correction=0.130156u.a ; G= -891.637005 u.a at 298,15 K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.67819600	-0.25801200	0.04245500
C	-0.40203700	0.75576800	0.91334200
H	0.16414700	0.11265600	1.57943100
H	-0.85272800	1.55691500	1.49145700
C	1.90975000	1.14865300	0.02684700
H	2.42979300	1.70162900	-0.75518300
H	2.22064000	1.56476700	0.98583100
C	2.36113900	-0.28683300	-0.05221000
O	1.65654900	-1.22572700	-0.34938800
O	3.66502500	-0.39658900	0.24767800
H	3.92919100	-1.32802000	0.17274900
N	0.46407300	1.28276000	-0.18381800
H	0.25521600	2.26535000	-0.32637800
O	-1.11136000	-0.11594500	-1.40895800
O	-3.08249100	0.53077300	0.11666600
H	-3.05187900	1.39385800	-0.31939900
O	-1.90267600	-1.62190300	0.59792200
H	-0.18343800	0.55330500	-1.13783800

12- Structures and energetics of transition states (TS-H2O), the zwitterionic and non-ionized conformers involved in the intermolecular concerted ZWP-H2O⇋ NE-H2O tautomerization process of glyphosate at SMD-B3LYP-D3/6-311++G(2d,2p) (Path B).

Structure of ZWP1.H2O at SMD-B3LYP-D3/6-311++G (2d,2p)
E=-968.239885620u.a. ; Zero-point correction=0.160163 u.a. ; G= -968.121293u.a at 298,15K.
Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.88734200	-0.58652000	-0.14689400
C	0.18028900	-0.25069300	-0.73909000
H	-0.35803400	-1.19060100	-0.81669400
H	0.22655300	0.21715000	-1.71905400
C	-1.99205700	0.89508200	-0.25181300
H	-2.37634500	1.76384400	0.28080200
H	-2.01613900	1.10542400	-1.31744000
C	-2.86147400	-0.29038500	0.08224400
O	-2.50831400	-1.22101000	0.77182300
O	-4.07468000	-0.16029900	-0.45916600
H	-4.62959300	-0.91366800	-0.19607600
N	-0.58714000	0.66139100	0.16978900
H	1.11104700	3.31717500	0.99270100
O	2.43572200	-1.68974100	-1.00425700
O	1.62679300	-1.09996000	1.38084000
H	1.32760600	-2.01871700	1.40465800
O	2.64087200	0.71430300	-0.00468000
H	-0.58398100	0.26619900	1.11331600
O	1.06330800	2.91801600	0.11640800
H	1.76364700	2.22450600	0.10649100
H	-0.09505800	1.58225100	0.21040400

Structure of NE14.H2O at SMD-B3LYP-D3/6-311++G (2d,2p)
E= -968.22811569u.a. ; Zero-point correction= 0.158365 u.a. ; G= -968.110207u.a at 298, 15 K.
Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.83535000	-0.62499800	-0.15268200
C	0.07534100	-0.39435700	-0.53485500
H	-0.38091400	-1.38740800	-0.50092800
H	0.02986700	-0.04527700	-1.56667100
C	-1.94986500	0.88506000	-0.08438500
H	-2.34722200	1.70643000	0.51494900
H	-1.95086500	1.22175400	-1.11983900
C	-2.92461800	-0.26490900	0.06407100
O	-2.71872900	-1.26681800	0.71634900
O	-4.07559800	-0.03143700	-0.58935800
H	-4.68771500	-0.76842700	-0.43010500
N	-0.58824500	0.58532100	0.33988000
H	1.29815600	3.19496800	0.88725300
O	2.41820000	-1.78816000	-0.87275900
O	1.93180700	-0.71573400	1.45201400
H	1.53518500	-1.52265500	1.81067300
O	2.61519000	0.71521500	-0.45019900
H	-0.60625000	0.21737800	1.28553400
O	1.08185800	2.78851600	0.03964000
H	2.11020600	1.56036200	-0.24040700
H	0.36003500	2.13318800	0.23611800

