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Computational Study of Glyphosate Dimerization Process: Mechanism and Effect of Solvent

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1-

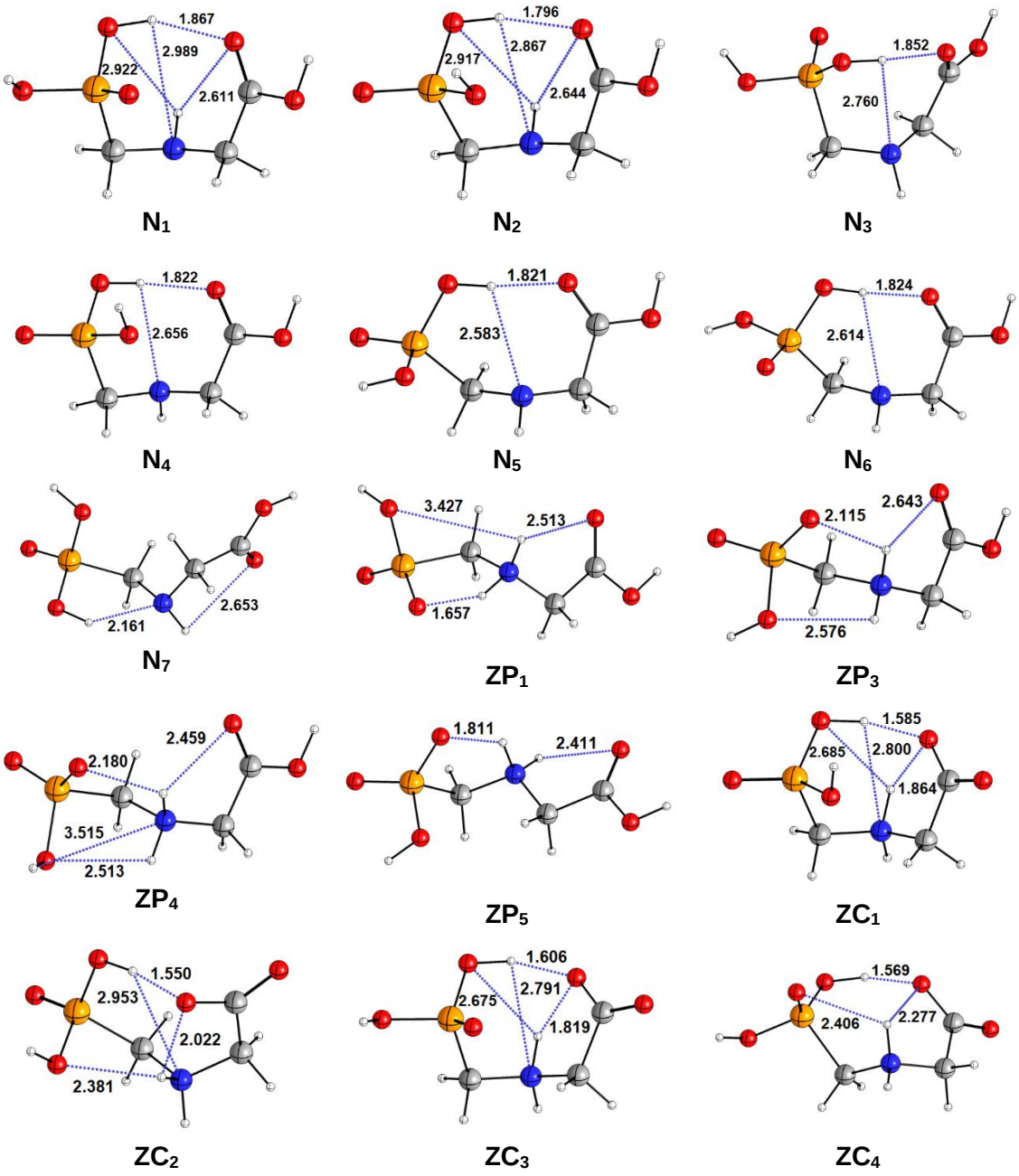

Fig. S1 Optimized structures and hydrogen-bond distances (in Å) of the non-ionized (N) and ionized (ZP and ZC) neutral conformers of Glyph monomer obtained in cyclohexane at the SMD-B3LYP-D3/6-311++G(2d,2p) level.

2-

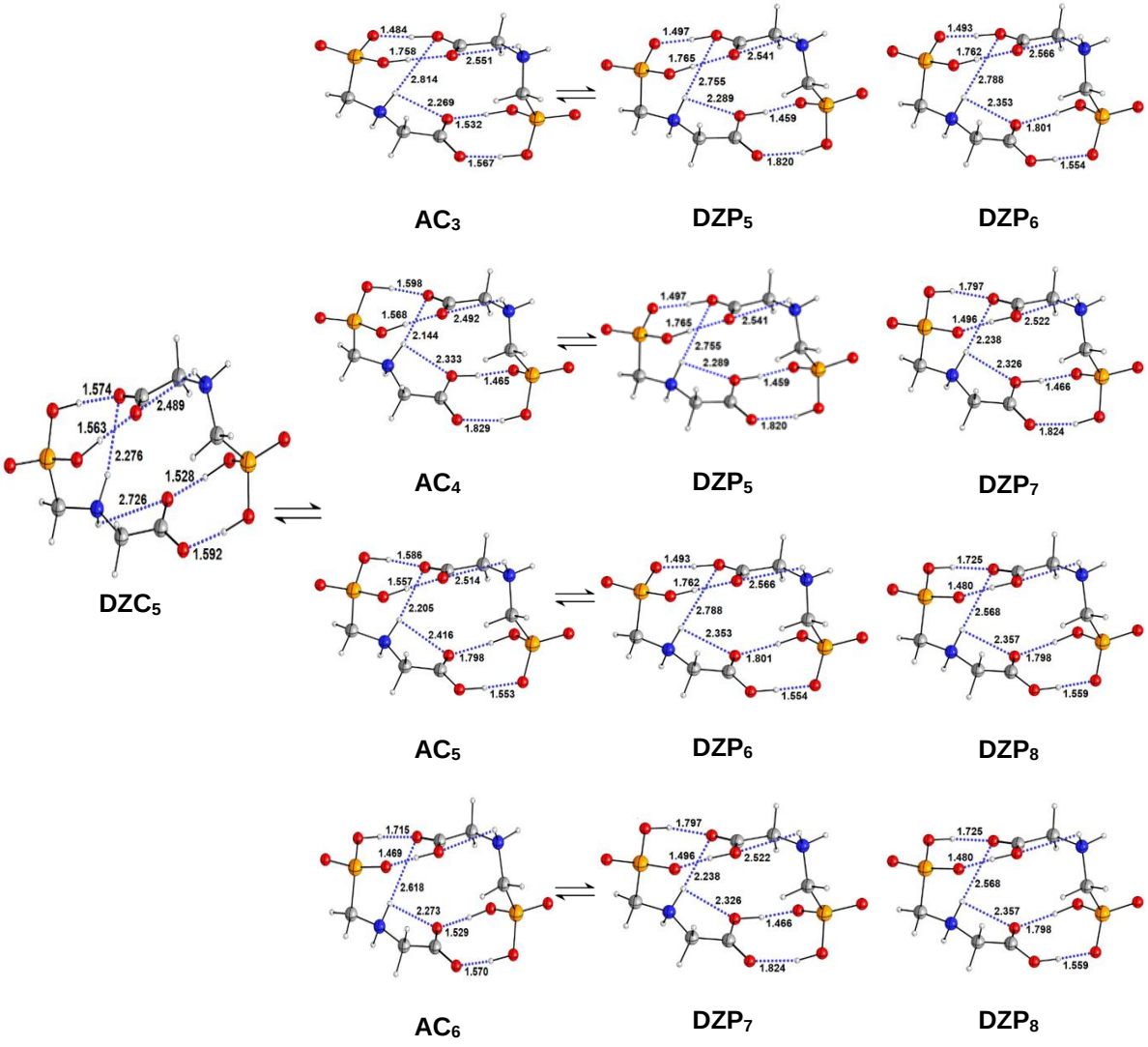

Fig. S2 Structure of DZP and AC tautomers involved in the tautomerization process of DZC_5 in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p) level.

3- Table S1 Relative electronic energies (kcal/mol) with inclusion of zero-point energy (ZPE) contributions (Δ(E+ZPE)) and relative Gibbs free energies (ΔG) (kcal.mol^{-1}) of the most stable non-ionized and ionized conformers of Glyph monomer calculated in the gas phase and in solution at B3LYP-D3/6-311++G(2d,2p) level and using the SMD model.

	Gas phase		Cyclohexane		Water	
Conformer	**Δ(E+ZPE)**[a]	**ΔG**[a]	**Δ(E+ZPE)**	**ΔG**	**Δ(E+ZPE)**[a]	**ΔG**[a]
N_1	0.0	0.0	0.0	0.0	4.4	5.5
N_2	1.1	1.2	0.3	0.6	3.3	4.8
N_3	2.1	2.2	1.7	1.7	6.0	7.0
N_4	2.8	2.8	1.6	1.9	4.8	6.1
N_5	3.7	3.3	2.1	2.0	4.8	6.3
N_6	3.8	3.3	2.3	2.1	5.0	6.2
N_7	4.0	2.9	2.9	1.8	6.1	6.0
ZP_1	-	-	11.2	10.1	0.0	0.0
ZP_2	-	-	-	-	0.2	0.2
ZP_3	-	-	14.6	14.1	0.3	0.8
ZP_4	-	-	15.5	14.8	0.5	0.9
ZP_5	-	-	10.9	10.7	0.8	1.3
ZC_1	-	-	10.0	10.5	1.0	2.4
ZC_2	-	-	11.4	11.5	2.0	3.0
ZC_3	-	-	11.2	11.5	2.5	3.9
ZC_4	-	-	11.3	11.6	2.8	3.9

[a] Energies were taken from our previous work: O. Fliss, K. Essalah and A. Ben Fredj, *Phys. Chem. Chem. Phys.*, 2021, **23**, 26306-26323.

4- Structures and energetics of Glyph monomers in cyclohexane, at SMD-B3LYP-D3/6-311++G(2d,2p) level.

N_1 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E (SCF) = -891.721191802 u.a. ; Zero-point correction = 0.133529 u.a. ; G = -891.624830 u.a. at 298,15K. $\Delta G_{solv.tot.}$ = -6.6 kcal.mol^{-1} ; $\Delta G_{solv.el.}$ = -4.6 kcal.mol^{-1} ; $E_{nonel.}$ = -1.93 kcal.mol^{-1}

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.35649700	-0.24256800	-0.14940100
C	-0.83781700	1.51264200	-0.10816600
H	-1.54042300	2.05780500	0.52153700
H	-0.94030500	1.90194900	-1.12203200
C	1.61572400	1.15976700	-0.34767200
H	1.39378600	1.12894000	-1.41333400
H	2.51353100	1.77525800	-0.23484300
C	2.02517800	-0.23606800	0.09495600
O	1.63018700	-0.80016000	1.09475400
O	2.95196600	-0.76130500	-0.71051700
H	3.18492700	-1.64124700	-0.37524400
N	0.51533500	1.75654200	0.37926800
H	0.58894100	1.57767000	1.37178400
O	-2.95803000	-0.14911800	-0.24324300
H	-3.32194000	-0.87484500	-0.76584600
O	-1.14294000	-0.77614200	1.34705200
H	-0.18906500	-0.92534600	1.49512100
O	-0.70216500	-1.04771200	-1.20375900

N_2 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(d,2p).
E(SCF) = -891.720831452 u.a. ; Zero-point correction = 0.133712 u.a. ; G = -891.623938 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.55421900	-0.17939700	-0.07867800
C	-0.86225100	1.51826200	-0.10080000
H	-1.55310600	2.11701500	0.49327500
H	-0.94006400	1.87889800	-1.12729500
C	1.59743700	1.16065800	-0.32735500
H	1.37808400	1.13316900	-1.39403000
H	2.48531700	1.79052700	-0.21390400
C	2.03395600	-0.22976500	0.10244000
O	1.61136900	-0.83850200	1.06393500
O	3.01711800	-0.70293400	-0.66998800
H	3.28187300	-1.57258500	-0.33119200
N	0.48835500	1.73253800	0.39877100
H	0.55684800	1.56367700	1.39269300
O	-1.12586700	-0.81806900	1.32292500
H	-0.15140200	-0.87531700	1.40462900
O	-0.60272700	-0.90308100	-1.18009000
H	-0.97939100	-1.74002800	-1.48071600
O	-2.99966900	-0.29080200	-0.33683300

N_3 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.718419732 u.a. ; Zero-point correction = 0.133437 u.a. ; G = -891.622129 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	1.37878500	-0.24726400	-0.14647500
C	0.86204600	1.49973200	-0.05941200
H	0.98827600	1.92416300	-1.06415200
H	1.55444600	2.00489100	0.61274100
C	-1.57919500	1.13290200	-0.33124500
H	-2.43919400	1.79969300	-0.25103500
H	-1.33637500	1.06401600	-1.39698500
C	-2.06824200	-0.24084700	0.10034100
O	-1.64720600	-0.89989200	1.02396900
O	-3.08346600	-0.65158100	-0.67267200
H	-3.34752200	-1.53695400	-0.37884200
N	-0.48647400	1.62722800	0.48011500
H	-0.65643000	2.57124500	0.78639300
O	2.98277000	-0.15352000	-0.18267600
H	3.34477000	-0.76123000	-0.83916000
O	1.11740600	-0.83363600	1.31147300
H	0.15051600	-0.86951500	1.46870400
O	0.77767000	-0.98995400	-1.27502600

N_4 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.718728771 u.a. ; Zero-point correction = 0.133641 u.a. ; G = -891.621858u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.57147100	-0.18337000	-0.07289700
C	-0.87657700	1.50360900	-0.09385900
H	-1.56476200	2.09103500	0.51302600
H	-0.94927900	1.87214100	-1.12499300
C	1.57443300	1.14136700	-0.30340900
H	1.36255000	1.09857900	-1.37711800
H	2.42441800	1.81547200	-0.18588800
C	2.06977400	-0.23476700	0.10958900
O	1.62979700	-0.92087800	1.00401400
O	3.11284900	-0.61629000	-0.64243200
H	3.39645800	-1.49407500	-0.34390300
N	0.45571000	1.60372700	0.48701600
H	0.61809500	2.53060400	0.84461600
O	-1.12031000	-0.84138500	1.30431600
H	-0.14435700	-0.81419900	1.40638500
O	-0.64839500	-0.88166400	-1.21221800
H	-0.98664300	-1.75044200	-1.46355900
O	-3.02146000	-0.27552400	-0.31094900

N_5 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.717512239 u.a. ; Zero-point correction = 0.133252 u.a. ; G = -891.621664 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.76313300	-0.17653100	0.13426900
C	-0.45303700	0.93125000	0.75585900
H	0.04028800	0.40099800	1.57114700
H	-0.92394700	1.81712100	1.19024600
C	1.89809100	1.17169900	0.00211900
H	2.46472400	1.73968500	-0.73735100
H	2.16838400	1.58557800	0.98305500
C	2.42675300	-0.25027000	-0.04786900
O	1.78439300	-1.23676700	-0.33069500
O	3.72808700	-0.30351100	0.26783700
H	4.01693000	-1.22808100	0.21800900
N	0.49492400	1.22821200	-0.31283800
H	0.24449800	2.05618900	-0.82675700
O	-0.98556900	-1.43302900	-0.44639300
H	-0.02155400	-1.29074500	-0.55732700
O	-2.30378700	0.60589900	-1.17887100
H	-3.25592800	0.74272300	-1.10671900
O	-2.84583900	-0.49372400	1.08573100

N_6 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.717272920 u.a. ; Zero-point correction = 0.133219u.a. ; G = -891.621452 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.75117100	-0.06932900	-0.06309900
C	-0.43267500	0.92468400	0.71186000
H	0.03343600	0.31244500	1.48408500
H	-0.87630200	1.79297200	1.20702000
C	1.93188900	1.17169200	0.01857700
H	2.52653500	1.73755000	-0.70006500
H	2.18962700	1.56460000	1.01194300
C	2.42823700	-0.26127400	-0.03823300
O	1.76670400	-1.23101100	-0.33551300
O	3.72360900	-0.34735800	0.29389100
H	3.99194400	-1.27779500	0.23928300
N	0.53775400	1.26205100	-0.32551500
H	0.30783800	2.11848600	-0.80185400
O	-2.61854600	-0.63381400	1.17797700
H	-3.53573100	-0.34622900	1.09859500
O	-1.00377100	-1.37796500	-0.56867400
H	-0.03176600	-1.26993400	-0.63560100
O	-2.57637000	0.66050700	-1.04662400

N_7 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.716351102 u.a. ; Zero-point correction = 0.133358 u.a. ; G = -891.621910 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
C	1.46170100	0.00308700	0.89154700
H	0.99047000	0.98455600	0.90803700
H	1.89187000	-0.15120100	1.88339300
C	2.61779400	0.02556000	-0.09592200
O	3.38321400	1.12170600	0.06601400
O	2.84858600	-0.83407000	-0.90867000
N	0.47546100	-1.02903100	0.62113800
H	-1.40097300	-0.83109600	1.67423000
C	-0.33041500	-0.82018600	-0.59269600
H	0.19504600	-0.31066700	-1.40337900
H	-0.66072800	-1.78553300	-0.97353800
P	-1.85752600	0.08897600	-0.17760200
O	-2.96906300	0.06170600	-1.14250400
O	-1.29571000	1.58068600	0.11307400
O	-2.22643300	-0.51491500	1.26094900
H	0.93343300	-1.92898800	0.56485400
H	-1.95535600	2.25095100	-0.10579000
H	4.12167400	1.06888200	-0.56021700

ZP_1 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.705211261 u.a. ; Zero-point correction = 0.135322 u.a. ; G = -891.608704 u.a. at 298,15K. $\Delta G_{solv.tot.}$ = -24.0 kcal.mol^{-1} ; $\Delta G_{solv.el}$ = -21.7 kcal.mol^{-1} ; $E_{nonel.}$ = -2.3 kcal.mol^{-1}

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	2.05175600	-0.10528000	0.14324200
C	0.27625400	0.39155400	0.48505500
H	0.10268300	1.45896400	0.55521000
H	-0.04518800	-0.09403400	1.40190600
C	-1.78741300	-0.86318700	-0.33329200
H	-2.12685200	-1.43237900	-1.19942500
H	-1.62102100	-1.56125800	0.48297600
C	-2.85040900	0.15334900	0.02230900
O	-2.76022600	1.33055700	-0.21246700
O	-3.90598600	-0.43456000	0.59504200
H	-4.58063300	0.24097200	0.77020200
N	-0.51417700	-0.19256300	-0.66488300
H	0.21173400	-0.87334600	-1.05601500
O	2.78758200	-0.23962700	1.42565000
O	2.62223100	1.17595900	-0.70232600
H	3.23009800	1.67761300	-0.14743300
O	1.81871400	-1.22087100	-0.85330600
H	-0.67704400	0.52864400	-1.36704800

ZP_3 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.700722395 u.a. ; Zero-point correction = 0.136325 u.a. ; G = -891.602425 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.97220400	-0.26163600	0.03266900
C	-0.33079400	0.21072700	0.78140200
H	0.17466000	-0.66958200	1.16721500
H	-0.39450800	0.98300300	1.54251600
C	1.89886200	1.06970700	-0.10990900
H	2.28637800	1.67618400	-0.92870700
H	1.96723700	1.64352600	0.81047900
C	2.71948500	-0.20082200	-0.02367700
O	2.33295700	-1.27514900	-0.39681300
O	3.92894600	0.05072400	0.48979000
H	4.44221600	-0.77330000	0.49159500
N	0.47814400	0.73679300	-0.37778100
H	-0.00718500	1.55825400	-0.74304100
O	-1.54969600	-0.85364900	-1.27605100
O	-2.52770300	1.26347700	-0.30151500
H	-3.19226300	1.50735600	0.35231800
O	-2.82670000	-0.89170600	1.07030700
H	0.37175800	0.01431000	-1.11059300