Structure of TS1.H2O at SMD-B3LYP-D3/6-311++G(2d,2p)
E (SCF) = -968.22237413 u.a.; Zero-point correction = 0.153755 u.a.; G= -968.108066u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.87697800	-0.55283900	-0.16485100
C	0.11963400	-0.33395100	-0.61384400
H	-0.34503700	-1.32096700	-0.59852800
H	0.09819400	0.03427500	-1.63906400
C	-1.96736100	0.88212500	-0.17705200
H	-2.37012300	1.73762200	0.36774400
H	-1.98331100	1.14041900	-1.23419600
C	-2.90474300	-0.27754000	0.07283600
O	-2.64144000	-1.24359400	0.75688800
O	-4.08987800	-0.09458000	-0.53075100
H	-4.67804700	-0.83591700	-0.31153200
N	-0.59149000	0.63339100	0.25314800
H	1.16303800	3.05194800	0.95575000
O	2.46976100	-1.66317700	-0.97296200
O	1.84158600	-0.89568400	1.42247100
H	1.53949900	-1.79782400	1.59556900
O	2.59379800	0.80979400	-0.21927800
H	-0.60308700	0.26921600	1.20226000
O	1.02547500	2.61537400	0.10366400
H	1.85670600	1.82144000	-0.03732500
H	0.22832200	1.90975800	0.22814700

Structure of ZWP3.H2O at SMD-B3LYP-D3/6-311++G (2d,2p)
E=-968.238756085u.a ; Zero-point correction= 0.160175 u.a ; G= -968.120557u.a at 298.15 K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	2.01725400	-0.28719900	-0.25556000
C	0.27358600	-0.86241800	-0.16615000
H	0.26114900	-1.91193600	0.11527100
H	-0.18791000	-0.74719800	-1.14205100
C	-1.94437400	-0.59561700	0.98155000
H	-1.93808200	-1.67403900	1.11492500
H	-2.37829400	-0.13889700	1.86953200
C	-2.78317200	-0.20892400	-0.21031700
O	-2.42279800	0.54166800	-1.08815200
O	-3.98611000	-0.78764900	-0.15066200
H	-4.52053700	-0.49839100	-0.90941300
N	-0.54714000	-0.10787200	0.83725200
H	0.08557500	3.07503000	1.01626900
O	2.76517800	-1.28788000	-1.08737200
O	2.48513600	-0.36101100	1.30815300
H	2.71333500	-1.26238400	1.57184700
O	2.04876100	1.17887200	-0.61216000
H	-0.09433200	-0.18867700	1.74960300
O	-0.11944600	2.62226100	0.19017100
H	0.73789100	2.25311500	-0.12122400
H	-0.54964800	0.90813300	0.59755900

Structure of NE5.H2O at SMD-B3LYP-D3/6-311++G (2d,2p)
E= -968.22710218 u.a ; Zero-point correction=0.157599 u.a. ; G= -968.110307 u.a. at 298.15 K.

Charge = 0; Multiplicity = 1
Coordinates (Angstroms)

	X	Y	Z
P	1.96297600	-0.33393100	-0.23660400
C	0.26193700	-0.95625000	-0.12088200
H	0.33156900	-2.02999300	0.08320300
H	-0.17782700	-0.83656600	-1.11040400
C	-1.92685000	-0.71369000	0.91474500
H	-2.00997900	-1.80501700	0.87614800
H	-2.39142800	-0.39084800	1.84699800
C	-2.75545200	-0.14445900	-0.21116900
O	-2.38480800	0.68658000	-1.01119900
O	-3.99132000	-0.67743100	-0.22165500
H	-4.49974200	-0.28137300	-0.94802900
N	-0.54651800	-0.23979800	0.87690300
H	0.22519500	2.85733000	1.13381600
O	2.83118600	-1.20841000	-1.06814500
O	2.45756700	-0.14525900	1.28415900
H	2.52993700	-0.98337800	1.76313600
O	1.93929000	1.15542100	-0.75816100
H	-0.13637900	-0.39402800	1.79075400
O	-0.07176300	2.45635400	0.30814000
H	1.22063400	1.73402200	-0.35246700
H	-0.43002100	1.56575500	0.56629700

Structure of TS2.H2O in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-968.22127480 u.a.; Zero-point correction = 0.154118 u.a.; G=-968.106610u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.97788600	-0.27422000	-0.26104300
C	0.25527100	-0.87391000	-0.14586500
H	0.29630700	-1.94756100	0.05291100
H	-0.19458500	-0.73078400	-1.12681600
C	-1.93582300	-0.66029900	0.93212800
H	-1.98797500	-1.75198700	0.92742500
H	-2.39727300	-0.31710200	1.85836600
C	-2.77677900	-0.13628800	-0.20538100
O	-2.42677300	0.69539700	-1.01354000
O	-3.99367600	-0.70710700	-0.20974700
H	-4.51447200	-0.33726800	-0.94148900
N	-0.55771400	-0.16635400	0.86998400
H	0.15848700	2.78856000	1.10064300
O	2.75247100	-1.14763700	-1.19697800
O	2.53184900	-0.36859500	1.26455100
H	2.74388800	-1.27693900	1.51946600
O	1.97502800	1.23565300	-0.55275100
H	-0.13263600	-0.32171400	1.77885900
O	-0.03016500	2.28812600	0.29417000
H	0.95670300	1.88956100	-0.11016300
H	-0.41862800	1.33929100	0.59561700