ZP_4 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.699191276 u.a. ; Zero-point correction = 0.136201 u.a. ; G = -891.601193 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.97591400	-0.25961400	0.05171300
C	-0.32454700	0.14199800	0.79842500
H	0.17919600	-0.76960500	1.10438400
H	-0.38029700	0.84820600	1.62142500
C	1.89544800	1.07149000	-0.03922800
H	2.28036300	1.73614600	-0.81291500
H	1.97117600	1.57524000	0.92056900
C	2.71083300	-0.20516100	-0.05489100
O	2.32309100	-1.24151700	-0.52271700
O	3.91574100	-0.00511700	0.48992500
H	4.42508000	-0.82923900	0.42653100
N	0.47120400	0.76466400	-0.32102200
H	-0.02194900	1.61584700	-0.59791400
O	-1.63457800	-0.73768300	-1.33227700
O	-2.46836700	1.32513800	-0.10016500
H	-2.92444500	1.42717000	-0.94326600
O	-2.79084200	-0.99427200	1.04565200
H	0.36039200	0.11543900	-1.11653700

ZP_5 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.706160627 u.a. ; Zero-point correction = 0.135939 u.a. ; G = -891.607774 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	1.95240100	0.03299300	0.19698800
C	0.83407500	-0.85306100	-1.01513800
H	1.18901300	-1.87412200	-1.12568700
H	0.74385900	-0.38508600	-1.99029200
C	-1.35818900	0.28846100	-0.54081100
H	-0.87334200	1.13824100	-0.06604300
H	-1.45050600	0.49669400	-1.60588300
C	-2.73050000	0.04088200	0.04178400
O	-3.11314600	-1.03623700	0.42357300
O	-3.46068900	1.15890800	0.04734000
H	-4.33778500	0.95580200	0.40990900
N	-0.51329100	-0.91535200	-0.34112000
H	-1.04222300	-1.75218500	-0.58303800
O	1.22397400	-0.25215100	1.48510500
H	-0.23538100	-0.94898900	0.67078200
O	1.65781300	1.60832100	-0.17749000
H	2.43107600	1.97982200	-0.61674500
O	3.36829800	-0.29825300	-0.10040300

ZC_1 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.706557500 u.a. ; Zero-point correction = 0.134792 u.a. ; G = -891.608080 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.51001800	-0.21834600	-0.05987500
C	-0.82606500	1.49101000	-0.04706400
H	-1.42094600	2.05251100	0.67020300
H	-0.95654400	1.93195400	-1.03219200
C	1.65336800	1.01322500	-0.55554500
H	1.24280800	0.88487500	-1.54983800
H	2.50814800	1.68310700	-0.58980900
C	2.08393400	-0.35374100	0.04577800
O	1.57521600	-0.59893200	1.19605000
O	2.86111400	-1.01956600	-0.61930100
N	0.61430800	1.62313900	0.35556100
H	0.81745700	2.60536500	0.52755800
O	-0.97865100	-0.94444900	1.23287600
H	0.03337900	-0.95544400	1.27850800
O	-0.66997100	-0.81957800	-1.29385300
H	-0.65906000	-1.78501600	-1.33187300
O	-2.97035800	-0.17913700	-0.19775100
H	0.77866000	1.08619200	1.23345100

ZC_2 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.704082884 u.a. ; Zero-point correction = 0.134664 u.a. ; G = -891.606488 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	1.62186600	-0.17022700	-0.16278100
C	0.50383200	1.23166400	-0.57425700
H	0.10878700	1.07783000	-1.57413900
H	1.11113400	2.13242300	-0.57966800
C	-2.01641700	1.11975900	-0.15191700
H	-2.74153200	1.66997400	0.44384300
H	-2.08176300	1.43785800	-1.18681400
C	-2.28187000	-0.40178100	0.00505900
O	-1.43768200	-0.99687700	0.75882400
O	-3.26613600	-0.84045600	-0.56934900
N	-0.64513100	1.43377400	0.38702900
H	-0.60844300	2.37864200	0.76195200
O	0.82292300	-1.51268300	-0.30062000
H	-0.09901700	-1.45649600	0.12721600
O	1.73967800	0.12661700	1.42586500
H	2.04100800	-0.63584000	1.93650900
O	2.86168000	-0.09568900	-0.94453200
H	-0.53922600	0.76744800	1.16880200

ZC_3 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.704377228 u.a. ; Zero-point correction = 0.134487 u.a. ; G = -891.606493 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.38380700	-0.26647800	-0.15045800
C	-0.80748000	1.47476300	0.07170100
H	-1.35070000	1.92210900	0.90122100
H	-1.01195100	2.03196100	-0.83899200
C	1.62550100	0.96257500	-0.60927800
H	1.11487200	0.74817900	-1.54220400
H	2.43412800	1.66680600	-0.77772200
C	2.18013200	-0.35127200	0.01696800
O	1.66567400	-0.63880200	1.15651900
O	3.03615700	-0.93815500	-0.62195300
N	0.65498900	1.57032900	0.38050800
H	0.86587000	0.99348300	1.22705600
O	-2.95352200	-0.09399600	0.11990700
H	-3.47089100	-0.44854500	-0.61429100
O	-0.89823500	-1.01535200	1.14330400
H	0.11178300	-1.04387600	1.19401000
O	-1.02541700	-0.80397200	-1.47332700
H	0.89290600	2.54056400	0.57228200

ZC_4 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -891.704871842 u.a. ; Zero-point correction = 0.135218 u.a. ; G = -891.606423 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	1.55308700	-0.14392200	0.05374900
C	0.35688600	0.99636300	-0.76579800
H	-0.16050200	0.51284300	-1.58860800
H	0.89786100	1.85933900	-1.14293800
C	-2.08567800	1.11667400	-0.09569700
H	-2.73037000	1.63131200	0.61432600
H	-2.29874500	1.46603900	-1.10077700
C	-2.29419400	-0.41639300	0.03498800
O	-1.39480000	-1.00551200	0.71567400
O	-3.30382700	-0.86349800	-0.49352200
N	-0.66305800	1.47043700	0.24473600
H	-0.56541000	2.47457100	0.38187900
O	2.78480500	-0.20463600	-0.96596900
H	3.56211500	0.23678300	-0.60182100
O	0.95538500	-1.58275700	-0.08199300
H	-0.00891100	-1.56127500	0.23329300
O	1.86317200	0.41191400	1.38825100
H	-0.45091000	1.02220600	1.14478600

5- Structures and energetics of Glyph dimers in the gas phase, at B3LYP-D3/6-311++G(2d,2p) level.

DZC_1 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.45995522 u.a. ; Zero-point correction = 0.274017 u.a. ; G = -1783.237450 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.43757300	-0.05883000	0.17216500
C	2.13850500	0.87748800	-0.74107000
H	1.19992000	0.33532600	-0.79512100
H	2.48887000	1.14246000	-1.73443400
C	0.85598400	3.03828400	-0.55642400
H	0.95592600	4.02766700	-0.11359000
H	0.99541900	3.10310300	-1.63016900
C	-0.52472400	2.45171900	-0.19347000
O	-0.52055600	1.73335500	0.84190000
O	-1.47121200	2.73265800	-0.94621500
H	-2.88417100	1.95502500	-0.75853500
N	1.89704200	2.13883800	0.03537700
H	2.80220000	2.59184100	0.18314000
O	3.68212300	-1.34334600	-0.69191200
O	2.69344100	-0.44754400	1.51279900
H	1.88034500	-1.01269500	1.35043800
O	4.57378400	0.85662600	0.36763200
H	1.51569300	1.85748400	0.95209500
P	-3.43757100	0.05866600	0.17211800
C	-2.13932200	-0.87807800	-0.74190700
H	-1.20081800	-0.33589400	-0.79729800
H	-2.49057900	-1.14374100	-1.73476900
C	-0.85584200	-3.03832000	-0.55647100
H	-0.95549700	-4.02757700	-0.11330000
H	-0.99538600	-3.10353000	-1.63017900
C	0.52478800	-2.45138400	-0.19381000
O	0.52058700	-1.73242100	0.84110500
O	1.47126600	-2.73248900	-0.94657500
H	2.88338500	-1.95501600	-0.75881500
N	-1.89703500	-2.13890500	0.03516000
H	-2.80195900	-2.59216500	0.18354100
O	-3.68253600	1.34311300	-0.69210400
O	-2.69241000	0.44736200	1.51208200
H	-1.87935600	1.01289800	1.34965500
O	-4.57385700	-0.85651800	0.36837300
H	-1.51543800	-1.85686400	0.95158100

DZC_2 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.45627430 u.a. ; Zero-point correction = 0.271283 u.a. ; G = -1783.236442 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	4.06902200	-0.06751900	0.07148600
C	3.11866800	1.37681500	-0.56460200
H	3.03561700	1.37307400	-1.64776000
H	3.59286000	2.29620400	-0.22852200
C	0.79931700	2.37876800	-0.16872700
H	1.15404300	3.26348200	0.35696500
H	0.72337200	2.59395100	-1.23011600
C	-0.56645000	1.91874800	0.37680600
O	-0.52815200	1.04738700	1.28228000
O	-1.57342400	2.42611700	-0.15978900
H	-2.84473000	1.77802300	0.26758300
N	1.76110600	1.25762500	0.02924300
H	1.84480900	1.05554200	1.02964000
O	3.84718700	-0.11005000	1.52755900
O	5.54528500	0.27022200	-0.45175100
H	5.96577400	-0.48341800	-0.88058200
O	3.67253700	-1.31675800	-0.78663000
H	1.28609600	0.40032300	-0.38517900
P	-4.10776000	0.01829500	-0.28556200
C	-2.57225700	-0.93114700	-0.61861300
H	-1.91695500	-0.39354000	-1.29408700
H	-2.85329000	-1.87828600	-1.07342000
C	-0.74591900	-2.25696700	0.55773000
H	-0.44953700	-2.51418100	1.57138500
H	-1.16497900	-3.14203500	0.08231300
C	0.50223000	-1.78253400	-0.20424800
O	0.38720500	-0.76216700	-0.92984000
O	1.53203300	-2.45400300	0.00603600
H	2.82055500	-1.81503900	-0.48091500
N	-1.81077900	-1.20177500	0.64547800
H	-2.48115800	-1.47315700	1.36492500
O	-3.67259200	1.23741600	0.57637100
O	-4.79774300	-0.91594800	0.85190900
H	-5.62006200	-1.29026100	0.51744600
O	-4.91391900	0.15812500	-1.50608600
H	-1.36449900	-0.28809400	0.96788100

DZC_3 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.45637025 u.a. ; Zero-point correction = 0.272457 u.a. ; G = -1783.236040 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.73642200	0.00472200	0.24509900
C	2.59177000	1.06052700	-0.75922200
H	1.80115000	0.47841700	-1.21847700
H	3.14401100	1.62995400	-1.50091900
C	0.81815100	2.85660800	-0.32162800
H	0.64930200	3.68551400	0.36193900
H	1.09477400	3.25169800	-1.29546200
C	-0.46152600	2.00529700	-0.42185300
O	-0.31042800	0.79044900	-0.14583600
O	-1.49489200	2.61058100	-0.75270400
H	-2.77996400	1.77091700	-0.66991000
N	1.94895400	2.02253800	0.20707100
H	2.68659600	2.60477800	0.60662200
O	3.97939500	-1.26675600	-0.63849700
O	2.80245000	-0.37510100	1.46973600
H	2.10402900	-1.09348400	1.29629500
O	4.90174800	0.81584800	0.62629300
H	1.58540500	1.43588500	0.96878300
P	-3.77611500	0.04928600	0.35544200
C	-3.01201000	-1.45280500	-0.38619700
H	-3.06721700	-1.40586400	-1.47024400
H	-3.52333200	-2.34688600	-0.03833400
C	-0.70107000	-2.41257700	-0.76422600
H	-1.01960800	-3.44166400	-0.60619200
H	-0.79698300	-2.15899100	-1.81528700
C	0.75068200	-2.20877800	-0.29441300
O	0.88156700	-1.98700100	0.93433100
O	1.63166600	-2.24588900	-1.17810000
H	3.11987400	-1.76257100	-0.84382900
N	-1.58065000	-1.49613600	0.02268000
H	-1.48943900	-1.70769700	1.01791300
O	-3.22263200	0.23610700	1.70536300
O	-5.32792800	-0.33825800	0.22168000
H	-5.87115500	0.40367400	-0.06644100
O	-3.63749900	1.20941300	-0.69255000
H	-1.16373200	-0.52338600	-0.05531300

DZC_4 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.45594771 u.a. ; Zero-point correction = 0.272391 u.a. ; G = -1783.235753 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.74557600	-0.01924900	0.26596200
C	2.61381800	1.04058200	-0.74749300
H	1.81693600	0.46147100	-1.20044500
H	3.17203600	1.59354100	-1.49713200
C	0.85748900	2.84960400	-0.33888100
H	0.69161000	3.69427300	0.32623600
H	1.13159400	3.22135200	-1.32221900
C	-0.42274200	1.99661800	-0.41251400
O	-0.28964100	0.81164500	-0.01796600
O	-1.44037500	2.56747400	-0.83713200
H	-2.72275000	1.72850400	-0.72595300
N	1.98318400	2.02104900	0.20671300
H	2.72530200	2.60195200	0.59941700
O	3.99289200	-1.28877800	-0.61972600
O	2.80073300	-0.40037200	1.48165000
H	2.10010500	-1.11142400	1.29804600
O	4.90890400	0.78859500	0.65994200
H	1.60698300	1.44703400	0.97264400
P	-3.81358000	0.07021900	0.33043100
C	-3.02585900	-1.44160600	-0.37635200
H	-3.09687100	-1.42463000	-1.46051400
H	-3.51667200	-2.33508300	0.00050500
C	-0.70702600	-2.34741100	-0.81090300
H	-1.03473100	-3.38022300	-0.70330000
H	-0.79513800	-2.04506400	-1.84974900
C	0.74336100	-2.18079400	-0.32424700
O	0.87088400	-2.00326300	0.91164200
O	1.62861900	-2.20265400	-1.20468100
H	3.12940000	-1.76748200	-0.84529900
N	-1.58724100	-1.46290300	0.01156300
H	-1.47413300	-1.70713000	0.99713000
O	-3.36213100	0.25645900	1.72138100
O	-5.37322400	-0.26371700	0.14425200
H	-5.81962700	-0.28498300	0.99797100
O	-3.59228700	1.18691500	-0.73462900
H	-1.17482100	-0.48407000	-0.03665800

DZC_5 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.45842117 u.a. ; Zero-point correction = 0.275007 u.a. ; G = -1783.233438 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.63189000	0.08185300	-0.07976100
C	2.29969900	-0.77133000	-1.03169000
H	2.68270100	-0.92827300	-2.03690700
H	1.36540000	-0.22930000	-1.09562200
C	1.15699000	-2.09912400	0.79542800
H	1.15563000	-3.09490500	1.23540300
H	1.56836100	-1.38945600	1.50326900
C	-0.26847400	-1.71716600	0.38366600
O	-0.57584100	-1.89523900	-0.81468800
O	-0.99591300	-1.24967400	1.29741400
H	-2.67613400	-1.47442000	1.01355200
N	2.03074400	-2.12810100	-0.42978300
H	1.53565400	-2.69375900	-1.12278400
O	4.77774800	-0.84268700	-0.04483700
H	2.94120400	-2.54827200	-0.21866400
O	3.02967500	0.39237700	1.34366700
H	2.21583100	0.99807300	1.34197300
O	3.79043100	1.43334500	-0.87204300
P	-3.79720500	-0.17075600	-0.30296100
C	-3.26116500	1.34924800	0.61325500
H	-3.76626700	1.34154000	1.57580900
H	-3.57914700	2.22568600	0.05599300
C	-0.99734400	2.06677300	-0.26841700
H	-1.21953500	1.52053600	-1.17860200
H	-1.32935200	3.09640400	-0.38366000
C	0.50356800	2.01354000	0.04175800
O	0.79997000	1.64898600	1.21127700
O	1.26567800	2.29211500	-0.90144100
H	2.92510300	1.93595300	-0.88021500
N	-1.77735700	1.44011500	0.85321400
H	-1.56634700	1.96569400	1.70063600
O	-3.62079300	-1.34654000	0.74760300
H	-1.38674600	0.49425500	1.04493000
O	-2.66096100	-0.35655500	-1.39638500
H	-1.96208300	-1.04428600	-1.21689600
O	-5.15973500	0.03916200	-0.79124300

DZC_6 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.45668360 u.a. ; Zero-point correction = 0.274394 u.a. ; G = -1783.233127 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.69221800	-0.07870300	-0.15714300
C	-2.43591400	0.98306200	0.68307200
H	-1.58968500	0.41023500	1.04869500
H	-2.89546100	1.53113500	1.50060200
C	-0.82252300	2.84284600	0.18655900
H	-0.69079800	3.67972700	-0.49765300
H	-1.08226100	3.21211000	1.17265600
C	0.47608600	2.01753100	0.22105200
O	0.57249700	1.13543600	-0.68950200
O	1.30094800	2.30116500	1.09654400
H	2.47884100	1.19017600	1.22260100
N	-1.92909500	1.97477300	-0.32567500
H	-2.72455200	2.51440800	-0.67169800
O	-3.88752600	-1.28325500	0.83018700
O	-2.89699400	-0.57058600	-1.43766700
H	-2.20735000	-1.28059300	-1.25413000
O	-4.85767900	0.75571100	-0.47992800
H	-1.54675800	1.43789000	-1.11652700
P	3.84469500	0.00767600	-0.07392600
C	3.05537100	-1.58455000	-0.55554200
H	3.38334400	-2.37389200	0.11424100
H	3.37875600	-1.82206800	-1.56543300
C	0.87195800	-2.01421800	0.70092200
H	1.24711100	-3.01091400	0.92444100
H	1.10195400	-1.34812600	1.52502100
C	-0.63623700	-2.06521100	0.40090900
O	-0.92775000	-2.13102000	-0.82385000
O	-1.40839800	-2.00089100	1.37516600
H	-3.01115000	-1.71810700	1.06520500
N	1.55448100	-1.50878100	-0.53360700
H	1.11583400	-2.01433600	-1.30848200
O	3.06172000	0.37423600	1.25085700
O	3.33534000	1.02515800	-1.19801800
H	2.38419900	1.24017400	-1.12571700
O	5.29624800	-0.15529800	-0.01375400
H	1.23343300	-0.52637000	-0.65491000

DZC_7 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.45447109 u.a. ; Zero-point correction = 0.273739 u.a. ; G = -1783.231887 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.41171100	0.32907700	0.10074300
C	2.27789600	-0.51638000	-1.07847400
H	2.66727800	-0.36548500	-2.08213100
H	1.25276900	-0.17249200	-1.03610100
C	1.53728800	-2.42870900	0.42655300
H	1.72194100	-3.49074300	0.57629500
H	1.90825200	-1.87043200	1.27838000
C	0.03797300	-2.17696700	0.21654500
O	-0.32938200	-2.02487800	-0.97935800
O	-0.64936100	-2.13905800	1.25082400
H	-2.01312100	-1.46841000	1.17699000
N	2.29480700	-1.99887400	-0.80397000
H	1.85464300	-2.47199900	-1.59494900
O	4.64191100	-0.47960800	0.17189400
H	3.27887700	-2.27162900	-0.72057000
O	2.61910400	0.40579300	1.46458400
H	1.72084400	0.84874000	1.37786100
O	3.52756300	1.77727800	-0.50334600
P	-3.48605200	-0.40316700	-0.17187100
C	-3.58968500	1.40061700	0.18949000
H	-4.30418400	1.52391000	0.99913300
H	-3.92712600	1.96312900	-0.67550500
C	-1.32218900	2.41009900	-0.43809300
H	-1.54091500	1.83866300	-1.33488600
H	-1.47520000	3.46805600	-0.62656400
C	0.12529100	2.11452800	-0.01428000
O	0.24487600	1.39000100	1.01121200
O	1.01195800	2.57480900	-0.75257200
H	2.62744300	2.21382500	-0.56709000
N	-2.25926100	1.94434200	0.64301700
H	-2.39530700	2.70058200	1.30959200
O	-2.86461500	-0.90407800	1.18933500
H	-1.72528600	1.22059600	1.15878900
O	-2.33322500	-0.44040500	-1.25880400
H	-1.61663800	-1.14917200	-1.16481400
O	-4.81475700	-0.89025300	-0.55517800