Structure of ZWP4.H_2O in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -968.23945592 u.a.; Zero-point correction = 0.160381u.a. G= -968.120145 u.a at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-2.03785600	-0.22123800	-0.26602000
C	-0.31062600	-0.85502400	-0.24490500
H	0.16576000	-0.60265000	-1.18723100
H	-0.33244300	-1.93484200	-0.12770800
C	1.91914900	-0.80141400	0.89935000
H	2.36569100	-0.53292400	1.85536800
H	1.90862700	-1.88439900	0.81269600
C	2.75029400	-0.18890900	-0.20131600
O	2.39546900	0.72822100	-0.90682200
O	3.94453900	-0.78267800	-0.27344700
H	4.47655700	-0.35398900	-0.96474300
N	0.52231100	-0.29078100	0.86794300
H	0.07887500	-0.52755400	1.75725900
O	-2.02670500	1.28432000	-0.39974200
O	-2.56296900	-0.61273800	1.23099400
H	-2.48021300	0.13186100	1.84122000
O	-2.79057700	-1.06548200	-1.24996200
H	0.53289100	0.74963700	0.80220500
O	0.25942800	2.52859400	0.43152100
H	0.88576400	2.50637000	-0.30224600
H	-0.59621800	2.23271800	0.04876300

Structure of NE9.H2O in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -968.22751609 u.a.; Zero-point correction = 0.157942u.a. G= -968.109807 u.a at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.98435500	-0.26864300	-0.24863500
C	-0.29613200	-0.93866500	-0.21840200
H	0.15392100	-0.67882100	-1.17532400
H	-0.39473100	-2.02794000	-0.17873700
C	1.90633700	-0.87304800	0.82368000
H	2.38202200	-0.69929400	1.78944100
H	1.98693800	-1.94539300	0.61728100
C	2.72709900	-0.14089300	-0.21036100
O	2.34820100	0.78640700	-0.89248300
O	3.97058600	-0.64990800	-0.28560400
H	4.47671700	-0.15011200	-0.94643600
N	0.52448500	-0.40077200	0.87987100
H	0.12725700	-0.71738800	1.75742500
O	-1.91484900	1.28037600	-0.55908500
O	-2.54288400	-0.42099900	1.25290600
H	-2.25582400	0.27944700	1.85535500
O	-2.86716800	-1.00181000	-1.19153000
H	0.47982200	1.40777400	0.74328500
O	0.18899800	2.34081000	0.55571400
H	0.78052000	2.63243200	-0.14869300
H	-1.12959200	1.77096300	-0.15202400

Structure of TS3.H2O in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -968.22083213 u.a.; Zero-point correction = 0.154171 u.a.; G= -968.106244u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.98336100	-0.29695700	-0.25215400
C	-0.24653500	-0.85579100	-0.15262800
H	0.19389400	-0.69700600	-1.13541200
H	-0.26585400	-1.93084400	0.04052100
C	1.93413800	-0.63429400	0.94425800
H	2.39004500	-0.27285700	1.86637200
H	1.98165800	-1.72605700	0.96427100
C	2.78722000	-0.13878200	-0.19653800
O	2.45168200	0.68361900	-1.02029200
O	3.99815100	-0.72208100	-0.18277100
H	4.52878200	-0.36845300	-0.91547800
N	0.55884500	-0.13619000	0.86108200
H	0.12689000	-0.27817700	1.76929700
O	-2.01504300	1.21920000	-0.52660300
O	-2.55839900	-0.54026200	1.24867500
H	-2.43759300	0.22920100	1.82043100
O	-2.74091500	-1.17764100	-1.19217400
H	-0.15478900	2.83288800	1.01106900
O	0.01382500	2.30381700	0.21848000
H	0.41614500	1.37357400	0.54410300
H	-0.98401700	1.88540700	-0.14351200

Structure of ZWP8 in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.750850763 u.a.; Zero-point correction = 0.136605u.a; G= -891.650008u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.58580300	-0.22857800	0.00009200
C	0.92579700	1.48568000	-0.04019900
H	1.50619400	2.04843600	-0.76661100
H	1.00156900	1.96944700	0.92863000
C	-1.54434300	0.99261800	0.45671000
H	-1.06592000	0.79530300	1.41357200
H	-2.29806600	1.75665500	0.60450100
C	-2.26844200	-0.27512300	0.01957500
O	-1.67591200	-1.16759300	-0.74623300
O	-3.40330300	-0.44886700	0.42565100
N	-0.50968000	1.55381100	-0.48915400
H	-0.58339400	1.11341500	-1.40946200
O	0.83505600	-0.98215800	-1.08823800
H	-0.66810600	-1.05446400	-0.89045200
O	1.12614500	-0.81826500	1.44174400
H	0.27532900	-1.27573700	1.39768500
O	3.07713200	-0.15293200	-0.01260300
H	-0.73791000	2.53841300	-0.63423400

13- Structures and energetics of transition states TS and non-ionized conformers involved in the nonconcerted ZWP ⇋ NE tautomerzation process of glyphosate, at SMD-B3LYP-D3/6-311++G(2d,2p) (Path C).