DZC_8 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.45483329 u.a. ; Zero-point correction = 0.273938 u.a. ; G = -1783.231684 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.53518600	-0.35968000	-0.23350000
C	-2.51872000	0.83408500	0.73548600
H	-1.57566800	0.39261500	1.04338700
H	-3.06597200	1.19256200	1.60247500
C	-1.21360300	2.95536500	0.41918100
H	-1.25602900	3.88966200	-0.13782300
H	-1.44067900	3.13668100	1.46410700
C	0.17659300	2.31066000	0.23841800
O	0.25082700	1.53047000	-0.74938600
O	1.05493300	2.60428600	1.06437700
H	2.18256900	1.49574800	1.10107600
N	-2.21367700	2.00102400	-0.15810500
H	-3.09132200	2.44467900	-0.43023600
O	-3.57969500	-1.63758400	0.67899700
O	-2.60148400	-0.63697000	-1.48399300
H	-1.76933200	-1.15734000	-1.27547100
O	-4.80989800	0.28086600	-0.58702000
H	-1.76087600	1.61768100	-1.00435800
P	3.52730400	0.27466000	-0.19609400
C	3.52613000	-1.56846400	-0.10705200
H	3.93548600	-1.91780200	0.83633600
H	4.15294900	-1.92008700	-0.92264400
C	1.24585000	-2.15147100	0.90792300
H	1.40256400	-3.06101500	1.47960200
H	1.49916900	-1.28921800	1.51749800
C	-0.21056700	-2.02576300	0.43349600
O	-0.36219300	-1.81571600	-0.79722000
O	-1.07524200	-2.10046500	1.32631200
H	-2.65508800	-1.94155400	0.93638700
N	2.15086000	-2.14784700	-0.29416500
H	2.21336600	-3.09612500	-0.65802400
O	2.75375900	0.65979500	1.12931800
O	2.52243900	0.51666600	-1.39780200
H	1.63495400	0.93893200	-1.15450100
O	4.90788800	0.73234300	-0.37601600
H	1.62708500	-1.61834800	-1.01327500

DZC_9 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.45053838 u.a. ; Zero-point correction = 0.271577 u.a. ; G = -1783.231210 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.63583600	-0.12687100	0.68579100
C	-2.22929700	1.04310700	0.47122500
H	-1.31245200	0.70729500	0.94236500
H	-2.50621300	2.00858000	0.88739100
C	-1.00683400	2.26243400	-1.37950000
H	-1.04075800	2.36468400	-2.45990800
H	-1.29145100	3.18900700	-0.88840500
C	0.39643700	1.80148900	-0.94097400
O	1.05044200	1.14470700	-1.77759200
O	0.72017300	2.07184200	0.24524000
H	2.11315400	1.76453200	0.65697600
N	-1.99442900	1.19938900	-0.99905900
H	-2.90997700	1.35869100	-1.42777000
O	-4.50733500	0.05509100	-0.48985400
O	-4.30895000	0.33693900	2.06915800
H	-4.15046600	-0.29722100	2.77644200
O	-3.04573000	-1.52817300	1.04359700
H	-1.66758400	0.25501400	-1.37644500
P	3.63602500	0.12554000	0.68648800
C	2.22659700	-1.04049500	0.46973800
H	1.30976000	-0.70191400	0.93892300
H	2.50016900	-2.00648500	0.88688200
C	1.00746700	-2.26014200	-1.38270500
H	1.04139300	-2.36096100	-2.46326100
H	1.29292500	-3.18707300	-0.89280900
C	-0.39603800	-1.80083900	-0.94321600
O	-1.04898100	-1.13999600	-1.77755800
O	-0.72077800	-2.07649300	0.24134600
H	-2.11247900	-1.76577500	0.65701200
N	1.99424100	-1.19681300	-1.00096000
H	2.91059400	-1.35630400	-1.42798400
O	4.51061900	-0.06122000	-0.48611000
O	4.30410400	-0.33802800	2.07245700
H	4.14294400	0.29629800	2.77898200
O	3.04905900	1.52943100	1.03917600
H	1.66792500	-0.25257000	-1.37871000

DZP_9 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.44840851 u.a. ; Zero-point correction = 0.271262 u.a. ; G = -1783.228391 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.60976700	0.05216700	0.53176500
C	2.01716200	-0.92419400	0.56797100
H	1.15649400	-0.34609900	0.88624300
H	2.14058400	-1.78888700	1.21378600
C	0.87857900	-2.57420700	-0.98025300
H	0.97602000	-2.96073700	-1.99273200
H	1.15415700	-3.33724400	-0.26007700
C	-0.55313000	-2.07150500	-0.78142200
O	-0.93264600	-1.13904700	-1.48003300
O	-1.21793800	-2.66477100	0.14839400
H	-2.17754700	-2.17834600	0.32587100
N	1.79719900	-1.40782500	-0.83717500
H	2.75529400	-1.56660600	-1.19853800
O	4.30460900	-0.53487000	-0.64774700
O	4.29557000	-0.40964000	1.92438400
H	4.39948400	0.34707000	2.51083500
O	3.31820700	1.53274300	0.67157600
H	1.42734300	-0.60107700	-1.36976700
P	-3.60976800	-0.05203800	0.53181400
C	-2.01717200	0.92422900	0.56785800
H	-1.15661500	0.34598300	0.88613800
H	-2.14036700	1.78901800	1.21358000
C	-0.87859900	2.57398400	-0.98062100
H	-0.97589300	2.96030800	-1.99319800
H	-1.15431600	3.33718200	-0.26067300
C	0.55307800	2.07129700	-0.78145600
O	0.93278700	1.13892600	-1.48009900
O	1.21777000	2.66467800	0.14836600
H	2.17741300	2.17832700	0.32608300
N	-1.79725800	1.40763500	-0.83738900
H	-2.75530700	1.56634400	-1.19887200
O	-4.30463500	0.53496800	-0.64769400
O	-4.29512300	0.40998900	1.92459600
H	-4.40107000	-0.34706800	2.51023100
O	-3.31827800	-1.53262400	0.67159200
H	-1.42732600	0.60079900	-1.36978000

AC_9 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.44871513 u.a. ; Zero-point correction = 0.270276 u.a. ; G = -1783.230895 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.60211000	0.04212800	0.55427500
C	2.05941100	-0.98541400	0.53340400
H	1.19677100	-0.46481400	0.93595800
H	2.23543800	-1.89269000	1.10497500
C	0.86682700	-2.50612900	-1.09813400
H	0.93499100	-2.80331700	-2.14154200
H	1.17020800	-3.32175800	-0.44918900
C	-0.56349600	-2.03442000	-0.81642400
O	-1.04886300	-1.19663600	-1.56626800
O	-1.10425500	-2.54427800	0.23554100
H	-2.09931300	-2.09451800	0.44415700
N	1.79153500	-1.34936100	-0.89445000
H	2.71331700	-1.49394300	-1.32535900
O	4.31470800	-0.32449600	-0.68760100
O	4.34031100	-0.45362000	1.89291600
H	4.39540500	0.24611300	2.55266400
O	3.24602000	1.51330900	0.89032400
H	1.40437800	-0.47281600	-1.33393500
P	-3.58716600	-0.06370700	0.57833900
C	-2.02593300	0.95292700	0.53070900
H	-1.14601800	0.41299500	0.86396000
H	-2.15831700	1.84180900	1.14094100
C	-0.89759300	2.53555000	-1.08038400
H	-0.96910100	2.86007800	-2.11634200
H	-1.18958900	3.33768200	-0.41073700
C	0.53102700	2.03785300	-0.80089300
O	0.89206900	1.06205200	-1.49303000
O	1.17629300	2.61990300	0.10365600
H	2.39233600	1.98486600	0.47066700
N	-1.82903300	1.38268500	-0.89323400
H	-2.78329700	1.54163000	-1.25263600
O	-4.33809300	0.43262000	-0.60509200
O	-4.25143500	0.43726100	1.96924600
H	-4.30808300	-0.29464500	2.59226900
O	-3.23953800	-1.52826000	0.79106800
H	-1.46999600	0.55869400	-1.40702200

NZP_1 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.45183808 u.a. ; Zero-point correction = 0.272254 u.a. ; G = -1783.230144 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-2.46319100	0.55703300	0.13674800
C	-3.63539400	-0.85340900	0.13318700
H	-4.50038900	-0.54280500	-0.45182000
H	-3.97341200	-0.98954000	1.16063900
C	-2.02480000	-2.78160400	0.26405500
H	-2.03601000	-2.56204700	1.33010000
H	-2.14220600	-3.86447900	0.17085200
C	-0.62650300	-2.46328000	-0.26442700
O	-0.43617400	-1.75181800	-1.25071300
O	0.32676600	-3.03954300	0.40642900
H	1.26259600	-2.73641200	0.07974100
N	-3.13022000	-2.11114700	-0.39883100
H	-2.99158600	-2.06782000	-1.39831600
O	-1.68329000	0.50012300	-1.24405900
H	-1.23347300	-0.38315200	-1.37840800
O	-1.43181000	0.07514100	1.27739100
H	-0.91792600	0.83228400	1.61145300
O	-2.98337700	1.93665900	0.36318800
P	3.03832100	-0.77455600	0.00226600
C	1.68509200	0.35022800	-0.57384100
H	0.74210300	0.20259100	-0.06781500
H	1.55084100	0.27271300	-1.64803700
C	1.33473100	2.86413800	-0.72714900
H	1.87506200	3.80325200	-0.61225700
H	1.08747700	2.71399700	-1.77316800
C	0.07411700	2.87148500	0.13240200
O	0.10652800	2.37825800	1.24682700
O	-0.96277000	3.39346100	-0.45929200
H	-1.81753900	3.04593200	-0.03787300
N	2.19176500	1.73955300	-0.25617600
H	3.15481100	1.76405400	-0.62010900
O	2.63042700	-2.20045800	-0.22813300
O	2.95625500	-0.44915600	1.61261400
H	2.53457200	-1.17194800	2.08864400
O	4.25737100	-0.11403900	-0.53734100
H	2.26444500	1.79300900	0.76557900

DN_1 structure in the gas-phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.45161029 u.a. ; Zero-point correction = 0.270763 u.a. ; G = -1783.231974 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	2.42539400	1.20031400	-0.67467200
C	3.90547200	0.23126000	-0.16614200
H	4.61783000	0.97383700	0.19403700
H	4.32448000	-0.17223100	-1.09008000
C	2.97629100	-1.98403500	0.50902000
H	3.05147400	-2.22554700	-0.55026400
H	3.34944400	-2.85871500	1.04924700
C	1.50429700	-1.85650400	0.86716800
O	1.05033200	-0.92311000	1.50955800
O	0.77221100	-2.86930600	0.44410100
H	-0.17542800	-2.66422900	0.61442300
N	3.78811600	-0.82728600	0.82268300
H	3.56810200	-0.46120900	1.73829400
O	1.60066400	1.52203000	0.65128300
H	1.33446100	0.70093000	1.13887100
O	1.45455100	0.08513600	-1.40962100
H	1.53860000	0.17432600	-2.36787600
O	2.71241600	2.35740500	-1.52996600
P	-2.27014400	-1.15994500	-0.75752500
C	-3.86172100	-0.30915700	-0.43565700
H	-4.58039700	-1.09676400	-0.21084900
H	-4.17113300	0.13463000	-1.38309100
C	-3.14331700	1.91104700	0.44294400
H	-3.14990800	2.21361700	-0.60221300
H	-3.60734600	2.72591800	1.00699700
C	-1.69745500	1.84349000	0.91124000
O	-1.26101000	0.98317800	1.65357100
O	-0.96373600	2.85418600	0.45853800
H	-0.03059300	2.69385600	0.69617600
N	-3.91497800	0.69731700	0.61814700
H	-3.75245100	0.29007600	1.52897600
O	-1.67946500	-1.56144100	0.69829500
H	-1.43773800	-0.76830900	1.22562100
O	-1.37658200	0.09236400	-1.22489800
H	-0.41315500	-0.04519900	-1.22848300
O	-2.31042600	-2.33136100	-1.64262100

6- Structures and energetics of Glyph dimers in cyclohexane, at SMD-B3LYP-D3/6-311++G(2d,2p) level.

DZC_1 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.48956489 u.a. ; Zero-point correction = 0.274343 u.a. ; G = -1783.265939 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.44822000	0.09696000	0.20584500
C	-2.25045200	-0.92312700	-0.74950700
H	-1.31007500	-0.39646700	-0.88730600
H	-2.66945800	-1.19778200	-1.71352900
C	-0.90072600	-3.03737200	-0.59224600
H	-0.97530300	-4.03565100	-0.16481700
H	-1.05307200	-3.08818200	-1.66501900
C	0.46867600	-2.43542100	-0.23406900
O	0.47229700	-1.71657300	0.79934700
O	1.42082100	-2.71630500	-0.98568200
H	2.79617600	-1.96036000	-0.75828100
N	-1.96411100	-2.17702600	0.02027700
H	-2.83830900	-2.68587700	0.16097900
O	-3.62906800	1.38906900	-0.66682800
O	-2.62840800	0.45287500	1.51196500
H	-1.80211200	0.99300000	1.31109500
O	-4.66153700	-0.69684900	0.46563800
H	-1.60005500	-1.90157500	0.94380400
P	3.44825200	-0.09704000	0.20582800
C	2.24976400	0.92251200	-0.74908700
H	1.30928900	0.39564300	-0.88547400
H	2.66783800	1.19654300	-1.71367900
C	0.90080200	3.03724900	-0.59247600
H	0.97572600	4.03571200	-0.16554800
H	1.05299100	3.08757400	-1.66530200
C	-0.46866400	2.43578900	-0.23390900
O	-0.47222700	1.71662200	0.79927100
O	-1.42101200	2.71732200	-0.98502300
H	-2.79615300	1.96068900	-0.75778200
N	1.96407800	2.17688500	0.02018000
H	2.83849800	2.68551200	0.16032600
O	3.62927600	-1.38908500	-0.66692100
O	2.62903600	-0.45338300	1.51224500
H	1.80264800	-0.99327000	1.31130000
O	4.66137300	0.69717700	0.46533500
H	1.60029700	1.90193900	0.94392800

DZC_2 structure in cyclohexane at SMD- B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.48196931 u.a. ; Zero-point correction = 0.271400 u.a. ; G = -1783.261973 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	4.07455400	-0.06433300	0.05125100
C	3.11431700	1.39014700	-0.53223500
H	3.02564600	1.41307900	-1.61484700
H	3.59108200	2.30174200	-0.17874000
C	0.79663900	2.38142500	-0.14756000
H	1.14674300	3.26921900	0.37565200
H	0.73220500	2.58894900	-1.21104000
C	-0.56934700	1.92743700	0.39183800
O	-0.54942400	1.06157400	1.30028800
O	-1.57498600	2.44435100	-0.14765200
H	-2.81387700	1.77886000	0.25165400
N	1.75932100	1.26289400	0.06495700
H	1.84262200	1.07631500	1.06746800
O	3.90865100	-0.14799600	1.51525900
O	5.53408400	0.28461300	-0.50969000
H	5.96820000	-0.47153500	-0.92367100
O	3.64960300	-1.30402600	-0.80928000
H	1.28956100	0.40476800	-0.34261800
P	-4.09745200	0.01658200	-0.30111600
C	-2.58922400	-0.98533400	-0.59415100
H	-1.93058100	-0.48872500	-1.29802800
H	-2.89694900	-1.94113400	-1.01264400
C	-0.74184400	-2.27628800	0.58243400
H	-0.44874000	-2.52520100	1.59900100
H	-1.15203400	-3.16662900	0.10958200
C	0.49788600	-1.79165700	-0.18061000
O	0.38054400	-0.77096000	-0.90342000
O	1.53642300	-2.45912600	0.01842500
H	2.80223800	-1.80250900	-0.48505200
N	-1.81930500	-1.23252700	0.66686800
H	-2.47501100	-1.51143500	1.39730400
O	-3.65593900	1.23907100	0.55184900
O	-4.86183400	-0.86042400	0.82802900
H	-5.64898700	-1.27768400	0.45797900
O	-4.85890600	0.17532500	-1.55199300
H	-1.38504600	-0.31798600	0.98038800

DZC_3 structure in cyclohexane at SMD- B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.48485805 u.a. ; Zero-point correction = 0.272725 u.a. ; G = -1783.263856 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.75577800	0.00026200	0.21654000
C	2.59924200	1.09520900	-0.72317600
H	1.80432600	0.51559000	-1.17965800
H	3.13705100	1.66229300	-1.47753400
C	0.81808600	2.86703700	-0.29803100
H	0.64114800	3.69901500	0.37997900
H	1.08965000	3.25668100	-1.27528900
C	-0.44643100	1.99986300	-0.38464500
O	-0.30709700	0.80518100	-0.02897300
O	-1.47725500	2.57378800	-0.78616500
H	-2.73935300	1.73462800	-0.70651300
N	1.96319100	2.05862300	0.24008200
H	2.68693100	2.67329600	0.61544600
O	3.94152300	-1.25109000	-0.71396400
O	2.87566700	-0.41019300	1.46866800
H	2.14658100	-1.09790500	1.28892700
O	4.97474100	0.74404500	0.57469800
H	1.60892300	1.49661800	1.02230000
P	-3.80935000	0.05283200	0.33112000
C	-3.02058400	-1.47233800	-0.32249400
H	-3.07651200	-1.47844100	-1.40748300
H	-3.52521000	-2.35363600	0.06527100
C	-0.71062700	-2.39244000	-0.72687800
H	-1.02364600	-3.42569600	-0.58643800
H	-0.82603400	-2.11798400	-1.77051400
C	0.74591200	-2.19997400	-0.28235900
O	0.91332700	-1.97052600	0.94077100
O	1.61324400	-2.26579400	-1.18120100
H	3.06971300	-1.74597000	-0.88732400
N	-1.58780900	-1.49737800	0.08710100
H	-1.49749100	-1.74119200	1.07406700
O	-3.34588800	0.29872100	1.70777400
O	-5.35393400	-0.33604800	0.12831800
H	-5.88561300	0.40007000	-0.19854200
O	-3.60576300	1.17901600	-0.74307400
H	-1.17667300	-0.52343500	0.02880000

DZC_4 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.48460586 u.a. ; Zero-point correction = 0.272615 u.a. ; G = -1783.264147 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.76321300	-0.01768600	0.24151100
C	2.62167000	1.08055800	-0.71229600
H	1.82396300	0.50271200	-1.16677300
H	3.16729400	1.63447400	-1.47086500
C	0.85072600	2.86209200	-0.31995800
H	0.67095200	3.70654500	0.34195300
H	1.12641800	3.23314600	-1.30315400
C	-0.41302800	1.99334000	-0.39247200
O	-0.28843900	0.82356300	0.04473400
O	-1.43103700	2.53764200	-0.86034900
H	-2.70046000	1.71527200	-0.72577300
N	1.98963500	2.05944500	0.23737700
H	2.71448400	2.67497700	0.60854100
O	3.95380300	-1.26953500	-0.68738200
O	2.86678300	-0.42442800	1.48328900
H	2.13502000	-1.10507800	1.29285800
O	4.98138300	0.72068600	0.61357500
H	1.62526500	1.50870600	1.02346500
P	-3.83944900	0.06768800	0.31709500
C	-3.02212500	-1.43430700	-0.36940600
H	-3.07054800	-1.41564700	-1.45494200
H	-3.52042700	-2.32990400	-0.00733900
C	-0.71170500	-2.35144600	-0.77087500
H	-1.03520200	-3.38444600	-0.65406200
H	-0.81263700	-2.05679300	-1.81052200
C	0.74117900	-2.18193400	-0.30604400
O	0.89765600	-1.97278800	0.92188600
O	1.61773200	-2.24451000	-1.19651100
H	3.07919900	-1.75289600	-0.87769000
N	-1.59219400	-1.46519200	0.04939500
H	-1.51030000	-1.72740200	1.03242400
O	-3.45046400	0.24928900	1.72965300
O	-5.39308000	-0.25044400	0.06194900
H	-5.85406600	-0.40829800	0.89475400
O	-3.59240600	1.20263700	-0.72321400
H	-1.17325300	-0.49189900	0.01590700