Structureof NE15 in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.740696176u.a.; Zero-point correction = 0.133726u.a. G= -891.643955 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.55958800	-0.15762300	-0.10224900
C	-0.77633800	1.47483400	-0.04812600
H	-1.41660300	2.06029000	0.61094600
H	-0.87737500	1.89379300	-1.05456900
C	1.63011900	1.07204800	-0.47319500
H	1.27880200	0.98844700	-1.50110300
H	2.46346900	1.77516800	-0.47144800
C	2.21391600	-0.26618200	-0.06283100
O	1.91089100	-0.65201400	1.18157800
O	2.93800500	-0.93493800	-0.77278100
N	0.59681300	1.52401900	0.46338400
H	1.30414400	0.04250200	1.53066000
O	-1.48524100	-0.83967300	1.34542800
H	-0.61271700	-1.19317800	1.56830400
O	-0.55892000	-0.99597800	-1.02746600
H	-0.75854500	-1.94334000	-1.06684400
O	-2.97455800	-0.08863000	-0.54633700
H	0.78737200	2.47819100	0.73562900

Structure of TS-1a in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.732384646 u.a.; Zero-point correction = 0.130175 u.a.; G=-891.638729u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.58862100	-0.15624600	-0.09231300
C	-0.75173400	1.45322500	0.00215900
H	-1.31260300	2.01703800	0.74522100
H	-0.88198200	1.94640400	-0.96118400
C	1.65479300	0.98549800	-0.61037000
H	1.19541800	0.77549800	-1.57078700
H	2.43384200	1.73111400	-0.74593600
C	2.26784600	-0.28651700	-0.01297200
O	1.81412700	-0.49893600	1.18890600
O	3.08471400	-0.97769600	-0.61401500
N	0.67042700	1.43627200	0.40713800
H	1.07166500	0.46837100	1.19220200
O	-1.41445900	-0.90783500	1.30800900
H	-0.52168300	-1.24824600	1.47009300
O	-0.69057400	-0.95435200	-1.14325800
H	-0.91745100	-1.89273000	-1.22849500
O	-3.02770100	-0.00849100	-0.41354900
H	0.91483200	2.35758000	0.75196900

Structure of TS-2a in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.747600338 u.a.; Zero-point correction =0.132095u.a.; G= -891.651426u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.55639800	-0.21738500	-0.02877100
C	-0.89759600	1.49159800	0.00984700
H	-1.49282700	2.05313300	0.72530600
H	-0.98268200	1.95716800	-0.96741500
C	1.59263100	1.00926800	-0.44606000
H	1.16347500	0.87411500	-1.43561300
H	2.39045000	1.74013600	-0.51508200
C	2.21012500	-0.31323600	0.01137500
O	1.58400800	-1.06835200	0.84711400
O	3.30834200	-0.58869400	-0.47516000
N	0.53360900	1.59605300	0.45827000
H	0.61958700	1.19993600	1.39797500
O	-0.80878800	-0.98072000	1.09035600
H	0.35682100	-0.99842000	0.97479100
O	-1.08888000	-0.83144300	-1.44214000
H	-0.25234800	-1.31543700	-1.39894700
O	-3.03999800	-0.17318600	0.03415500
H	0.73982000	2.59115100	0.55709100

Structure of ZWP9 in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.750133623u.a. Zero-point correction =0.135576u.a.; G= -891.651209 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.66018100	-0.25804400	0.09415200
C	-0.47022000	0.96340200	0.76182100
H	0.07144300	0.50707700	1.58503500
H	-0.98155200	1.84862700	1.12532000
C	1.96585000	1.13282300	0.02694100
H	2.56145100	1.67070000	-0.70705300
H	2.16699400	1.54950300	1.00949500
C	2.45292100	-0.30773600	0.00967400
O	1.68470300	-1.31472700	-0.34466900
O	3.61988600	-0.48882100	0.31100200
N	0.52747700	1.38937700	-0.29393900
H	0.43121400	2.39489200	-0.44444600
O	-0.82606100	-1.19943300	-0.75756100
H	0.68841000	-1.16411900	-0.51158200
O	-2.53295200	0.58717400	-0.98174400
H	-3.22587400	1.11028300	-0.55637100
O	-2.50830100	-0.76613800	1.21643500
H	0.30879300	0.95268300	-1.19341600