DZC_5 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.48802482 u.a. ; Zero-point correction = 0.275165 u.a. ; G = -1783.263323 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.64377200	0.08372700	-0.07281000
C	2.35869300	-0.82942300	-1.03095300
H	2.77031700	-1.00708600	-2.02155400
H	1.43366600	-0.27499400	-1.14015800
C	1.14452600	-2.13189700	0.77967800
H	1.11028900	-3.13371300	1.20395800
H	1.56564700	-1.44729800	1.50576900
C	-0.26705200	-1.70864500	0.37142600
O	-0.58430800	-1.85488000	-0.82980800
O	-0.98946200	-1.25088200	1.29567400
H	-2.63328100	-1.44850800	1.02723100
N	2.03716600	-2.17245400	-0.42942800
H	1.55103800	-2.72660600	-1.13845200
O	4.86535800	-0.73744600	-0.01837500
H	2.91612400	-2.64484100	-0.20413400
O	3.01996700	0.37501600	1.34717200
H	2.19368700	0.96631100	1.33163900
O	3.72786500	1.44058200	-0.87062900
P	-3.79247200	-0.18124000	-0.29217100
C	-3.27732500	1.36079400	0.58617900
H	-3.79710300	1.38161200	1.54065300
H	-3.58905100	2.22225200	0.00235000
C	-1.01193100	2.10136000	-0.26239000
H	-1.24397600	1.57635500	-1.18287700
H	-1.32766500	3.13791500	-0.35701700
C	0.48692900	2.02054700	0.03421300
O	0.79707800	1.63374800	1.19209500
O	1.24653000	2.31514400	-0.90981400
H	2.83989100	1.91515700	-0.87513300
N	-1.79887300	1.46826500	0.84925300
H	-1.62636900	2.00596600	1.69816900
O	-3.58870500	-1.33987800	0.77313100
H	-1.39643500	0.53365400	1.05567300
O	-2.68222600	-0.37832000	-1.40675400
H	-1.94454500	-1.02778100	-1.20964700
O	-5.16995200	-0.01718400	-0.76887400

DZC_6 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.48621382 u.a. ; Zero-point correction = 0.274844 u.a. ; G = -1783.261582 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.71219500	-0.07851000	-0.15672600
C	-2.47538500	1.02784900	0.64993000
H	-1.63993200	0.45401400	1.04114100
H	-2.94230000	1.58060600	1.46027600
C	-0.80322800	2.83539500	0.19345600
H	-0.63935600	3.67449800	-0.48139200
H	-1.06989900	3.20300800	1.17821100
C	0.47160900	1.98281700	0.23319300
O	0.58361000	1.12416100	-0.69643200
O	1.28662800	2.22772100	1.13467500
H	2.46248900	1.17260200	1.22553900
N	-1.93427800	2.01287300	-0.34307000
H	-2.69562300	2.60688600	-0.67516100
O	-3.83987300	-1.27011400	0.86143500
O	-2.93461800	-0.57633100	-1.44517700
H	-2.21106900	-1.25298800	-1.24885500
O	-4.94084000	0.66751800	-0.46809700
H	-1.57602300	1.49008500	-1.15231600
P	3.84904600	0.01875700	-0.08118000
C	3.08127100	-1.58711300	-0.53349800
H	3.40617300	-2.35639800	0.16119100
H	3.42178300	-1.85014000	-1.53162300
C	0.88339900	-2.03622000	0.68394800
H	1.23394600	-3.04471900	0.89343600
H	1.13121700	-1.38759000	1.51719800
C	-0.62423900	-2.04642500	0.39851500
O	-0.93852600	-2.07770800	-0.82113000
O	-1.38631400	-2.00011100	1.38491700
H	-2.94415100	-1.68415100	1.08229200
N	1.57908100	-1.53124600	-0.54231700
H	1.18846600	-2.05291900	-1.32951200
O	3.11350400	0.40103800	1.26234100
O	3.31162800	1.02615300	-1.20136200
H	2.35243500	1.21629200	-1.12276300
O	5.30880200	-0.11527100	-0.05131100
H	1.24289400	-0.55844400	-0.68349800

DZC_7 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.48541602 u.a. ; Zero-point correction = 0.273486 u.a. ; G = -1783.263789 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.43007100	0.35622200	0.11946900
C	2.41124800	-0.56323600	-1.10410200
H	2.88775100	-0.44998300	-2.07515200
H	1.39229300	-0.19985200	-1.16743500
C	1.56248300	-2.44115300	0.40724700
H	1.69586400	-3.51235800	0.54523700
H	1.94569800	-1.91566000	1.27433000
C	0.07886700	-2.12797000	0.19511700
O	-0.28180800	-1.89530300	-0.98871800
O	-0.62278400	-2.14110700	1.22377400
H	-1.98254900	-1.48648900	1.14554600
N	2.36526400	-2.03741900	-0.80123100
H	1.94933100	-2.50718300	-1.60746500
O	4.73082000	-0.32103900	0.26865600
H	3.32817100	-2.36626900	-0.69625200
O	2.57927800	0.38937800	1.45065400
H	1.66869300	0.80778700	1.33157100
O	3.45128800	1.80597900	-0.49649900
P	-3.50142900	-0.42026200	-0.16234900
C	-3.62064700	1.37387600	0.21999100
H	-4.32601200	1.48291900	1.03985000
H	-3.98090200	1.93929600	-0.63442600
C	-1.37163900	2.40102900	-0.42810900
H	-1.61179200	1.85011600	-1.33212500
H	-1.51206400	3.46324800	-0.59900900
C	0.07634600	2.08298000	-0.03844800
O	0.21798400	1.34374600	0.97301100
O	0.95723700	2.55151800	-0.78360200
H	2.52147500	2.18937100	-0.57972400
N	-2.29868400	1.94026500	0.66134800
H	-2.45323300	2.70886300	1.31149900
O	-2.85757900	-0.95372400	1.17522100
H	-1.76043600	1.23502600	1.19371100
O	-2.38508300	-0.46541200	-1.28291900
H	-1.60244100	-1.10033000	-1.15781700
O	-4.83628900	-0.92040800	-0.52459200

DZC_8 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.48621956 u.a. ; Zero-point correction = 0.274051 u.a. ; G = -1783.262870 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.56643300	-0.36064100	-0.24646700
C	-2.62196200	0.90293100	0.70803900
H	-1.71258200	0.45750600	1.10377900
H	-3.22047600	1.29364000	1.52604400
C	-1.19007500	2.94173000	0.42437500
H	-1.19018600	3.88559800	-0.11776300
H	-1.43117300	3.11660900	1.46722300
C	0.17917000	2.26311600	0.25732900
O	0.25284500	1.46819200	-0.71814900
O	1.06713900	2.55582200	1.07811500
H	2.20844500	1.48973100	1.08588500
N	-2.22316500	2.04095900	-0.18313700
H	-3.05169500	2.55825100	-0.47572300
O	-3.54157000	-1.61146400	0.70709500
O	-2.60749200	-0.63265700	-1.47979700
H	-1.76688900	-1.13545700	-1.24641100
O	-4.89106900	0.14828800	-0.63479200
H	-1.77853900	1.63875800	-1.02240800
P	3.55513400	0.25986300	-0.21397200
C	3.52583600	-1.57856800	-0.12219900
H	3.95101000	-1.93292500	0.81263900
H	4.13175000	-1.94388900	-0.94797100
C	1.24872100	-2.11449100	0.92073800
H	1.40059000	-3.01385200	1.50911800
H	1.51380500	-1.24556300	1.51539700
C	-0.20816100	-1.98118100	0.46307100
O	-0.38604100	-1.79949100	-0.76788400
O	-1.06473100	-2.02988100	1.37013100
H	-2.59835900	-1.87214000	0.97069800
N	2.14645800	-2.15069300	-0.28351000
H	2.21299500	-3.11304800	-0.61162400
O	2.83118800	0.68695400	1.12442100
O	2.54287200	0.54475600	-1.39934000
H	1.63954000	0.92270900	-1.13109500
O	4.94272800	0.69729500	-0.42339700
H	1.63008800	-1.64984300	-1.02403700

DZC_9 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.47475011 u.a. ; Zero-point correction = 0.271528 u.a. ; G = -1783.254692 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.60912300	0.14249600	0.69255400
C	2.29097800	-1.11641900	0.43457100
H	1.37113500	-0.87500900	0.95662700
H	2.65130500	-2.07971500	0.78766900
C	1.01130500	-2.27521700	-1.41237600
H	1.02879500	-2.35564600	-2.49480600
H	1.30796200	-3.21085900	-0.94743400
C	-0.38381700	-1.82824200	-0.94117000
O	-1.05913900	-1.15712200	-1.74887300
O	-0.69461100	-2.13575200	0.24088500
H	-2.02447000	-1.74674400	0.70510100
N	2.00915800	-1.22070000	-1.03041700
H	2.90126500	-1.37830400	-1.50378700
O	4.48134200	0.11013700	-0.49741300
O	4.34264900	-0.35275700	2.03426300
H	4.11716600	0.19230600	2.79725300
O	2.93033900	1.47256300	1.14858700
H	1.67273800	-0.27249400	-1.37210600
P	-3.60920200	-0.14213800	0.69258300
C	-2.29104300	1.11667300	0.43407100
H	-1.37121600	0.87544300	0.95623400
H	-2.65134300	2.08012200	0.78678000
C	-1.01111600	2.27460200	-1.41323500
H	-1.02843000	2.35455600	-2.49570300
H	-1.30775800	3.21047000	-0.94873500
C	0.38384500	1.82765400	-0.94158000
O	1.05948300	1.15663300	-1.74909900
O	0.69429800	2.13544700	0.24050300
H	2.02423100	1.74703300	0.70503900
N	-2.00908000	1.22032500	-1.03094100
H	-2.90110800	1.37774800	-1.50451200
O	-4.48154700	-0.11017800	-0.49730500
O	-4.34258200	0.35350200	2.03423000
H	-4.11714200	-0.19143800	2.79732100
O	-2.93033400	-1.47203200	1.14897100
H	-1.67258700	0.27197000	-1.37216900

DZC_{10} structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.48543818 u.a. ; Zero-point correction = 0.274345 u.a. ; G = -1783.262119 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.86445100	-0.00336300	0.18280700
C	-3.03864900	-1.64227200	0.03241100
H	-3.26116100	-2.03283400	-0.95670700
H	-3.42667200	-2.32952600	0.77796300
C	-0.71658600	-2.37720000	-0.72702000
H	-1.03276300	-3.41465500	-0.63757600
H	-0.87716000	-2.03379100	-1.74393200
C	0.75312400	-2.22126400	-0.30946600
O	0.93247100	-1.97423100	0.91178700
O	1.60993700	-2.32141200	-1.21034100
H	3.07866800	-1.75990400	-0.91553500
N	-1.54785100	-1.54113300	0.19437000
H	-1.26615200	-1.78262600	1.14763400
O	-3.37730800	0.72986500	-1.12643500
O	-3.13144800	0.70218200	1.41609200
H	-2.21180000	0.98255800	1.20874000
O	-5.30934900	-0.18058800	0.35756600
H	-1.22654700	-0.55815900	0.10145500
P	3.69047000	0.01147900	0.19361700
C	2.40554800	0.99967500	-0.68900000
H	1.57053500	0.38159600	-1.00473200
H	2.84348600	1.49288200	-1.55250600
C	0.76015600	2.87439700	-0.33536500
H	0.63710400	3.76454000	0.27966300
H	1.02158900	3.17070300	-1.34597900
C	-0.54744600	2.07571200	-0.31179500
O	-0.57709200	1.08463200	0.48231000
O	-1.46356600	2.48096100	-1.04024900
H	-2.69421900	1.46807800	-1.05765400
N	1.87357800	2.05294300	0.23837800
H	2.64626700	2.64867700	0.54139000
O	3.92203700	-1.22527800	-0.74618400
O	2.92594500	-0.45671200	1.49886500
H	2.19632600	-1.13525500	1.32437900
O	4.85956200	0.86093800	0.47265100
H	1.50574200	1.57615500	1.07072200

DZC_{12} structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.48432344 u.a. ; Zero-point correction = 0.274976 u.a. ; G = -1783.259247 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.65471500	0.02353800	0.16531400
C	2.31292000	0.94208500	-0.70565900
H	1.44658700	0.31231800	-0.88183800
H	2.68489600	1.33952300	-1.64577800
C	0.76530600	2.91073200	-0.43621800
H	0.71376600	3.85383200	0.10533100
H	0.98606500	3.10663900	-1.48013100
C	-0.56866600	2.16955300	-0.27089600
O	-0.60355400	1.30092500	0.64531000
O	-1.48905300	2.50174500	-1.03876700
H	-2.69714900	1.48157200	-1.04463900
N	1.87049800	2.08832100	0.15399300
H	2.68424100	2.66480800	0.37720000
O	3.86646900	-1.26127800	-0.71557400
O	2.96548100	-0.38448900	1.52968900
H	2.15349500	-0.96666900	1.37724900
O	4.82067800	0.90664700	0.32972500
H	1.51114500	1.69781200	1.03405400
P	-3.82057100	-0.01954100	0.20094100
C	-2.99213800	-1.65579800	0.01636000
H	-3.41829300	-2.18044900	-0.83487900
H	-3.11805000	-2.25169800	0.91600700
C	-0.69938900	-2.65654200	-0.57451000
H	-1.05534700	-3.50136500	0.01110000
H	-0.79720200	-2.86939500	-1.63329700
C	0.74682800	-2.31937600	-0.16387700
O	0.81711300	-1.64305100	0.89959600
O	1.67571300	-2.69889900	-0.89716900
H	3.07885200	-1.89077600	-0.74315400
N	-1.52969600	-1.45705300	-0.22239300
H	-1.06544300	-1.05370800	0.60700100
O	-3.33413400	0.69891700	-1.12609900
O	-3.05924500	0.67622400	1.40667400
H	-2.13678000	0.98390500	1.17977400
O	-5.26357100	-0.19615700	0.39243700
H	-1.42490900	-0.75377400	-0.95678700

DZP_9 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.47427923 u.a. ; Zero-point correction = 0.271818 u.a. ; G = -1783.255085 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.63416700	0.05955800	0.53029000
C	2.06390300	-0.94582300	0.55571400
H	1.19704600	-0.39324000	0.90394300
H	2.21452200	-1.81999900	1.18282800
C	0.88981500	-2.57954800	-0.97629400
H	0.98138400	-2.97575400	-1.98561300
H	1.16815000	-3.33672300	-0.25150600
C	-0.53669400	-2.07212400	-0.77787000
O	-0.92572400	-1.14131500	-1.47158700
O	-1.20755200	-2.67345100	0.14756000
H	-2.15264900	-2.19177600	0.31758600
N	1.81902400	-1.41846400	-0.84739800
H	2.75492400	-1.60763700	-1.23566100
O	4.36929300	-0.49946700	-0.63943800
O	4.31736300	-0.39549100	1.93008400
H	4.37925000	0.35502900	2.53184700
O	3.32214000	1.53616200	0.66784100
H	1.44947300	-0.61206100	-1.37811400
P	-3.63415400	-0.05959200	0.53040700
C	-2.06387300	0.94575200	0.55579600
H	-1.19699000	0.39309600	0.90384000
H	-2.21439900	1.81983700	1.18306200
C	-0.88981600	2.57962100	-0.97604800
H	-0.98127400	2.97590900	-1.98534800
H	-1.16813300	3.33676900	-0.25122500
C	0.53660500	2.07201800	-0.77749400
O	0.92571900	1.14141900	-1.47144500
O	1.20755800	2.67346800	0.14778600
H	2.15266800	2.19180600	0.31777400
N	-1.81911700	1.41860400	-0.84726500
H	-2.75503700	1.60790700	-1.23542400
O	-4.36937800	0.49955500	-0.63920200
O	-4.31721600	0.39532800	1.93030600
H	-4.37907300	-0.35525400	2.53199400
O	-3.32212400	-1.53621000	0.66778600
H	-1.44966200	0.61225700	-1.37814000

AC_9 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.47409896 u.a. ; Zero-point correction = 0.270993 u.a. ; G = -1783.255090 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.62097700	-0.04734400	0.55365500
C	-2.07846800	0.99253800	0.50772700
H	-1.20405600	0.48002000	0.89638500
H	-2.24803900	1.89881400	1.08257000
C	-0.87803600	2.53238200	-1.08852800
H	-0.92235800	2.84701500	-2.12918100
H	-1.18595400	3.34227200	-0.43620700
C	0.54102300	2.03764600	-0.77453500
O	0.90735100	1.02767700	-1.41051000
O	1.19432000	2.66839000	0.09385200
H	2.36937300	1.99731100	0.49131800
N	-1.82363000	1.38768800	-0.91539400
H	-2.74783500	1.56699100	-1.32767300
O	-4.38688400	0.40515200	-0.63968500
O	-4.30629500	0.47602100	1.93057700
H	-4.33604700	-0.23600800	2.57939700
O	-3.26355200	-1.50370500	0.79430200
H	-1.45034800	0.55605800	-1.40248300
P	3.61444500	0.06458200	0.52973600
C	2.13614200	-1.05126400	0.54159600
H	1.26594400	-0.59061600	0.99911500
H	2.38925500	-1.95742100	1.08585100
C	0.86742500	-2.56702900	-1.02990200
H	0.93049700	-2.90622900	-2.06079100
H	1.16360600	-3.36102500	-0.35222300
C	-0.55459100	-2.06908700	-0.77043600
O	-1.02212200	-1.22386900	-1.52086100
O	-1.13079900	-2.58214100	0.26679300
H	-2.09324300	-2.11736100	0.45147300
N	1.80998000	-1.41565800	-0.87276900
H	2.69913000	-1.58716200	-1.35211300
O	4.30956900	-0.20142400	-0.74781900
O	4.43271800	-0.43613200	1.82087300
H	4.47494900	0.23806400	2.50928400
O	3.20001500	1.50269000	0.93999200
H	1.41313300	-0.54588400	-1.30409200

NZP_1 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.47493189 u.a. ; Zero-point correction = 0.272603 u.a. ; G = -1783.252879 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-2.46753700	0.61485900	0.14268700
C	-3.68782700	-0.75113700	0.14542900
H	-4.54674400	-0.40708200	-0.43026000
H	-4.02190600	-0.88093300	1.17528900
C	-2.14408000	-2.73561500	0.24451900
H	-2.16009400	-2.55438800	1.31773600
H	-2.28424100	-3.81193100	0.11105500
C	-0.73716000	-2.43527800	-0.26746500
O	-0.52052300	-1.73510600	-1.25589400
O	0.20282000	-3.02505900	0.41452700
H	1.14102000	-2.73910600	0.09237000
N	-3.23110100	-2.02121100	-0.39987400
H	-3.11458800	-1.98371200	-1.40259300
O	-1.71305000	0.55079900	-1.25413400
H	-1.28562400	-0.34138600	-1.39446200
O	-1.43174800	0.09074600	1.25656700
H	-0.85246900	0.81958700	1.54879900
O	-2.93447600	2.01292800	0.38754600
P	3.04238700	-0.85008800	0.01270300
C	1.79378700	0.34586300	-0.64507500
H	0.81223600	0.21501600	-0.20988000
H	1.73279600	0.27950000	-1.72711200
C	1.43244900	2.85979100	-0.71943300
H	1.97015300	3.79558100	-0.56887100
H	1.19057200	2.74531500	-1.77131800
C	0.17563500	2.83905500	0.13783500
O	0.19795400	2.29894000	1.23212600
O	-0.85684700	3.40370000	-0.42265600
H	-1.71469000	3.06545300	-0.00056100
N	2.29886900	1.72386100	-0.28782100
H	3.24779400	1.79961300	-0.66693400
O	2.53910600	-2.24802900	-0.21730700
O	2.92536400	-0.49344000	1.61336600
H	2.37441500	-1.13478600	2.07593000
O	4.34457400	-0.32406000	-0.47589700
H	2.39203500	1.75572100	0.73302600

DN_1 structure in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.46921447 u.a. ; Zero-point correction = 0.270550 u.a. ; G = -1783.249786 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	2.41217200	-1.19988600	0.69127400
C	3.91149400	-0.25755600	0.19366900
H	4.62171200	-1.01170700	-0.14698900
H	4.32365300	0.15811800	1.11576100
C	3.01428700	1.95711300	-0.53662100
H	3.10451100	2.23737800	0.51196200
H	3.39240700	2.80551600	-1.11472400
C	1.54059000	1.83821200	-0.88399200
O	1.07511000	0.91466600	-1.53337500
O	0.81217200	2.85154200	-0.45298900
H	-0.13493200	2.64817900	-0.62453100
N	3.80967200	0.78127100	-0.81586200
H	3.60793400	0.40074700	-1.72998900
O	1.59349700	-1.51968600	-0.63919300
H	1.35143500	-0.69676200	-1.13788300
O	1.43574800	-0.07019800	1.39080900
H	1.60019300	-0.02725700	2.34315800
O	2.66873300	-2.36338500	1.55158400
P	-2.26755600	1.15987200	0.76452000
C	-3.86613800	0.33043200	0.42942800
H	-4.57141000	1.12921100	0.20038800
H	-4.18891900	-0.10858000	1.37508300
C	-3.16745800	-1.89314900	-0.46237000
H	-3.18828900	-2.21160400	0.57793900
H	-3.63120900	-2.69515500	-1.04463500
C	-1.71907900	-1.82831100	-0.92035100
O	-1.27545100	-0.96684500	-1.65822400
O	-0.98675800	-2.84161800	-0.47261500
H	-0.05314600	-2.67700200	-0.70659800
N	-3.92880500	-0.67150200	-0.62678800
H	-3.78129200	-0.26309100	-1.53991500
O	-1.65684200	1.56579600	-0.68066100
H	-1.43060100	0.77085500	-1.21370200
O	-1.38711200	-0.09474400	1.24301400
H	-0.42118400	0.03221600	1.25573100
O	-2.30639300	2.33201400	1.65440100

7- Structures and energetics of Glyph dimers in aqueous solution, at SMD-B3LYP-D3/6-311++G(2d,2p) level.

DZC_1 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54799641 u.a. ; Zero-point correction = 0.272516 u.a. ; G = -1783.325128 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.45915700	-0.11049900	0.26578200
C	2.40013300	0.96844600	-0.75932200
H	1.48387800	0.42394400	-0.97956000
H	2.90505700	1.21680700	-1.68823800
C	0.90876000	2.97476900	-0.71272100
H	0.94324600	4.00967700	-0.37918100
H	1.03825800	2.93840900	-1.78922300
C	-0.42325800	2.36528300	-0.28772600
O	-0.41308200	1.64325300	0.74236100
O	-1.41917200	2.66414700	-0.99505700
H	-2.73595300	1.92895700	-0.73775300
N	2.03884400	2.24027100	-0.06144200
H	2.86209600	2.84171200	-0.00720700
O	3.61326400	-1.40876500	-0.61127800
O	2.56411500	-0.45668300	1.52418300
H	1.71201900	-0.94504100	1.25421200
O	4.75080700	0.51610600	0.64372700
H	1.73746700	2.02455800	0.89514700
P	-3.45916600	0.11049900	0.26587400
C	-2.40037600	-0.96857200	-0.75933300
H	-1.48416700	-0.42408300	-0.97979800
H	-2.90547600	-1.21702800	-1.68813000
C	-0.90876800	-2.97470200	-0.71268100
H	-0.94320400	-4.00962200	-0.37917200
H	-1.03829800	-2.93833900	-1.78917800
C	0.42326200	-2.36513100	-0.28776200
O	0.41321800	-1.64327600	0.74244400
O	1.41919100	-2.66416700	-0.99501700
H	2.73595300	-1.92909800	-0.73763600
N	-2.03891100	-2.24030600	-0.06139400
H	-2.86210200	-2.84182100	-0.00705700
O	-3.61327600	1.40870800	-0.61127700
O	-2.56390900	0.45664700	1.52412100
H	-1.71178500	0.94492000	1.25404100
O	-4.75083300	-0.51594400	0.64402700
H	-1.73747300	-2.02448000	0.89515000

DZC_5 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54645155 u.a. ; Zero-point correction = 0.272416 u.a. ; G = -1783.324892 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.67725100	0.11409300	-0.08074700
C	2.47842700	-0.87953400	-1.04401300
H	2.93145100	-1.06339400	-2.01534000
H	1.57070000	-0.30518400	-1.19459600
C	1.16405500	-2.19006400	0.70595500
H	1.10352700	-3.20760500	1.08489400
H	1.58388000	-1.55502000	1.47708000
C	-0.23633000	-1.72314300	0.34118000
O	-0.51904600	-1.54995100	-0.87106900
O	-1.01493100	-1.56827700	1.32080500
H	-2.54945300	-1.46447500	0.98537900
N	2.09601000	-2.21045000	-0.46830500
H	1.64772600	-2.74461800	-1.21637000
O	5.02890600	-0.49589200	-0.01707800
H	2.94026300	-2.72208700	-0.20244700
O	3.05918800	0.35739900	1.35019000
H	2.14459900	0.81993100	1.31558200
O	3.63778300	1.48753800	-0.86644100
P	-3.78920500	-0.18175400	-0.29780500
C	-3.35976000	1.39039200	0.53841500
H	-3.93338300	1.43196700	1.46038600
H	-3.64815500	2.22624900	-0.09253500
C	-1.05958000	2.10949000	-0.20675100
H	-1.28009400	1.57211100	-1.12338700
H	-1.32638100	3.15424100	-0.33662500
C	0.42019400	1.96546400	0.10779900
O	0.73182100	1.38723400	1.18326400
O	1.20697900	2.41379100	-0.76416500
H	2.72067000	1.92186200	-0.81380400
N	-1.90720000	1.54345900	0.89021500
H	-1.83037000	2.16052400	1.70014500
O	-3.53264300	-1.32111200	0.76811300
H	-1.49615800	0.65222700	1.19445400
O	-2.74715300	-0.38737600	-1.46588500
H	-1.88125700	-0.86127000	-1.20803000
O	-5.19864900	-0.11925800	-0.75591000

DZC_8 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54483243 u.a. ; Zero-point correction = 0.272011 u.a. ; G = -1783.323529 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.65214300	-0.24573700	-0.19722200
C	-2.61800500	0.99747900	0.65559800
H	-1.73718000	0.48317800	1.03132900
H	-3.16328300	1.42468200	1.49192800
C	-1.04125500	2.90065200	0.35891700
H	-0.96091100	3.83391800	-0.19504900
H	-1.27638000	3.11308500	1.39570500
C	0.27305200	2.13756700	0.22319900
O	0.36684700	1.32760800	-0.73558400
O	1.16665300	2.40296700	1.06724400
H	2.32546100	1.42606900	1.08689300
N	-2.16150000	2.10660800	-0.23796400
H	-2.94690500	2.72323100	-0.45202900
O	-3.63604800	-1.46404700	0.80401000
O	-2.81488900	-0.64506400	-1.48100100
H	-1.95529900	-1.13064700	-1.25115600
O	-5.01449500	0.23023800	-0.54098500
H	-1.81902900	1.70859300	-1.11954400
P	3.67904000	0.16541900	-0.17263600
C	3.43592500	-1.64683500	-0.11582900
H	3.78748500	-2.04473900	0.83209900
H	4.03121100	-2.07073000	-0.92022600
C	1.10612100	-1.96746400	0.84888500
H	1.32036100	-2.77646100	1.53870600
H	1.29809800	-1.01772100	1.34237300
C	-0.34931600	-1.97974000	0.40192500
O	-0.58336900	-1.79725500	-0.82144700
O	-1.20020100	-2.12052900	1.31864500
H	-2.68558400	-1.79040800	1.00125500
N	2.02032400	-2.08761400	-0.32997300
H	2.02730500	-3.06384300	-0.63067200
O	3.08271100	0.73457000	1.16930800
O	2.76868400	0.68065100	-1.35774900
H	1.80706600	0.91178200	-1.10134800
O	5.12633700	0.43288900	-0.37987900
H	1.59538800	-1.56434500	-1.10350500

DZC_{10} structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54308139 u.a. ; Zero-point correction = 0.272831 u.a. ; G = -1783.320694 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.88282600	-0.08426800	0.13125200
C	-2.89797300	-1.52981800	-0.43854800
H	-2.87762600	-1.52663400	-1.52450600
H	-3.37187900	-2.44203400	-0.08937800
C	-0.57856900	-2.47265800	-0.62802500
H	-0.93069300	-3.48459400	-0.44034000
H	-0.61919500	-2.26797900	-1.69269200
C	0.84410700	-2.29392800	-0.11088900
O	0.97256600	-1.75036400	1.01947100
O	1.77068500	-2.68039500	-0.86691400
H	3.09852300	-1.78792400	-0.85110100
N	-1.49105000	-1.51384000	0.06612600
H	-1.48784400	-1.72253800	1.06679800
O	-3.69561800	1.04430500	-0.94675600
O	-3.16688600	0.40971900	1.46718900
H	-2.27886500	0.82351200	1.29512900
O	-5.29931300	-0.46529400	0.34569600
H	-1.08446000	-0.56850200	0.00162900
P	3.69833300	0.09320000	0.09846100
C	2.34733800	1.05351100	-0.67468100
H	1.52281600	0.38800700	-0.91633500
H	2.71419300	1.51418200	-1.58764800
C	0.67016700	2.88181900	-0.35565400
H	0.57542900	3.81719200	0.19265300
H	0.87887100	3.09685400	-1.39784000
C	-0.62730700	2.09930900	-0.19778000
O	-0.68170300	1.22705500	0.71022500
O	-1.55890200	2.42219300	-0.97762100
H	-2.81298300	1.57625100	-0.91836900
N	1.82932900	2.13174300	0.22268400
H	2.58142500	2.79099100	0.43326800
O	3.87514200	-1.13870500	-0.87411500
O	3.11078100	-0.42743000	1.46834400
H	2.28224400	-1.01288900	1.33906700
O	4.94113000	0.88474000	0.27330600
H	1.51984700	1.71079000	1.10516200

DZC_{11} structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54270978 u.a. ; Zero-point correction = 0.272879 u.a. ; G = -1783.320221 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.48111800	-0.05102400	0.39880900
C	2.46250500	0.93301700	-0.76053100
H	1.59748300	0.33797000	-1.04372400
H	3.03718900	1.17301100	-1.65015500
C	0.82508600	2.81971700	-0.90131800
H	0.78378000	3.87917400	-0.65760600
H	0.99629800	2.70304400	-1.96582000
C	-0.48211900	2.16536900	-0.46578000
O	-0.46995000	1.56508600	0.64190200
O	-1.46485500	2.29043000	-1.23807900
H	-2.74981700	1.46472300	-0.90195000
N	1.97269200	2.21176900	-0.15137400
H	2.74568800	2.87557900	-0.09160300
O	3.74048700	-1.40213100	-0.37790900
O	2.51825900	-0.35049800	1.61676900
H	1.67792200	-0.84396200	1.32196200
O	4.73114300	0.63435700	0.80936700
H	1.63391800	2.02583200	0.79961300
P	-3.59326200	-0.05904400	0.49553000
C	-2.74469700	-1.58591200	-0.06452100
H	-3.44794400	-2.23589800	-0.57630700
H	-2.33426300	-2.09682800	0.80103400
C	-0.64918800	-2.39179300	-1.25662800
H	-1.14781600	-3.34599900	-1.10898200
H	-0.31642200	-2.32028200	-2.28706600
C	0.54932000	-2.25035500	-0.32387000
O	0.41075100	-1.49261100	0.67193200
O	1.58988900	-2.87575100	-0.65117700
H	2.93656200	-2.01010000	-0.44271100
N	-1.62564500	-1.27705300	-1.00984300
H	-1.08236800	-0.49525400	-0.63309900
O	-3.59180100	0.90223700	-0.76081200
O	-2.64587500	0.58208800	1.58390300
H	-1.78170000	0.97774800	1.21154400
O	-4.94750900	-0.37265000	1.01286000
H	-2.02543000	-0.96544700	-1.89586300

DZC_{12} structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54401029 u.a. ; Zero-point correction = 0.272845 u.a. ; G = -1783.321449 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.67494400	0.06797500	0.10028200
C	2.32647500	1.03350800	-0.66920600
H	1.48710300	0.37396700	-0.87558300
H	2.68268100	1.46361700	-1.60100400
C	0.69698600	2.90687000	-0.38332200
H	0.62302800	3.85358800	0.14854600
H	0.90873600	3.09462000	-1.42951300
C	-0.61387400	2.15016600	-0.19797000
O	-0.72327500	1.43299700	0.83049400
O	-1.49392800	2.33872500	-1.07692900
H	-2.72213200	1.44311500	-1.05221800
N	1.84173000	2.14403000	0.20857100
H	2.61028900	2.78916600	0.40218300
O	3.82892100	-1.17368600	-0.86429900
O	3.09020300	-0.43638400	1.47740400
H	2.24019500	-0.98997700	1.34378600
O	4.92802400	0.84657100	0.25798700
H	1.52685700	1.75184400	1.10270700
P	-3.84313100	-0.06959000	0.14935900
C	-2.94205000	-1.63473300	-0.14257300
H	-3.26384800	-2.06524300	-1.08693200
H	-3.15395300	-2.32757100	0.66690700
C	-0.64053800	-2.62417200	-0.50594300
H	-1.02832500	-3.45832400	0.07481600
H	-0.71899200	-2.83691500	-1.56528700
C	0.79836000	-2.33233700	-0.07956300
O	0.91921600	-1.69098300	1.00179000
O	1.72670900	-2.73024100	-0.82316600
H	3.05254700	-1.82125500	-0.82323200
N	-1.46761300	-1.41476200	-0.19165600
H	-1.13292400	-1.05453500	0.70881400
O	-3.54628700	0.83104000	-1.10915900
O	-3.13336500	0.60479500	1.39481700
H	-2.21123500	0.97708100	1.19821800
O	-5.28372500	-0.34569000	0.37030300
H	-1.24813600	-0.68679100	-0.87770700

DZC_{13} structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.53962415 u.a. ; Zero-point correction = 0.271156 u.a. ; G = -1783.319833 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.78102400	0.01791300	0.22400900
C	2.58326900	1.04950000	-0.69971600
H	1.76885600	0.41503000	-1.03867600
H	3.07278500	1.49283600	-1.56175400
C	0.81321000	2.80411400	-0.50086200
H	0.66842400	3.77039200	-0.02279600
H	1.01717800	2.95440700	-1.55591000
C	-0.43689300	1.95511900	-0.28894500
O	-0.37790700	1.03752000	0.56045400
O	-1.44244200	2.27714600	-0.98095300
H	-2.73020900	1.69216000	-0.54435300
N	1.99755900	2.14337800	0.13489800
H	2.71524300	2.84108000	0.33939500
O	3.97629400	-1.24175700	-0.70775600
O	3.01192300	-0.43926700	1.52792000
H	2.20854400	-1.03031900	1.32972900
O	5.04853700	0.72354900	0.53549200
H	1.67409000	1.74185900	1.02184700
P	-3.91730200	-0.02067500	0.32767500
C	-2.90462200	-1.21875500	-0.61422000
H	-2.78991600	-0.87069700	-1.63714800
H	-3.40963900	-2.18077600	-0.61503300
C	-0.61368200	-2.16706100	-0.86226900
H	-0.98477300	-3.18553100	-0.95408200
H	-0.59303000	-1.70709300	-1.84544100
C	0.78938700	-2.16003300	-0.27147100
O	0.91336800	-1.81773900	0.93377500
O	1.71957900	-2.47680000	-1.05937900
H	3.12853500	-1.79065700	-0.82296800
N	-1.55330000	-1.38471500	-0.00710800
H	-1.64019200	-1.83755800	0.90408100
O	-3.68349600	-0.16847900	1.78747200
O	-5.42951200	-0.37643600	-0.04482000
H	-5.72248900	-0.00110500	-0.88726400
O	-3.69972100	1.39450000	-0.30789700
H	-1.12605000	-0.44842200	0.19101900

DZP_1 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54845414 u.a. ; Zero-point correction = 0.274414 u.a. ; G = -1783.324946 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.53202500	-0.18200400	-0.20338000
C	-2.40895100	0.89710900	0.76573200
H	-1.47386900	0.36494500	0.91930700
H	-2.84816600	1.13858200	1.72919300
C	-0.97255900	2.94528100	0.66311900
H	-1.00979200	3.97010200	0.29791800
H	-1.08022800	2.94552900	1.74274400
C	0.33956400	2.32454700	0.23337500
O	0.39783500	1.59481500	-0.74867000
O	1.33983100	2.67132200	0.99603300
H	2.22534700	2.19931400	0.73971200
N	-2.10311100	2.18279300	0.05788700
H	-2.94033500	2.76770000	0.04416400
O	-3.55040400	-1.50721100	0.54238300
O	-2.71871300	-0.35096100	-1.59211300
H	-1.88436100	-0.84521900	-1.42860900
O	-4.82091000	0.51727000	-0.50465500
H	-1.85811300	1.97473100	-0.91579800
P	3.53189700	0.18212700	-0.20346900
C	2.40889900	-0.89737900	0.76532000
H	1.47374700	-0.36521200	0.91843200
H	2.84779400	-1.13865100	1.72897800
C	0.97263200	-2.94548900	0.66299700
H	1.00955400	-3.97034100	0.29784400
H	1.08039600	-2.94582400	1.74263300
C	-0.33935400	-2.32454400	0.23336700
O	-0.39774700	-1.59473500	-0.74852400
O	-1.33972700	-2.67139300	0.99601700
H	-2.22482000	-2.19948900	0.73944400
N	2.10344700	-2.18332900	0.05783900
H	2.94065700	-2.76831500	0.04513400
O	3.54995800	1.50692500	0.54310300
O	2.71852400	0.35147500	-1.59204200
H	1.88352700	0.84468700	-1.42820100
O	4.82105500	-0.51648000	-0.50496900
H	1.85922700	-1.97601500	-0.91619200

DZP_2 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54605514 u.a. ; Zero-point correction = 0.273888 u.a. ; G = -1783.323189 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.49771100	-0.11947900	0.27496900
C	2.42814600	0.98835100	-0.72534700
H	1.51527700	0.44716600	-0.96376000
H	2.92504700	1.28711500	-1.64321400
C	0.93106200	2.99153700	-0.59877600
H	0.94968900	4.01235600	-0.22126600
H	1.06161300	3.00492000	-1.67570000
C	-0.38224500	2.35185600	-0.20208100
O	-0.45047900	1.61192800	0.77192600
O	-1.37177200	2.69354300	-0.98021000
H	-2.25350000	2.20151500	-0.74851700
N	2.05495000	2.23260500	0.02354000
H	2.87573300	2.83596900	0.09473100
O	3.74805500	-1.32542700	-0.76057500
O	2.62398000	-0.61212000	1.42551900
H	1.35578900	-1.23996000	1.02043500
O	4.79951600	0.54321500	0.59965500
H	1.77156100	1.98273400	0.97710500
P	-3.53683200	0.15650700	0.16524000
C	-2.35705000	-0.90364000	-0.75517400
H	-1.42260600	-0.36120000	-0.87151500
H	-2.75440900	-1.15310700	-1.73475600
C	-0.94588100	-2.97525000	-0.61619800
H	-0.99845500	-3.98698500	-0.21745100
H	-1.06796100	-3.01169100	-1.69342300
C	0.41150000	-2.40442300	-0.26587500
O	0.41529100	-1.63537200	0.78712300
O	1.38783400	-2.70994800	-0.94057200
H	2.94783000	-1.89840800	-0.82860200
N	-2.07082600	-2.18382200	-0.02976700
H	-2.91480700	-2.76029400	-0.02581300
O	-3.56337100	1.47676500	-0.58874500
O	-2.77373400	0.35181400	1.57916700
H	-1.94088800	0.85476600	1.43641200
O	-4.81731100	-0.57319700	0.42783600
H	-1.84923700	-1.97199200	0.94751200