Structure of ZWC22 in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.748243862u.a. Zero-point correction =0.134980u.a.; G= -891.649777u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.66627600	-0.20412500	0.12709900
C	-0.38516000	0.93843500	0.74129900
H	0.15626300	0.43679200	1.53752500
H	-0.87159000	1.81663900	1.15469700
C	2.03831600	1.12038100	0.02388100
H	2.64084200	1.64729900	-0.71199900
H	2.23223100	1.54183300	1.00546200
C	2.42770200	-0.35919400	-0.00431300
O	1.58682900	-1.22627800	-0.39514200
O	3.59938400	-0.59345600	0.34453100
N	0.59908100	1.38514700	-0.31168500
H	0.48641300	2.38954500	-0.45560800
O	-0.90746400	-1.24911800	-0.76285500
H	0.11167700	-1.24951300	-0.61661600
O	-2.49511100	0.59058400	-0.98768800
H	-3.20279200	1.13384800	-0.61165000
O	-2.48868400	-0.70889600	1.25404700
H	0.40273800	0.94899700	-1.21484700

Structure of NE16 in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.740115570 u.a.; Zero-point correction =0.132340 u.a.; G= -891.645815u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.55039100	-0.15491000	-0.13256300
C	0.77063600	1.47749700	-0.05674500
H	0.83107800	1.90106800	-1.06463400
H	1.42947400	2.06665000	0.58061200
C	-1.65238400	1.09487900	-0.40309300
H	-2.48495000	1.79530300	-0.33301500
H	-1.34489800	1.06386500	-1.44846600
C	-2.22285500	-0.26446800	-0.04642900
O	-1.84306800	-0.75247400	1.13813200
O	-3.00448700	-0.86918200	-0.75418400
N	-0.58117500	1.50520500	0.50627700
H	-0.76196100	2.44248400	0.83621000
O	0.50932600	-1.00322400	-0.99478300
H	0.62807000	-1.96259000	-0.93184700
O	1.41159300	-0.85131900	1.30652900
H	2.17477700	-0.68057900	1.87643700
O	2.94706400	-0.09593600	-0.63789100
H	-1.19503100	-0.10935700	1.50439000

Structure of TS-1b in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.731600753u.a.; Zero-point correction =0.130031 u.a.; G= -891.639066u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.64188600	-0.14524400	-0.13882000
C	0.72671100	1.42015800	0.01274600
H	0.75820600	1.92260200	-0.95270400
H	1.29961000	2.02165600	0.71693000
C	-1.72261300	1.04311600	-0.49285800
H	-2.44849600	1.85083300	-0.51702600
H	-1.30789400	0.90781400	-1.48804000
C	-2.39121300	-0.25691500	-0.03068400
O	-1.80888300	-0.72217600	1.03631400
O	-3.33941300	-0.76525400	-0.62143700
N	-0.65953000	1.29729600	0.51510300
H	-0.88628900	2.11924300	1.06275900
O	0.76452500	-1.19950600	-0.94751900
H	0.03397500	-1.59255300	-0.44577400
O	1.64834400	-0.80248700	1.31990300
H	2.08362200	-0.25520200	1.98998900
O	2.95850700	0.07556800	-0.78106500
H	-1.00626800	0.19589500	1.12567300

Structureof TS-2b in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.746993869 u.a.; Zero-point correction =0.131176 u.a.; G= -891.652031u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.63505400	-0.23341100	-0.11292900
C	0.44971300	1.00199700	-0.74780100
H	-0.08552400	0.57011900	-1.58823500
H	0.98762500	1.87977600	-1.09196300
C	-1.98799600	1.12043000	-0.02611600
H	-2.59806500	1.63942700	0.70931100
H	-2.20162800	1.53106700	-1.00831200
C	-2.39441400	-0.35087400	0.00013000
O	-1.57828500	-1.27493700	0.36388900
O	-3.56772900	-0.56640500	-0.31793100
N	-0.55640700	1.43375100	0.29400700
H	-0.48733700	2.44602800	0.40809500
O	0.79115700	-1.21298500	0.73000000
H	-0.36441900	-1.18548600	0.54346600
O	2.49019300	0.53573400	1.01360400
H	3.20949400	1.06222100	0.63711500
O	2.46973600	-0.74953300	-1.23221700
H	-0.33549900	1.03744000	1.21037100