DZP_3 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54605521 u.a. ; Zero-point correction = 0.273898 u.a. ; G = -1783.323173 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.49851600	-0.11948200	0.27505700
C	2.42878000	0.98817300	-0.72527200
H	1.51629400	0.44660600	-0.96434100
H	2.92606600	1.28741000	-1.64278900
C	0.93081800	2.99068900	-0.59884800
H	0.94932600	4.01161000	-0.22162400
H	1.06132600	3.00374800	-1.67577700
C	-0.38242300	2.35095500	-0.20202900
O	-0.45077700	1.61146600	0.77226500
O	-1.37185100	2.69230600	-0.98048700
H	-2.25380200	2.20085900	-0.74841000
N	2.05478000	2.23209200	0.02373200
H	2.87533700	2.83570500	0.09539400
O	3.74870100	-1.32545900	-0.76060700
O	2.62471400	-0.61227800	1.42543100
H	1.35610800	-1.23898000	1.02034700
O	4.80036500	0.54312200	0.59965100
H	1.77113900	1.98192800	0.97715000
P	-3.53746800	0.15636400	0.16518900
C	-2.35783900	-0.90386000	-0.75533800
H	-1.42360200	-0.36119800	-0.87261100
H	-2.75576000	-1.15387900	-1.73455100
C	-0.94557900	-2.97473100	-0.61574400
H	-0.99761000	-3.98625100	-0.21640400
H	-1.06780400	-3.01180700	-1.69292900
C	0.41155100	-2.40296100	-0.26608900
O	0.41542700	-1.63410600	0.78708500
O	1.38766700	-2.70792900	-0.94132400
H	2.94816600	-1.89804000	-0.82866100
N	-2.07075700	-2.18354200	-0.02944100
H	-2.91442100	-2.76046100	-0.02490400
O	-3.56385900	1.47679600	-0.58850700
O	-2.77417300	0.35108400	1.57909300
H	-1.94143100	0.85418700	1.43652500
O	-4.81821900	-0.57288200	0.42766300
H	-1.84903600	-1.97106700	0.94769600

DZP_4 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54366255 u.a. ; Zero-point correction = 0.273835 u.a. ; G = -1783.322054 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.50598500	-0.09331500	0.20404600
C	2.35172000	1.00747600	-0.70560200
H	1.43100400	0.45996300	-0.89419400
H	2.78415200	1.33004400	-1.64775400
C	0.90322000	3.04547000	-0.48715600
H	0.93656700	4.03624000	-0.03697200
H	1.05478000	3.13677400	-1.55720500
C	-0.45848400	2.45061500	-0.19911200
O	-0.48780700	1.65843200	0.83670000
O	-1.41654900	2.76147000	-0.89696700
H	-2.94348200	1.87797000	-0.88577700
N	2.01723800	2.23277500	0.09102900
H	2.85263500	2.81771900	0.15876900
O	3.72423900	-1.27407100	-0.86668300
O	2.71452000	-0.62672600	1.39499400
H	1.43350900	-1.26069100	1.03890700
O	4.80697400	0.59994600	0.46162200
H	1.76318000	1.96176100	1.04583100
P	-3.50567800	0.09314000	0.20381700
C	-2.35162700	-1.00801200	-0.70569900
H	-1.43076100	-0.46084600	-0.89450800
H	-2.78418900	-1.33075000	-1.64773500
C	-0.90330300	-3.04601800	-0.48635800
H	-0.93573000	-4.03610100	-0.03458600
H	-1.05542300	-3.13905100	-1.55618300
C	0.45811200	-2.44990400	-0.19961000
O	0.48728500	-1.65791300	0.83641500
O	1.41605500	-2.75986700	-0.89801800
H	2.94413600	-1.87764000	-0.88624800
N	-2.01753400	-2.23323500	0.09124000
H	-2.85296900	-2.81818100	0.15852100
O	-3.72339500	1.27410400	-0.86672000
O	-2.71446200	0.62601700	1.39517200
H	-1.43372200	1.26085500	1.03958200
O	-4.80686500	-0.59986600	0.46108000
H	-1.76401500	-1.96219800	1.04617200

DZP_5 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54542468 u.a. ; Zero-point correction = 0.274471 u.a. ; G = -1783.321482 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.68450100	0.18897500	0.07087700
C	2.63075100	-0.77711600	-1.08870700
H	3.18888300	-0.90833700	-2.01177400
H	1.72538100	-0.22161200	-1.30682300
C	1.31367600	-2.22807600	0.54989400
H	1.26950300	-3.26808900	0.86615000
H	1.71816300	-1.63245700	1.36146800
C	-0.08542800	-1.77234800	0.21218100
O	-0.43107500	-1.48445000	-0.92760300
O	-0.84939500	-1.76030400	1.27068200
H	-1.82912200	-1.50618500	1.06323200
N	2.23248000	-2.14922700	-0.62397400
H	1.78804000	-2.62333900	-1.41456300
O	5.03987400	-0.43342100	0.19410400
H	3.07677700	-2.68037900	-0.39902000
O	2.89999200	0.45346100	1.35176600
H	1.54664000	0.97526900	1.19725300
O	3.79670600	1.56439500	-0.76618600
P	-3.82741200	-0.27226100	-0.16419600
C	-3.50173200	1.45748900	0.36514900
H	-4.13097700	1.64993900	1.22988600
H	-3.75073800	2.16715500	-0.41750500
C	-1.16501600	2.06716600	-0.33830300
H	-1.37060400	1.41202100	-1.18161500
H	-1.37750700	3.09058700	-0.62888700
C	0.29773600	1.91543300	0.00348500
O	0.53792200	1.23915200	1.09326200
O	1.14037400	2.37484400	-0.75827400
H	2.92477200	2.01876900	-0.76173800
N	-2.07623100	1.69201200	0.78588500
H	-2.05083100	2.43680900	1.48441100
O	-3.28263400	-1.17070700	0.93839400
H	-1.71347600	0.85517500	1.25195600
O	-2.93336800	-0.48941100	-1.49003100
H	-2.04468100	-0.86505500	-1.28663600
O	-5.27592500	-0.34678000	-0.53131200

DZP_6 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54674527 u.a. ; Zero-point correction = 0.275854 u.a. ; G = -1783.320942 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.69266300	0.25023700	-0.02262400
C	2.58170600	-0.74869500	-1.09741200
H	3.07599900	-0.84023000	-2.06158200
H	1.64597500	-0.22470500	-1.24853900
C	1.33969200	-2.27219200	0.52930000
H	1.29587000	-3.32396700	0.80541500
H	1.74554200	-1.70969300	1.36163900
C	-0.06135700	-1.80625800	0.21005000
O	-0.43261400	-1.55941700	-0.93153100
O	-0.79868100	-1.73811600	1.28526500
H	-1.78292700	-1.48774300	1.08842600
N	2.25885000	-2.14536100	-0.64140600
H	1.84054500	-2.63876100	-1.43391800
O	5.04425500	-0.38801700	0.06801400
H	3.12766200	-2.63438600	-0.41376200
O	3.03119900	0.20429500	1.45195000
H	2.18483200	0.70228300	1.46398300
O	3.54344300	1.65749800	-0.58181100
P	-3.80748800	-0.29882500	-0.14053700
C	-3.50593800	1.44860300	0.34009800
H	-4.13713100	1.65652800	1.19975400
H	-3.76523600	2.13261700	-0.46188700
C	-1.17530100	2.06863200	-0.37412200
H	-1.34981700	1.38061800	-1.19779600
H	-1.39966000	3.07761300	-0.70650200
C	0.26471700	1.94458600	0.05295500
O	0.58071500	1.44928100	1.12696300
O	1.08917800	2.37821500	-0.86683700
H	2.06907100	2.13834100	-0.67482200
N	-2.08512400	1.71508000	0.75309100
H	-2.06956900	2.47823200	1.43187300
O	-3.23553300	-1.15931400	0.97847700
H	-1.70412000	0.89854200	1.24287700
O	-2.92493200	-0.53496700	-1.47029500
H	-2.03626300	-0.91215400	-1.26980200
O	-5.25897900	-0.40450800	-0.48831400

DZP_7 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54424986 u.a. ; Zero-point correction = 0.274246 u.a. ; G = -1783.319735 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.71137500	0.14137900	-0.00833100
C	2.57851300	-0.86106600	-1.05831900
H	3.09146900	-1.07329800	-1.99256500
H	1.68641900	-0.28591200	-1.27824100
C	1.22376100	-2.15661900	0.68702200
H	1.15121400	-3.17197100	1.07036600
H	1.65348800	-1.52256100	1.45536600
C	-0.17323700	-1.67465100	0.37915000
O	-0.43068300	-1.44278000	-0.87727500
O	-0.96898700	-1.54587900	1.30432400
H	-2.73938200	-1.51812600	0.99844400
N	2.15154800	-2.18557400	-0.48793600
H	1.71276300	-2.72211900	-1.23998400
O	5.06901900	-0.48494800	0.05366200
H	2.98489600	-2.70774400	-0.20696300
O	3.00845400	0.46189300	1.30640900
H	1.64617800	0.99406200	1.20961800
O	3.77551900	1.47838500	-0.91113900
P	-3.80316000	-0.20110600	-0.36324100
C	-3.43504300	1.36451400	0.53274900
H	-4.01353300	1.38560700	1.45152000
H	-3.71100000	2.21911200	-0.07820800
C	-1.13716700	2.08594800	-0.18387600
H	-1.37584300	1.57108400	-1.11002300
H	-1.38452400	3.13818700	-0.28930000
C	0.34104000	1.92441300	0.07166600
O	0.63693900	1.26018000	1.15571500
O	1.14500900	2.37588400	-0.73532200
H	2.91389600	1.94957900	-0.86206200
N	-1.98228200	1.50654600	0.90381100
H	-1.90396300	2.10438400	1.72810700
O	-3.68082400	-1.32522600	0.79238500
H	-1.59332400	0.59967100	1.18362200
O	-2.69565400	-0.43454300	-1.38246500
H	-1.38166300	-1.05538700	-1.02848100
O	-5.22533800	-0.13680200	-0.82118100

DZP_8 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54522886 u.a. ; Zero-point correction = 0.275609 u.a. ; G = -1783.319358 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.69813500	0.21965700	-0.03391200
C	2.57467000	-0.77687400	-1.09899800
H	3.07644700	-0.89964900	-2.05597200
H	1.65480900	-0.23244800	-1.27163300
C	1.29624000	-2.25281100	0.55931500
H	1.20819000	-3.30716300	0.81513500
H	1.74541700	-1.72756300	1.39302900
C	-0.09928700	-1.72190100	0.32806800
O	-0.41802400	-1.49353700	-0.91475100
O	-0.84065200	-1.57917400	1.29449100
H	-2.54784200	-1.39185000	1.13216400
N	2.21202200	-2.15652200	-0.62181300
H	1.78390300	-2.65170600	-1.40753400
O	5.04587400	-0.42744200	0.05158900
H	3.06913500	-2.66432600	-0.38943700
O	3.04592100	0.18568200	1.44485200
H	2.20566100	0.69385600	1.46141000
O	3.55590300	1.62513500	-0.59947100
P	-3.78081100	-0.27249400	-0.27443600
C	-3.48397800	1.42354200	0.37493000
H	-4.10013400	1.56233200	1.25835700
H	-3.75970200	2.16511400	-0.36890600
C	-1.16069600	2.05283600	-0.35464300
H	-1.34108000	1.37110900	-1.18186500
H	-1.39634500	3.06486400	-0.67008900
C	0.28353400	1.93638600	0.05839900
O	0.61191600	1.46075300	1.13750500
O	1.09937200	2.35556400	-0.87647100
H	2.07962000	2.11721600	-0.68822900
N	-2.05574800	1.67619600	0.77679400
H	-2.03349100	2.42568000	1.47073000
O	-3.51010600	-1.20387600	1.01382200
H	-1.66276900	0.85298000	1.24548400
O	-2.72614000	-0.57770100	-1.33020400
H	-1.38504400	-1.12501000	-1.02488900
O	-5.22824400	-0.35361400	-0.64384100

DZP_{10} structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54269027 u.a. Zero-point correction = 0.273693 u.a. ; G = -1783.320983 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.59806700	-0.21973800	0.19524500
C	2.49744500	0.88618500	-0.77031900
H	1.55496700	0.36932400	-0.93208400
H	2.94421800	1.12759700	-1.73033300
C	1.07999100	2.94779000	-0.64731200
H	1.13778900	3.97384900	-0.28868800
H	1.17056700	2.94104700	-1.72863800
C	-0.23087800	2.34363800	-0.18840700
O	-0.29203100	1.59969200	0.77451400
O	-1.24989400	2.72736700	-0.92369900
H	-2.11839400	2.29325700	-0.59995600
N	2.20805500	2.17140000	-0.05440000
H	3.05080800	2.74797800	-0.04020500
O	3.58915200	-1.54118300	-0.55727400
O	2.78013200	-0.38012900	1.58219700
H	1.93946200	-0.86547100	1.42077100
O	4.90049500	0.45219700	0.50102700
H	1.96283100	1.95914500	0.91857100
P	-3.52962600	0.22885500	0.30267900
C	-2.28812300	-0.73844500	-0.63950200
H	-1.33747500	-0.22026600	-0.57639500
H	-2.57987400	-0.84126700	-1.68042200
C	-0.97373500	-2.86994600	-0.67669200
H	-1.03617500	-3.90596800	-0.34783800
H	-1.07107500	-2.83128500	-1.75671800
C	0.35072000	-2.29725100	-0.22276800
O	0.43519000	-1.61478400	0.78991800
O	1.33772800	-2.63588400	-1.00864900
H	2.23567800	-2.19696000	-0.74583900
N	-2.10177100	-2.11045400	-0.06459500
H	-2.96320700	-2.64575700	-0.18915200
O	-3.33910200	-0.04379800	1.76393300
O	-4.95001800	-0.44425500	-0.10996600
H	-5.24118900	-0.17025000	-0.99002900
O	-3.47299100	1.64213500	-0.24231700
H	-1.94133400	-2.02105300	0.94359400

DZP_{11} structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54241171 u.a. ; Zero-point correction = 0.273587 u.a ; G = -1783.321038 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.59288400	0.22497700	0.21076600
C	-2.50382000	-0.88275000	-0.76613400
H	-1.56200100	-0.36703700	-0.93497900
H	-2.95937200	-1.12107300	-1.72277600
C	-1.08528600	-2.94501500	-0.65732400
H	-1.14277400	-3.97254700	-0.30292700
H	-1.18038200	-2.93326500	-1.73824700
C	0.22812300	-2.34415600	-0.20122500
O	0.29319200	-1.60227400	0.76296800
O	1.24457600	-2.72797300	-0.94029500
H	2.11464000	-2.29591000	-0.61908100
N	-2.21004600	-2.17010900	-0.05594600
H	-3.05267300	-2.74676000	-0.03850900
O	-3.58693500	1.54662100	-0.54150300
O	-2.76227000	0.38255500	1.59038100
H	-1.92377100	0.86933700	1.42253600
O	-4.89436700	-0.44339800	0.52809100
H	-1.95908200	-1.96073700	0.91617500
P	3.52255600	-0.24185200	0.29642200
C	2.28779600	0.72997200	-0.65067000
H	1.33473700	0.21666200	-0.58448000
H	2.58184400	0.82366300	-1.69142900
C	0.97754200	2.86354900	-0.70199900
H	1.04295500	3.90234500	-0.38256400
H	1.07123200	2.81456800	-1.78192900
C	-0.34584900	2.29695100	-0.23771200
O	-0.42634200	1.62372100	0.78155300
O	-1.33634300	2.63001300	-1.02154100
H	-2.23384000	2.19581300	-0.74861300
N	2.10566800	2.10708900	-0.08613900
H	2.96728500	2.64089100	-0.21641600
O	3.31261800	0.01650100	1.76011500
O	4.95036500	0.37157600	-0.18298400
H	5.24170700	1.08644100	0.39854900
O	3.47414300	-1.64681100	-0.26439300
H	1.94493400	2.02631900	0.92271800

DZP_{12} structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54161784 u.a. ; Zero-point correction = 0.273649 u.a. ; G = -1783.319289 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.87049000	-0.11438700	0.16780400
C	2.68415800	0.94632500	-0.76076800
H	1.82752900	0.34543100	-1.04893200
H	3.15272300	1.35003900	-1.65335300
C	0.98395100	2.78057500	-0.49259400
H	0.88155100	3.74882100	-0.00571700
H	1.12152000	2.93291200	-1.55876500
C	-0.25706500	1.96502500	-0.20587800
O	-0.24432700	1.04360500	0.59944200
O	-1.30408800	2.36935600	-0.87538900
H	-2.16347100	1.90621100	-0.54909400
N	2.18405100	2.09326200	0.06743800
H	2.93387100	2.77625300	0.18789800
O	3.90260900	-1.44159600	-0.57194700
O	3.10715000	-0.30423400	1.58517500
H	2.33123700	-0.89715500	1.48214800
O	5.14534200	0.62456000	0.43223900
H	1.94514200	1.73968600	0.99995300
P	-4.03029000	0.05334100	0.30751800
C	-3.01998100	-1.19257700	-0.58699100
H	-2.88320500	-0.87014400	-1.61563200
H	-3.52002500	-2.15653200	-0.57194200
C	-0.74087700	-2.16763300	-0.79993700
H	-1.09414000	-3.19626100	-0.82955700
H	-0.74277600	-1.76153200	-1.80634100
C	0.65540800	-2.10423100	-0.22732900
O	0.86104300	-1.79776600	0.93883400
O	1.57559600	-2.37072900	-1.12230100
H	2.51334300	-2.09246500	-0.81435600
N	-1.66976700	-1.35438600	0.03491300
H	-1.76633100	-1.78470800	0.95693200
O	-4.12971900	-0.33491100	1.75129900
O	-5.48537800	-0.16928600	-0.37361800
H	-5.58290700	0.33057600	-1.19524200
O	-3.52248100	1.43528900	-0.06220200
H	-1.23658700	-0.42676000	0.20444000

AC_1 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54799223 u.a. ; Zero-point correction = 0.273204 u.a. ; G = -1783.324869 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.47001900	-0.13608400	0.26502000
C	2.42402500	0.95955100	-0.75700800
H	1.50414300	0.42241000	-0.97979900
H	2.93033000	1.21007000	-1.68443700
C	0.94083700	2.97214700	-0.68847200
H	0.96819600	4.00539100	-0.34780100
H	1.05694100	2.94526500	-1.76701300
C	-0.36616100	2.34662900	-0.24872700
O	-0.41113500	1.62805700	0.74249700
O	-1.37248000	2.67472000	-1.00950500
H	-2.25251700	2.19385500	-0.74021400
N	2.07240500	2.23349400	-0.05245200
H	2.89638100	2.83606200	-0.01498200
O	3.60258600	-1.43210400	-0.61727100
O	2.56813900	-0.47064600	1.52099700
H	1.70898600	-0.94870200	1.25061600
O	4.76988500	0.47260500	0.64267800
H	1.79803600	2.02197700	0.91319700
P	-3.50577300	0.15309500	0.21752200
C	-2.37557700	-0.90027200	-0.77034700
H	-1.44272200	-0.36210700	-0.91659000
H	-2.81640300	-1.12571900	-1.73709800
C	-0.93456300	-2.94791000	-0.71206600
H	-0.98356300	-3.97882600	-0.36736100
H	-1.05252100	-2.92370900	-1.79024500
C	0.40271200	-2.35249600	-0.28514900
O	0.40150700	-1.62845100	0.74359300
O	1.39708200	-2.66360300	-0.99083200
H	2.71808500	-1.94427100	-0.73861100
N	-2.06327600	-2.19376600	-0.08503500
H	-2.90176200	-2.77582600	-0.06311900
O	-3.55402300	1.48731800	-0.51270100
O	-2.68778300	0.32327800	1.60357300
H	-1.86350100	0.83301100	1.43850400
O	-4.78246200	-0.56786200	0.52148300
H	-1.79387400	-1.99454400	0.88376300