Structureof ZWP10 in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.748701076 u.a.; Zero-point correction =0.135821 u.a.; G= -891.649670u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.52509500	-0.24161000	0.13245500
C	0.85876400	1.45679600	-0.16815400
H	1.40576300	1.91961400	-0.98436500
H	0.93825500	2.07591000	0.71972200
C	-1.56108600	0.93174200	0.46689900
H	-1.00349400	0.66644000	1.36297700
H	-2.22822900	1.75092500	0.70303500
C	-2.40032200	-0.27287100	0.06143700
O	-1.81407300	-1.28246100	-0.55243400
O	-3.58213300	-0.30492800	0.34890100
N	-0.58616300	1.41682000	-0.58211400
H	-0.65869400	0.85650400	-1.43490400
O	3.01031800	-0.16664400	-0.50687600
H	3.67623100	0.05268200	0.15855400
O	0.72228700	-1.15013600	-0.78323800
H	-0.79659300	-1.21545900	-0.62200000
O	1.58488500	-0.52821600	1.60207000
H	-0.86091900	2.36487900	-0.84351000

Structureof ZWC32 in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.747840286 u.a.; Zero-point correction =0.135098u.a.; G= -891.649434u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.35181300	-0.25439500	0.14739700
C	0.78602500	1.48448100	0.04008700
H	1.40275700	1.99645200	-0.69387200
H	0.91917200	1.95106900	1.01252500
C	-1.69368200	1.01253500	0.48430200
H	-1.32914900	0.95613000	1.50436700
H	-2.57122700	1.65287600	0.45783000
C	-2.09782500	-0.37405000	-0.03168900
O	-1.61099500	-0.76131300	-1.13871700
O	-2.91598000	-0.98919400	0.67594600
N	-0.64315100	1.66365000	-0.37424000
H	-0.76457800	1.30847100	-1.32861200
O	2.93446200	-0.14238400	0.03447800
H	3.37690300	-0.14684600	0.89551200
O	1.01457600	-0.90915800	-1.25239000
H	0.01992000	-0.95734100	-1.35342400
O	0.83121100	-0.94753200	1.35089100
H	-0.82224400	2.66841300	-0.40346400

Structureof NE17in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.739526509u.a. Zero-point correction =0.132445u.a.; G= -891.645231u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.39663300	-0.23920100	-0.13193700
C	-0.73940000	1.44684800	-0.07489100
H	-1.39956600	2.01344300	0.58077800
H	-0.84759800	1.85243400	-1.08594800
C	1.66940000	1.06265200	-0.48084700
H	1.32993400	0.97881800	-1.51343900
H	2.50861900	1.75870400	-0.47258900
C	2.24121500	-0.27919000	-0.06433400
O	1.91708900	-0.67660600	1.17080700
O	2.97667200	-0.94357100	-0.76699700
N	0.63047000	1.52853600	0.44075800
H	1.30387400	0.00707400	1.52497100
O	-2.89648600	-0.10498300	-0.67620000
H	-3.49210300	0.37011600	-0.07910900
O	-1.49022100	-0.62049900	1.41917400
H	-1.61226000	-1.56808600	1.57884000
O	-0.64363300	-1.20392900	-0.97305000
H	0.81063100	2.49060800	0.69080400

Structureof TS-1c in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.731193442u.a.; Zero-point correction = 0.129937 u.a.; G=-891.638003u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.46683200	-0.23907900	-0.16000500
C	-0.73128200	1.41495300	0.04001500
H	-1.28618200	1.90683800	0.83678600
H	-0.89869600	1.96403200	-0.88662000
C	1.66137600	0.95957600	-0.63000100
H	1.17019200	0.69930700	-1.56273000
H	2.40829500	1.72430500	-0.82458700
C	2.33463300	-0.27638900	-0.02027600
O	1.89144800	-0.50017300	1.18328900
O	3.18038500	-0.93549300	-0.61742900
N	0.69895600	1.40737700	0.40873900
H	1.12187400	0.44293800	1.18965900
O	-3.02740500	0.03060700	-0.30260400
H	-3.42947800	0.49982000	0.44349700
O	-1.36094900	-0.95756700	1.26580300
H	-0.48907200	-1.34782400	1.42993500
O	-0.93637600	-1.02147500	-1.30095300
H	0.94765800	2.32909500	0.74968300