AC_2 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54552535 u.a. ; Zero-point correction = 0.272838 u.a. ; G = -1783.323337 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.49230400	0.06756200	0.24147700
C	-2.36196100	-1.01484100	-0.71622400
H	-1.45510700	-0.45517500	-0.93422000
H	-2.82711300	-1.33045300	-1.64527400
C	-0.86041700	-3.01193200	-0.57180900
H	-0.88824900	-4.02730000	-0.18134200
H	-1.00555200	-3.03653500	-1.64628700
C	0.47999900	-2.38598600	-0.20416100
O	0.50539700	-1.64247300	0.81018300
O	1.45320800	-2.69578200	-0.93999000
H	2.75050400	-1.91864600	-0.78899000
N	-1.98134000	-2.24273000	0.05075600
H	-2.80190200	-2.84230700	0.14710600
O	-3.75184000	1.25792100	-0.81041200
O	-2.67067800	0.59922700	1.41386400
H	-1.41423900	1.24441700	1.03813900
O	-4.78188700	-0.63297300	0.53582500
H	-1.67493400	-1.97164400	0.99143400
P	3.49483100	-0.08941300	0.17958900
C	2.32221300	0.97737300	-0.72719400
H	1.39973500	0.41890100	-0.86998100
H	2.73496500	1.24929000	-1.69418500
C	0.88036000	3.02213900	-0.56813100
H	0.92520700	4.03096800	-0.16168200
H	1.00911200	3.06616300	-1.64425000
C	-0.47368900	2.43721000	-0.22744000
O	-0.47384200	1.65435200	0.81431800
O	-1.44983400	2.74521500	-0.90133200
H	-2.97482100	1.86424700	-0.85013300
N	2.00936700	2.23575500	0.02158100
H	2.84448100	2.82506500	0.04578000
O	3.61553000	-1.36202400	-0.73634600
O	2.71359100	-0.48827300	1.49742700
H	1.84437700	-0.97018400	1.27869600
O	4.79120200	0.57447200	0.46521200
H	1.77362900	2.00871700	0.99261800

AC_3 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54693672 u.a. ; Zero-point correction = 0.273826 u.a. ; G = -1783.323153 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.64975200	0.20439600	0.04287400
C	2.61285100	-0.77514600	-1.10763000
H	3.16917900	-0.86175900	-2.03765800
H	1.69744900	-0.22800800	-1.30627100
C	1.32995900	-2.30341700	0.49320300
H	1.26255600	-3.36229300	0.73469500
H	1.75569400	-1.78025300	1.34164000
C	-0.06128900	-1.79371700	0.19554100
O	-0.41799700	-1.47889700	-0.93399200
O	-0.80316300	-1.77329100	1.26754400
H	-1.78390100	-1.49262700	1.08031000
N	2.24348800	-2.16679000	-0.68271000
H	1.79760600	-2.61635000	-1.48731700
O	5.02065800	-0.33794300	0.21252500
H	3.09570400	-2.69723700	-0.48549900
O	2.87409500	0.31451700	1.41279000
H	1.95566100	0.75711200	1.31321800
O	3.60710300	1.62261700	-0.65399000
P	-3.80244600	-0.28342500	-0.13211300
C	-3.48802000	1.46215100	0.34228000
H	-4.11268900	1.67243600	1.20647500
H	-3.75390600	2.14521100	-0.45844100
C	-1.15285100	2.09048700	-0.38793800
H	-1.35345100	1.42541300	-1.22359000
H	-1.36991700	3.11031900	-0.68792300
C	0.30618500	1.93468300	0.00725000
O	0.55342600	1.32882800	1.08436100
O	1.14511500	2.39295400	-0.80982200
H	2.65594000	1.99209500	-0.69582600
N	-2.06394500	1.72254000	0.74003000
H	-2.04008800	2.47647100	1.42784100
O	-3.22361300	-1.14399700	0.98430300
H	-1.67138300	0.90339700	1.21547600
O	-2.93734100	-0.53210600	-1.47098800
H	-2.03522100	-0.87862800	-1.27503100
O	-5.25786300	-0.38772600	-0.46535300

AC_4 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54495180 u.a. ; Zero-point correction = 0.272896 u.a. ; G = -1783.322444 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.71010300	0.10627800	-0.04319800
C	2.52281000	-0.89953400	-1.02894300
H	2.99899100	-1.14138700	-1.97553400
H	1.62725100	-0.32217800	-1.23055700
C	1.16069900	-2.10084200	0.76065900
H	1.10669500	-3.08634900	1.21691300
H	1.57213100	-1.40266400	1.48082100
C	-0.23982400	-1.67182700	0.35875900
O	-0.51033600	-1.53491000	-0.86048700
O	-1.03668500	-1.49638100	1.32275800
H	-2.59187000	-1.48368700	0.95710300
N	2.09889700	-2.19824800	-0.40423300
H	1.64489300	-2.75713500	-1.12963600
O	5.05441700	-0.55145600	-0.00709100
H	2.92819200	-2.71484900	-0.10483900
O	3.05761800	0.47727900	1.28458600
H	1.70210300	1.03001800	1.21642500
O	3.77961800	1.41984200	-0.98004000
P	-3.80289700	-0.19098800	-0.32793300
C	-3.38394600	1.35428700	0.56640600
H	-3.95601300	1.36219000	1.49001500
H	-3.67297600	2.21272100	-0.03315800
C	-1.09530200	2.11222100	-0.15387100
H	-1.33390200	1.62438100	-1.09401200
H	-1.35164500	3.16504500	-0.22862000
C	0.38661900	1.95526700	0.08794200
O	0.69477800	1.30674600	1.17731800
O	1.17913300	2.39756600	-0.73478800
H	2.93537000	1.91780500	-0.91006300
N	-1.92910400	1.49699300	0.92590100
H	-1.85509300	2.07798800	1.76299600
O	-3.56721900	-1.36261200	0.70972000
H	-1.52417200	0.58713500	1.18672500
O	-2.73255700	-0.36114400	-1.47601200
H	-1.87268100	-0.84327200	-1.21274100
O	-5.20129800	-0.11289800	-0.81374600

AC_5 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54577097 u.a. ; Zero-point correction = 0.273896 u.a. ; G = -1783.322453 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.70787400	0.15520700	-0.11150600
C	2.47851200	-0.84311500	-1.05184500
H	2.90835300	-1.02166000	-2.03476100
H	1.55988200	-0.28491500	-1.18445100
C	1.18325200	-2.17468700	0.69307800
H	1.10356900	-3.19886100	1.05169600
H	1.61397500	-1.56386700	1.47648100
C	-0.21083300	-1.68126900	0.34133200
O	-0.52165900	-1.55960700	-0.87059800
O	-0.96201400	-1.45663600	1.33022900
H	-2.51724700	-1.44734200	1.02047600
N	2.11460400	-2.18492900	-0.48013100
H	1.67531900	-2.72845400	-1.22600200
O	5.03425100	-0.54064800	-0.09365800
H	2.96661700	-2.68103600	-0.21046400
O	3.16249200	0.20265400	1.40967000
H	2.33724100	0.73243600	1.45718700
O	3.58018800	1.54410900	-0.72200900
P	-3.79354400	-0.22126800	-0.27665000
C	-3.37906300	1.37523200	0.52407600
H	-3.94985200	1.43237200	1.44677200
H	-3.67681300	2.19303700	-0.12596900
C	-1.09235200	2.08370600	-0.24470100
H	-1.29617200	1.50530600	-1.14042900
H	-1.36519400	3.12056900	-0.42313900
C	0.37094600	1.96641000	0.09900600
O	0.74708100	1.52299800	1.17589600
O	1.14304500	2.35219700	-0.88559500
H	2.12797200	2.09486800	-0.74210500
N	-1.92698800	1.55541000	0.87400500
H	-1.85953900	2.20550300	1.65938400
O	-3.50334500	-1.33749100	0.80601100
H	-1.51504400	0.67458200	1.21205300
O	-2.76408300	-0.42815600	-1.45460900
H	-1.88763600	-0.88963900	-1.20246300
O	-5.21051500	-0.18729600	-0.71217700

AC_6 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54527078 u.a. ; Zero-point correction = 0.273656 u.a. ; G = -1783.321264 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.65151000	0.17554200	0.02637100
C	2.59525000	-0.80274400	-1.10825300
H	3.15168800	-0.91888300	-2.03517700
H	1.69372700	-0.23777900	-1.31961900
C	1.28856300	-2.28588300	0.52895000
H	1.19174900	-3.34467000	0.76132600
H	1.75071100	-1.78593300	1.37171800
C	-0.10298100	-1.73694600	0.31551300
O	-0.40513700	-1.43701500	-0.91513400
O	-0.85239500	-1.64757000	1.28171100
H	-2.54099400	-1.39092000	1.12310300
N	2.19365300	-2.17822200	-0.66108700
H	1.73627200	-2.63035600	-1.45723200
O	5.02014800	-0.37621700	0.18363000
H	3.03537300	-2.72520400	-0.46263500
O	2.89262400	0.29915200	1.40380600
H	1.98089300	0.75832000	1.31507600
O	3.61292900	1.59026800	-0.67846400
P	-3.77158800	-0.25354000	-0.27177800
C	-3.46361800	1.43713200	0.38202500
H	-4.07524200	1.57225100	1.26949000
H	-3.74407500	2.18261900	-0.35619200
C	-1.13887600	2.08867500	-0.35589900
H	-1.34672100	1.44270600	-1.20405200
H	-1.36874600	3.11518300	-0.62291200
C	0.32540900	1.93739200	0.02067100
O	0.58790900	1.35272800	1.10607300
O	1.15364300	2.38026300	-0.81568600
H	2.66504700	1.96770700	-0.71355300
N	-2.03297800	1.68171000	0.77199600
H	-2.00350400	2.41408900	1.48276600
O	-3.50223700	-1.19033300	1.01293300
H	-1.62681200	0.85249000	1.21759500
O	-2.72095800	-0.56422000	-1.33098400
H	-1.37864500	-1.07592700	-1.02428400
O	-5.21987200	-0.32904300	-0.64022400

AC_7 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54358209 u.a. ; Zero-point correction = 0.272830 u.a. ; G = -1783.321886 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-3.66281100	-0.29829400	-0.19727100
C	-2.65978000	0.96735100	0.66298900
H	-1.77105400	0.47208000	1.04581400
H	-3.21658300	1.38749300	1.49520900
C	-1.11241400	2.90013700	0.35320800
H	-1.04319000	3.82806600	-0.21235500
H	-1.34968000	3.12200900	1.38714400
C	0.22499800	2.19279400	0.25455600
O	0.34789700	1.44118700	-0.80480900
O	1.08776300	2.38122500	1.10293000
H	2.47914600	1.33482600	1.16281200
N	-2.22377300	2.08552700	-0.23323600
H	-3.01881500	2.69907700	-0.42370900
O	-3.61587800	-1.51746800	0.80078600
O	-2.80909100	-0.66577800	-1.47811200
H	-1.92953000	-1.12002100	-1.24255700
O	-5.03555200	0.14634300	-0.54045900
H	-1.91321000	1.70319900	-1.13223300
P	3.69806900	0.17059900	-0.23283500
C	3.47532900	-1.64924100	-0.10009100
H	3.80960600	-2.02555100	0.86234400
H	4.07180800	-2.10476600	-0.88589800
C	1.14105400	-1.92368600	0.84960700
H	1.34946100	-2.71769500	1.55826100
H	1.33937700	-0.96392600	1.32215000
C	-0.31458900	-1.93292500	0.40502700
O	-0.54890900	-1.71994500	-0.81375400
O	-1.16624400	-2.09995300	1.31686600
H	-2.65500900	-1.81568600	0.99923900
N	2.05534900	-2.07382100	-0.32281600
H	2.04018700	-3.05069900	-0.61929000
O	3.26304300	0.73889100	1.21215000
O	2.68879700	0.65575200	-1.26980500
H	1.31686200	1.08053000	-0.93491500
O	5.15779500	0.41604100	-0.46236800
H	1.65616300	-1.53238900	-1.09724300

AC_8 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54204454 u.a. ; Zero-point correction = 0.272383 u.a. ; G = -1783.321305 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.52519400	-0.16553600	0.25186500
C	2.48574000	0.95055800	-0.75427700
H	1.55719200	0.42769200	-0.97496000
H	2.98922600	1.20075400	-1.68338700
C	1.03385100	2.98623100	-0.66089400
H	1.08437600	4.01732000	-0.31664400
H	1.13877000	2.96146100	-1.74070200
C	-0.27668800	2.37826000	-0.20464200
O	-0.33344900	1.64289000	0.76543400
O	-1.29516500	2.74479400	-0.94695400
H	-2.15856300	2.29328800	-0.62505200
N	2.15710700	2.22372400	-0.03774600
H	2.99060300	2.81258700	0.00387600
O	3.63384500	-1.45780500	-0.63944100
O	2.63260200	-0.49818800	1.51463100
H	1.76801100	-0.97430200	1.25817700
O	4.83615200	0.42480200	0.62078800
H	1.87953700	2.00642100	0.92596700
P	-3.48144100	0.20026400	0.31202600
C	-2.24884000	-0.75731900	-0.65033500
H	-1.29629900	-0.24094800	-0.59737300
H	-2.55664300	-0.85041500	-1.68769400
C	-0.92774500	-2.88552200	-0.71993300
H	-1.00417200	-3.92574600	-0.40921000
H	-1.03391800	-2.82524400	-1.79802900
C	0.42142400	-2.33881500	-0.27004400
O	0.44412800	-1.65201300	0.78294400
O	1.40546400	-2.65227900	-0.99059300
H	2.74198000	-1.95886500	-0.75040000
N	-2.05464100	-2.13197400	-0.08963900
H	-2.91857600	-2.66523500	-0.20152600
O	-3.24313700	-0.03350500	1.77315100
O	-4.89757900	-0.51477100	-0.04352000
H	-5.22498600	-0.26190700	-0.91703800
O	-3.48128100	1.60442200	-0.26219100
H	-1.86918000	-2.04715900	0.91407100

AC_{10} structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54450453 u.a. ; Zero-point correction = 0.274062 u.a. ; G = -1783.320718 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.69415200	0.01471900	0.12530100
C	2.39159200	1.01965300	-0.67540200
H	1.54148300	0.37757900	-0.89342300
H	2.77292200	1.44016200	-1.60127700
C	0.77129200	2.90388500	-0.39398300
H	0.68905100	3.85215200	0.13461700
H	0.97109300	3.09007300	-1.44300900
C	-0.51568200	2.13205100	-0.18727400
O	-0.66548800	1.41311300	0.79392700
O	-1.40000300	2.34287300	-1.12127300
H	-2.25448900	1.76962100	-0.99464300
N	1.91691800	2.14452500	0.19342300
H	2.68848600	2.79238400	0.36670300
O	3.82067600	-1.23489200	-0.83045100
O	3.05638100	-0.45646700	1.49052000
H	2.19090200	-0.98201000	1.33700800
O	4.96998500	0.74913100	0.30905900
H	1.62193200	1.76695600	1.10074700
P	-3.88603700	-0.02167300	0.11340100
C	-3.00872800	-1.61089800	-0.18165600
H	-3.32446500	-2.03043600	-1.13304100
H	-3.22299500	-2.31314700	0.61867800
C	-0.69502000	-2.59757100	-0.53227900
H	-1.07757500	-3.43451600	0.04810300
H	-0.76688500	-2.81479500	-1.59130500
C	0.74110600	-2.29767700	-0.10296800
O	0.85982200	-1.64412700	0.97098900
O	1.67306500	-2.70544600	-0.83816100
H	3.01352700	-1.85003100	-0.80700500
N	-1.53215500	-1.39600700	-0.22441700
H	-1.20737800	-1.03335000	0.67782500
O	-3.48726200	0.92653000	-1.00933900
O	-3.22910900	0.51141700	1.49383600
H	-2.35827400	0.93511900	1.33509300
O	-5.33357300	-0.31867900	0.34461600
H	-1.31571900	-0.66535800	-0.90704200

AC_{11} structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54184701 u.a. ; Zero-point correction = 0.272576 u.a. ; G = -1783.320721 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.51651400	-0.16694200	0.26865500
C	2.48288600	0.94496900	-0.74822200
H	1.55551600	0.42153800	-0.97229600
H	2.99224200	1.19069800	-1.67532700
C	1.03270400	2.98322200	-0.67344900
H	1.08493800	4.01661500	-0.33650800
H	1.14246200	2.95006200	-1.75260300
C	-0.28150700	2.38210500	-0.21874600
O	-0.34329000	1.65134800	0.75438300
O	-1.29697200	2.74792400	-0.96610400
H	-2.16147900	2.29784800	-0.64814400
N	2.15078800	2.22157200	-0.03958600
H	2.98480000	2.80946400	0.00516300
O	3.63570900	-1.46047400	-0.61965500
O	2.61450100	-0.49990400	1.52474800
H	1.75553100	-0.98166600	1.26169700
O	4.82279300	0.42734000	0.64756800
H	1.86651000	2.00843600	0.92310900
P	-3.46925900	0.21099000	0.30639000
C	-2.24385400	-0.74814300	-0.66343300
H	-1.28875700	-0.23682000	-0.60923900
H	-2.55610200	-0.83170100	-1.69990700
C	-0.92789100	-2.87808400	-0.75062700
H	-1.00920000	-3.92191700	-0.45359100
H	-1.02999900	-2.80302500	-1.82817100
C	0.42080700	-2.34088800	-0.28762300
O	0.43911200	-1.66834000	0.77472900
O	1.40790100	-2.64677000	-1.00705400
H	2.74451100	-1.95921400	-0.74515100
N	-2.05350300	-2.12793300	-0.11390200
H	-2.91839900	-2.65875500	-0.23023300
O	-3.20190500	0.00147600	1.76838600
O	-4.89268700	-0.46321600	-0.10388900
H	-5.14352300	-1.16270200	0.51427800
O	-3.49047500	1.60288200	-0.29084400
H	-1.86523100	-2.05226200	0.89010600

AC_{12} structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54156235 u.a. ; Zero-point correction = 0.272654 u.a. ; G = -1783.320138 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.81605200	-0.05189800	0.17027000
C	2.62457400	1.00928400	-0.72913400
H	1.77697100	0.39765500	-1.02525600
H	3.09320000	1.42517400	-1.61590900
C	0.92192800	2.83082400	-0.45698400
H	0.82139800	3.79895900	0.03013700
H	1.06825600	2.98077200	-1.52206400
C	-0.31772500	2.01295500	-0.17004500
O	-0.30077100	1.11240600	0.65865800
O	-1.35994400	2.38684400	-0.86147500
H	-2.21783800	1.91353000	-0.53411000
N	2.11510200	2.13732000	0.11534500
H	2.86200700	2.81935800	0.26086900
O	3.93909000	-1.32818500	-0.74826400
O	3.06458400	-0.45980100	1.50042600
H	2.22199800	-1.00585000	1.33385400
O	5.11349400	0.61636400	0.43530600
H	1.85019000	1.76912800	1.03585400
P	-4.00814500	0.00749000	0.28002000
C	-2.94530800	-1.17891700	-0.63218200
H	-2.77966700	-0.81407600	-1.64233400
H	-3.43290700	-2.14870600	-0.67432900
C	-0.66287100	-2.16383700	-0.78928800
H	-1.03738100	-3.18311700	-0.84897200
H	-0.63383500	-1.74006500	-1.78844200
C	0.73837600	-2.14383200	-0.19699200
O	0.87401100	-1.72413100	0.98128900
O	1.65852700	-2.53139100	-0.96593400
H	3.07492900	-1.86287400	-0.80952000
N	-1.61541400	-1.35243400	0.02540600
H	-1.73775800	-1.79085800	0.93982700
O	-4.10557800	-0.42321000	1.71203800
O	-5.45036700	-0.24634200	-0.41893500
H	-5.55846300	0.27064200	-1.22854300
O	-3.55240000	1.41921800	-0.04588300
H	-1.18653500	-0.43079800	0.21926500