Structure of TS-2c in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.745313971u.a.; Zero-point correction =0.131388u.a.; G= -891.650380 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.44901700	-0.24677300	-0.15006100
C	-0.83747300	1.47857700	0.03400200
H	-1.44629800	1.98319800	0.77914000
H	-0.90412600	2.01226800	-0.90881100
C	1.65508900	1.01200600	-0.40408000
H	1.24347900	0.93795700	-1.40744000
H	2.45962800	1.73896400	-0.41631300
C	2.25596800	-0.33900800	-0.01389100
O	1.62830600	-1.12368900	0.79466800
O	3.34813100	-0.60371600	-0.51795200
N	0.58494000	1.55269900	0.51496000
H	0.65158000	1.09954000	1.43016700
O	-2.98173600	-0.16172100	0.31515400
H	-3.58969500	-0.07304600	-0.43201300
O	-0.76692000	-1.02779300	0.99551500
H	0.41272500	-1.05550100	0.90089800
O	-1.28017400	-0.74054300	-1.54645800
H	0.79101800	2.53956500	0.67696700

Structureof ZWP11 in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) =-891.748328887u.a.; Zero-point correction = 0.135238u.a.; G= -891.650234u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-1.68721600	-0.12057500	-0.07670900
C	-0.45556200	0.98880000	0.72138800
H	0.04947900	0.44172700	1.51118500
H	-0.92102600	1.87219600	1.14424500
C	2.00036300	1.12034900	0.06855600
H	2.63604800	1.66214900	-0.62815700
H	2.18221400	1.49595300	1.07117600
C	2.43613800	-0.33636400	0.01800500
O	1.64144700	-1.30182400	-0.39179000
O	3.58457300	-0.57230000	0.34994900
N	0.58164500	1.43127800	-0.28801300
H	0.51497300	2.44350500	-0.40420800
O	-2.22932000	-0.99454200	1.17315800
H	-3.03681500	-0.62108600	1.55091100
O	-0.84039900	-1.04868800	-0.93243300
H	0.66187800	-1.10389100	-0.60141100
O	-2.79629500	0.65893000	-0.71337300
H	0.38428300	1.02980600	-1.20879200

Structureof NE18 in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.739701679u.a. Zero-point correction = 0.132487 u.a.; G= -891.645153u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.45049000	-0.20107500	0.04520500
C	0.72668500	1.44942900	-0.12901800
H	0.79929500	1.73259000	-1.18340700
H	1.38711000	2.10679800	0.43539300
C	-1.69276700	1.06887100	-0.46824000
H	-2.54551300	1.74675600	-0.42200300
H	-1.39276400	0.99727400	-1.51429300
C	-2.22217900	-0.28651500	-0.04082900
O	-1.85585900	-0.68352400	1.18215200
O	-2.96093600	-0.96478400	-0.72659600
N	-0.63090000	1.55681100	0.41363900
H	-0.80405200	2.52500500	0.64250700
O	2.88005300	-0.10823400	-0.67765800
H	3.59630300	0.11040400	-0.06439700
O	0.59623700	-1.06149000	-0.99407900
H	0.67953700	-2.01788900	-0.86504500
O	1.50506000	-0.74212000	1.42859200
H	-1.24783600	0.00801300	1.52693400

Structureof TS-1d in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.730671010 u.a.; Zero-point correction =0.129711 u.a.; G= -891.638082 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.52642000	-0.22134200	0.05670300
C	0.72185700	1.40840400	-0.04303000
H	0.82921400	1.79121400	-1.05663500
H	1.28175700	2.05813400	0.62750300
C	-1.68501400	0.95887700	-0.63710100
H	-2.42255400	1.73389500	-0.82555400
H	-1.20994500	0.68547100	-1.57505200
C	-2.36185500	-0.26778400	-0.01455400
O	-1.87561700	-0.51531300	1.16543300
O	-3.24141600	-0.90402700	-0.58938700
N	-0.69456300	1.39636100	0.38132100
H	-0.93877900	2.31203600	0.74002600
O	2.94146500	-0.00310200	-0.64490000
H	3.54254800	0.55782200	-0.13338400
O	0.86460100	-1.15313100	-1.05781900
H	0.16316700	-1.71825300	-0.70262700
O	1.53104400	-0.78609800	1.42879200
H	-1.09032000	0.42167600	1.15708900

Structureof TS-2d in aqueous solution at SMD-B3LYP-D3/6-311++G (2d,2p).
E (SCF) = -891.745361825u.a. Zero-point correction = 0.130998 u.a.; G= -891.651055 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	1.66094400	-0.10986300	0.05917900
C	0.43918800	1.02574600	-0.69950700
H	-0.05761000	0.51012300	-1.51511300
H	0.94009100	1.90537800	-1.08985100
C	-2.02048700	1.10742700	-0.07068600
H	-2.67351800	1.63278200	0.62212000
H	-2.20643200	1.47573900	-1.07499400
C	-2.38194800	-0.37480500	-0.00678800
O	-1.54824900	-1.26003800	0.41282900
O	-3.53587500	-0.64047500	-0.35443800
N	-0.61139900	1.47109400	0.29219600
H	-0.56993500	2.48785100	0.37324700
O	2.23150000	-0.91815000	-1.20739500
H	3.04620100	-0.53175600	-1.55688400
O	0.80557100	-1.12190800	0.84981900
H	-0.35076300	-1.12877100	0.62497800
O	2.72662900	0.60801200	0.81370200
H	-0.41952200	1.10920200	1.22919400

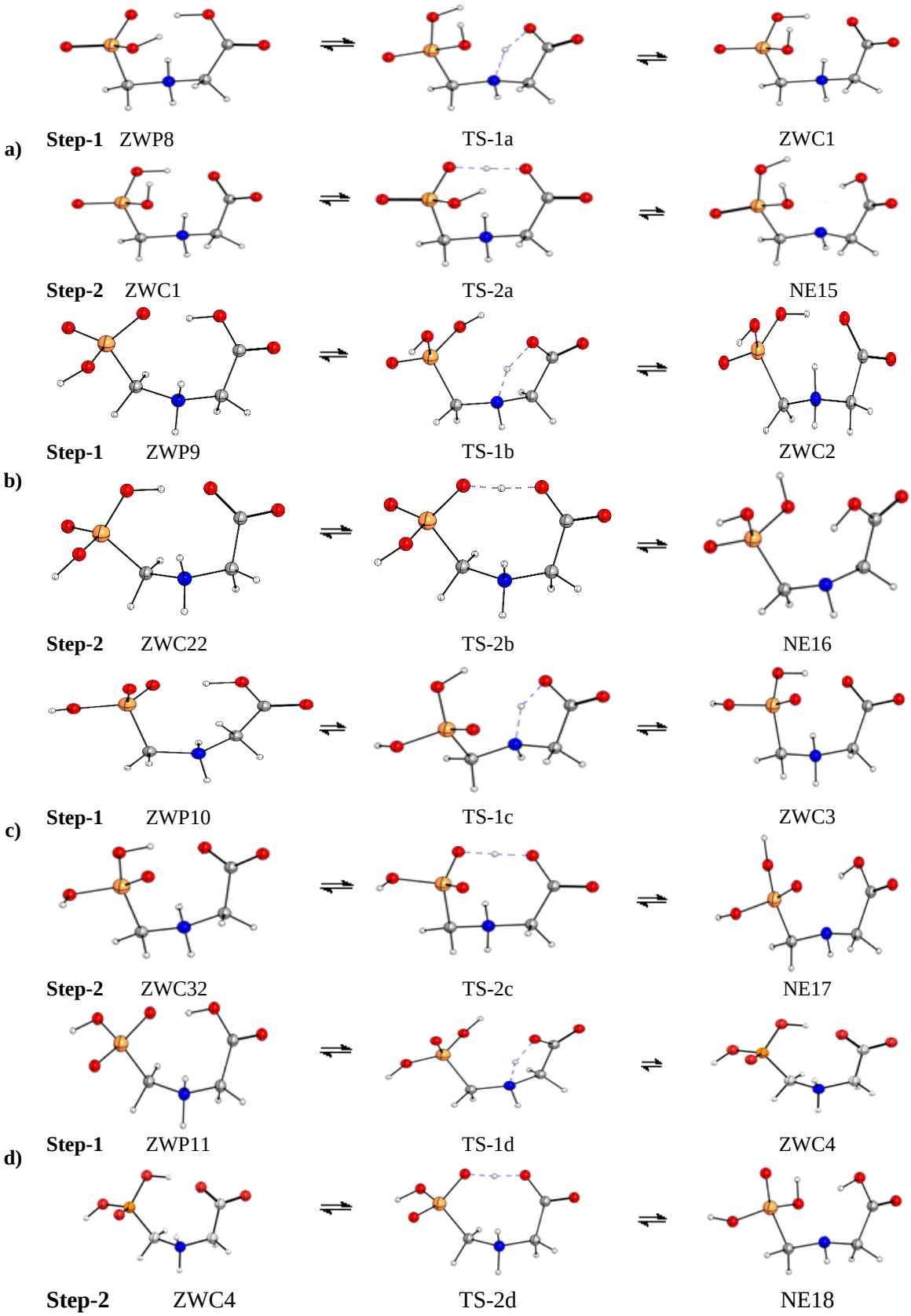


Fig.S110 Structures of non-ionized (NE), carboxylate (ZWC) and phosphonate (ZWP) zwitterionic tautomers involved in the nonconcerted tautomerization process of glyphosate, together with the corresponding transition states (TS), optimized in aqueous solution using SMD solvation model at DFT-D3/6-311++G(2d,2p) level.