NZP_2 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.52621249 u.a. ; Zero-point correction = 0.271964 u.a. ; G = -1783.305563 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	-2.28139500	0.87194200	0.21414600
C	-3.68026000	-0.29715000	0.29562700
H	-4.52481700	0.22576700	-0.15051700
H	-3.91168300	-0.44227800	1.35001900
C	-2.51013500	-2.49142100	0.18114800
H	-2.46830400	-2.39751500	1.26380300
H	-2.79334300	-3.52643600	-0.02681600
C	-1.10535400	-2.35433800	-0.37381800
O	-0.82625300	-1.69667400	-1.37395200
O	-0.21212800	-3.06031600	0.28697800
H	0.71864600	-2.87545400	-0.07984700
N	-3.51749400	-1.59166200	-0.36492000
H	-3.35933200	-1.45667400	-1.35724200
O	-1.69258500	0.80748700	-1.26668800
H	-1.37018000	-0.10406900	-1.47932700
O	-1.20663200	0.16432900	1.17066500
H	-0.41345100	0.71951500	1.29630000
O	-2.56759200	2.29938100	0.55793700
P	2.73981200	-1.19925800	0.10861900
C	2.06027600	0.23619700	-0.81232600
H	0.98874900	0.29500800	-0.64463900
H	2.25462700	0.13812500	-1.87597200
C	1.94610100	2.74371300	-0.76354600
H	2.57149300	3.61664600	-0.58274700
H	1.71183200	2.67671000	-1.82078900
C	0.69569300	2.84127900	0.07828400
O	0.61038400	2.28731300	1.16104600
O	-0.26408200	3.55413700	-0.47844700
H	-1.10537000	3.41219400	0.02079700
N	2.69091900	1.52036800	-0.34544500
H	3.64887600	1.56398300	-0.69671900
O	2.16745700	-2.45098800	-0.52291200
O	2.09846700	-0.97853100	1.58849200
H	1.14209900	-1.12937000	1.59750200
O	4.22222000	-1.03801300	0.25284800
H	2.74794400	1.51797400	0.67732000

DN_2 structure in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.51140515 u.a. ; Zero-point correction = 0.270132 u.a. ; G = -1783.291370 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	2.42387700	-1.15300700	0.68830200
C	3.93876700	-0.19744100	0.32804000
H	4.68865900	-0.93993600	0.05988700
H	4.24876700	0.23793500	1.27864600
C	3.02645300	1.97552800	-0.44661300
H	3.04997300	2.23902900	0.60830400
H	3.38938600	2.84942900	-0.99358300
C	1.58589600	1.81109800	-0.87927300
O	1.19043100	0.93339100	-1.63274400
O	0.78480400	2.75668000	-0.39888200
H	-0.14138400	2.54237100	-0.64407300
N	3.89750800	0.83753800	-0.70279000
H	3.67286500	0.42342800	-1.60013300
O	1.73583400	-1.54558400	-0.69772900
H	1.50978500	-0.74539000	-1.23021200
O	1.35703900	-0.07849600	1.26501900
H	1.68154100	0.40308000	2.04083100
O	2.63430000	-2.34506500	1.54610400
P	-2.38222400	1.13244500	0.71623900
C	-3.92603400	0.21436600	0.39573300
H	-4.67023200	0.97056500	0.15126300
H	-4.21982800	-0.22629400	1.34848300
C	-3.07370600	-1.96652300	-0.42891600
H	-3.08499200	-2.25126100	0.61993800
H	-3.45732000	-2.82283600	-0.98949700
C	-1.63811200	-1.81029400	-0.88148200
O	-1.25380900	-0.94944600	-1.65879500
O	-0.82886100	-2.74544000	-0.38965900
H	0.09339200	-2.53443300	-0.64694800
N	-3.93234000	-0.81100300	-0.64769100
H	-3.72208700	-0.39000200	-1.54552100
O	-1.77133500	1.57103700	-0.70792800
H	-1.54418200	0.78532700	-1.25433200
O	-1.42757000	-0.01568400	1.27764600
H	-0.46114900	0.10902600	1.18362600
O	-2.53255300	2.33263600	1.58117300

8- Structures and energetics of transition states (TS) for DZP_9 and AC_9 conversions in the gas phase at B3LYP-D3/6-311++G(2d,2p) level.

Structure of TS_1 in the gas phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.44801571 u.a. ; Zero-point correction = 0.268072 u.a. ; G = -1783.231120 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-3.60576400	-0.04731100	0.52980800
C	-2.02474200	0.93530500	0.56214600
H	-1.16635000	0.36560600	0.90122900
H	-2.16263100	1.80568100	1.19752300
C	-0.86255500	2.56500500	-0.98760500
H	-0.95065500	2.94007800	-2.00489100
H	-1.14605300	3.33455200	-0.27719600
C	0.56858500	2.06551200	-0.77177500
O	0.97250700	1.16345300	-1.49561000
O	1.20334900	2.62779400	0.19700500
H	2.17523100	2.14553000	0.37484500
N	-1.78508100	1.40006200	-0.84457900
H	-2.72866300	1.56428700	-1.23032000
O	-4.31072800	0.49035000	-0.66088700
O	-4.30224400	0.40128600	1.91552100
H	-4.39173400	-0.34881800	2.51291000
O	-3.30421500	-1.53576400	0.70417700
H	-1.40907700	0.57538400	-1.35607200
P	3.60830600	0.04033500	0.53461000
C	2.01820100	-0.93731900	0.55184600
H	1.15767700	-0.36432200	0.87975700
H	2.14088500	-1.81023600	1.18662600
C	0.85829000	-2.55802200	-1.00659800
H	0.94006400	-2.92882400	-2.02623600
H	1.13525500	-3.33386500	-0.30075800
C	-0.56815800	-2.04230800	-0.77789100
O	-0.93206400	-1.09569000	-1.48304600
O	-1.22952500	-2.61515500	0.14677600
H	-2.28452100	-2.07522100	0.36730900
N	1.79308100	-1.40381600	-0.85736100
H	2.74528600	-1.57174300	-1.22467700
O	4.31073400	-0.51841100	-0.65267100
O	4.29191900	-0.44288800	1.92170600
H	4.39152200	0.30440800	2.52073100
O	3.31181400	1.51867500	0.70561800
H	1.42953600	-0.58982500	-1.38289200

Structure of TS_2 in the gas phase at B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.44863432 u.a. ; Zero-point correction = 0.268101 u.a. ; G = -1783.232787 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	3.58584400	0.06623900	0.57821400
C	2.03441100	-0.95835200	0.52658200
H	1.15369700	-0.42689500	0.87109700
H	2.17691300	-1.85054900	1.12977300
C	0.89551500	-2.52828600	-1.08805600
H	0.95964000	-2.84262200	-2.12739600
H	1.19350200	-3.33546400	-0.42692900
C	-0.53120800	-2.03281300	-0.79348700
O	-0.91612200	-1.08300000	-1.50733000
O	-1.14948900	-2.59010800	0.14554900
H	-2.38182200	-1.96863000	0.50175200
N	1.82927300	-1.37668000	-0.89885000
H	2.77680800	-1.53878200	-1.26955300
O	4.34618400	-0.40235700	-0.60715900
O	4.25505200	-0.42197800	1.96794300
H	4.29645000	0.30607200	2.59672400
O	3.22509800	1.53285100	0.80546400
H	1.46943500	-0.54274400	-1.40211900
P	-3.60410300	-0.03784800	0.55579000
C	-2.06169600	0.98821000	0.52200700
H	-1.19906600	0.47048700	0.92813200
H	-2.23511700	1.90024600	1.08671800
C	-0.86055000	2.49108900	-1.11745500
H	-0.91966900	2.77657100	-2.16463400
H	-1.16510600	3.31455500	-0.47898300
C	0.56574800	2.01321800	-0.81595300
O	1.04901700	1.17142100	-1.57120100
O	1.09884800	2.50943000	0.23675500
H	2.15002300	2.03978900	0.46673900
N	-1.79376200	1.34148900	-0.90827700
H	-2.71400100	1.49029000	-1.33989800
O	-4.32220900	0.31436400	-0.68666100
O	-4.33977900	0.46938300	1.89198000
H	-4.38996600	-0.22381800	2.55890500
O	-3.24503300	-1.50601300	0.90622800
H	-1.41226400	0.46162300	-1.34487100

9- Structures and energetics of transition states (TS) for DZP_9 and AC_9 conversions in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p) level.

Structure of TS_1 in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.47353191 u.a. ; Zero-point correction = 0.268771 u.a. ; G = -1783.256299 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-3.62746800	-0.06924900	0.52835900
C	-2.10712600	0.99715500	0.55118900
H	-1.23686300	0.49083200	0.95674900
H	-2.31334900	1.88801500	1.13839900
C	-0.87573400	2.57000600	-0.99671600
H	-0.94778000	2.93779900	-2.01757200
H	-1.16362700	3.34614900	-0.29577800
C	0.54676400	2.06311100	-0.76160600
O	0.98689600	1.19430900	-1.50277200
O	1.15574100	2.59636900	0.24564500
H	2.11710800	2.13190600	0.41430400
N	-1.81748100	1.41725800	-0.85791400
H	-2.72705100	1.60553000	-1.29575600
O	-4.35940200	0.35690600	-0.68987600
O	-4.37360800	0.39084800	1.88513500
H	-4.40021500	-0.32651000	2.52889100
O	-3.25256800	-1.53424300	0.77746600
H	-1.43729600	0.57643400	-1.33976900
P	3.63612100	0.04906600	0.53654100
C	2.08011500	-0.97419300	0.52802400
H	1.21236500	-0.44318200	0.90668300
H	2.24300000	-1.86902800	1.12226900
C	0.87031300	-2.54339900	-1.03629000
H	0.93244100	-2.89837000	-2.06269300
H	1.15861500	-3.33060200	-0.34833100
C	-0.54752200	-2.02688700	-0.77543300
O	-0.92433000	-1.06769000	-1.45949800
O	-1.20367000	-2.61722000	0.14095600
H	-2.25701100	-2.06071000	0.39860500
N	1.81947700	-1.39911800	-0.88630200
H	2.74445000	-1.59141000	-1.29347000
O	4.38122000	-0.44520800	-0.65412100
O	4.32945700	-0.45039300	1.91716700
H	4.37555500	0.27590300	2.54915600
O	3.29788200	1.51411200	0.74119400
H	1.45409000	-0.57406600	-1.39106000

Structure of TS_2 in cyclohexane at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.47345810 u.a. ; Zero-point correction = 0.267610 u.a. ; G = -1783.259166 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	3.56640200	0.09840500	0.62135200
C	2.08906200	-1.01431900	0.49274500
H	1.18534300	-0.56356100	0.89085600
H	2.29521100	-1.93423400	1.03326000
C	0.93264900	-2.50355100	-1.17300800
H	0.98063600	-2.76862600	-2.22676900
H	1.25029200	-3.33768000	-0.55637200
C	-0.48970800	-2.03320400	-0.83164300
O	-0.88254400	-1.04027800	-1.48334100
O	-1.10831700	-2.64969500	0.06737800
H	-2.27740400	-1.94385800	0.56306500
N	1.86886100	-1.35719800	-0.94817700
H	2.79465000	-1.52655300	-1.35486100
O	4.39829200	-0.22483700	-0.56287700
O	4.25020700	-0.40990400	1.99702400
H	4.17753600	0.25951300	2.68686500
O	3.09973000	1.52690900	0.92664100
H	1.50668600	-0.50183600	-1.41596700
P	-3.57691900	-0.06353800	0.59320800
C	-2.19033200	1.15212100	0.48033000
H	-1.30182200	0.82689300	1.01288400
H	-2.52313700	2.09912600	0.89820100
C	-0.87826400	2.45598400	-1.24420500
H	-0.90794300	2.64863800	-2.31257000
H	-1.17753800	3.33779300	-0.68628400
C	0.52841900	1.97802300	-0.86172200
O	1.11113600	1.21457000	-1.63378200
O	0.95437000	2.39483900	0.27106200
H	2.04155100	1.95470800	0.55267300
N	-1.85461200	1.35468900	-0.96185100
H	-2.73387600	1.50437900	-1.46223300
O	-4.33171600	0.04325300	-0.67182000
O	-4.37363300	0.45764100	1.88810200
H	-4.38239300	-0.19263300	2.60037800
O	-3.03537000	-1.43881400	1.08466400
H	-1.47795800	0.43269300	-1.31072200

10- Structures and energetics of transition states (TS) involved in DZP⇋AC⇋DZC tautomerzation processes of Glyph dimers in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p) level.

Structure of TS_1 in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54629517 u.a. ; Zero-point correction = 0.269941 u.a. ; G = -1783.326452 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

	Coordinates (Angstroms)		
	X	Y	Z
P	3.48053800	-0.16423400	0.22181200
C	2.40566500	0.94326300	-0.76281400
H	1.47458000	0.41469100	-0.95456100
H	2.87825500	1.19412300	-1.70779000
C	0.94838200	2.97423700	-0.65629400
H	0.97986600	3.99927600	-0.29150400
H	1.05883400	2.97339400	-1.73559700
C	-0.35981200	2.34432900	-0.22630800
O	-0.41103400	1.61699500	0.75794100
O	-1.36276900	2.67941400	-0.98973200
H	-2.24282200	2.19472900	-0.73347000
N	2.08231300	2.21869700	-0.04586400
H	2.91300900	2.81262100	-0.02050600
O	3.48796100	-1.48788700	-0.57437800
O	2.64104400	-0.37325900	1.56911400
H	1.79316400	-0.85792300	1.36957400
O	4.80394000	0.44696400	0.52811100
H	1.82743200	2.00299300	0.92390300
P	-3.51292600	0.14995600	0.20019000
C	-2.37007400	-0.90548100	-0.77063100
H	-1.43899000	-0.36285100	-0.91105100
H	-2.79972600	-1.14005800	-1.74018800
C	-0.91778700	-2.94220400	-0.68486400
H	-0.95286100	-3.97029000	-0.32963700
H	-1.02601600	-2.93108400	-1.76424700
C	0.39857400	-2.31919800	-0.24964600
O	0.41394800	-1.60537800	0.76617500
O	1.39831700	-2.61999000	-0.98763200
H	2.44460700	-2.03843200	-0.72476800
N	-2.05721800	-2.19419700	-0.07431500
H	-2.89113400	-2.78333000	-0.06298100
O	-3.55147000	1.48121500	-0.53506600
O	-2.70888100	0.32366000	1.59407300
H	-1.88158300	0.83100900	1.43637300
O	-4.79223000	-0.57114500	0.49167200
H	-1.80675900	-1.99059100	0.89881100

Structure of TS_2 in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54606622 u.a. ; Zero-point correction = 0.268945 u.a. ; G = -1783.326885 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	3.46117900	-0.10794400	0.25747400
C	2.39810200	0.97236400	-0.76228000
H	1.48310200	0.42503200	-0.98027200
H	2.89847100	1.22444400	-1.69259600
C	0.89166900	2.96525100	-0.69970600
H	0.91100400	3.99986800	-0.36352100
H	1.00968300	2.93385400	-1.77769900
C	-0.41721700	2.32960300	-0.25944400
O	-0.42182900	1.62275500	0.76048700
O	-1.42120800	2.61410200	-0.99839400
H	-2.45519800	2.02981000	-0.72348600
N	2.03445000	2.24326100	-0.06117500
H	2.85229200	2.85343400	-0.02190600
O	3.60646600	-1.40558200	-0.62121900
O	2.57097000	-0.45133300	1.51988100
H	1.71669700	-0.93931700	1.25534100
O	4.75582900	0.51646600	0.62806900
H	1.75380000	2.02920900	0.90211400
P	-3.46766100	0.13945500	0.22946900
C	-2.38215600	-0.94776600	-0.76505900
H	-1.45498300	-0.41134500	-0.95412600
H	-2.85574000	-1.19173100	-1.71150200
C	-0.91510700	-2.97227400	-0.69428100
H	-0.95418400	-4.00202400	-0.34520500
H	-1.03915900	-2.95241700	-1.77179600
C	0.41829500	-2.36226200	-0.27426500
O	0.41289400	-1.63679000	0.75327200
O	1.41250000	-2.66414500	-0.98361700
H	2.72785800	-1.92723700	-0.73879300
N	-2.04685000	-2.22476200	-0.06210000
H	-2.87682700	-2.81790800	-0.02127200
O	-3.49778900	1.46911200	-0.55593200
O	-2.62923400	0.35254900	1.57821300
H	-1.78952200	0.84847300	1.37916600
O	-4.78126800	-0.49265500	0.53859900
H	-1.76343600	-2.00962000	0.89967100

Structure of TS_3 in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54502764 u.a. ; Zero-point correction = 0.270209 u.a. ; G = -1783.324659 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	3.45511300	-0.11958500	0.28153000
C	2.41495100	0.99318500	-0.73749100
H	1.50175200	0.45686100	-0.98724000
H	2.93154700	1.27476500	-1.64998600
C	0.91511100	2.99473200	-0.64054400
H	0.93508300	4.02263500	-0.28323600
H	1.03928800	2.98589300	-1.71836400
C	-0.39334700	2.35851000	-0.22163000
O	-0.44723300	1.63087500	0.76257100
O	-1.39267400	2.68722700	-0.99210000
H	-2.26984500	2.19337400	-0.74289100
N	2.04311200	2.24897700	-0.00818900
H	2.86329200	2.85443200	0.05207300
O	3.71604900	-1.33364500	-0.72101800
O	2.53396300	-0.60347400	1.42357800
H	1.49181900	-1.13634100	1.06017900
O	4.73325100	0.53118500	0.68882700
H	1.75900400	2.01641100	0.94958400
P	-3.51429400	0.13136600	0.18722000
C	-2.33792200	-0.90778300	-0.76121000
H	-1.40889000	-0.35760200	-0.88366800
H	-2.74633900	-1.14884900	-1.73837200
C	-0.89850700	-2.95960000	-0.65695700
H	-0.94105500	-3.97890100	-0.27749600
H	-1.02020300	-2.97475400	-1.73479600
C	0.44696300	-2.36616900	-0.27917600
O	0.44500200	-1.61337600	0.76016300
O	1.42914400	-2.67082800	-0.96899300
H	2.89839700	-1.89734100	-0.81889500
N	-2.03125500	-2.19231800	-0.05435800
H	-2.86885700	-2.77714800	-0.04498700
O	-3.56711000	1.46035100	-0.55085600
O	-2.73409900	0.32100900	1.59261500
H	-1.91069100	0.83705900	1.44338300
O	-4.78375300	-0.61377700	0.46058500
H	-1.79340600	-1.98542700	0.92035100

Structure of TS_4 in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54390075 u.a. ; Zero-point correction = 0.269707 u.a. ; G = -1783.324466 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-3.48937900	0.07610800	0.25336600
C	-2.37888200	-1.00865000	-0.72558600
H	-1.47336700	-0.44993100	-0.95125600
H	-2.85572200	-1.31796500	-1.65069700
C	-0.85937400	-2.99216200	-0.59041500
H	-0.87359700	-4.01216200	-0.21124600
H	-0.99225000	-3.00694100	-1.66677500
C	0.45840800	-2.34464100	-0.19838600
O	0.48907100	-1.61210200	0.80360200
O	1.44482300	-2.64717900	-0.95394000
H	2.48039700	-2.03354900	-0.73979900
N	-1.99217400	-2.24254900	0.03067900
H	-2.80691800	-2.85235900	0.11155900
O	-3.74930200	1.27529400	-0.78808800
O	-2.64808200	0.59106600	1.41882700
H	-1.38859900	1.23478600	1.03294400
O	-4.78192300	-0.61426700	0.55780400
H	-1.70090000	-1.98034700	0.97872900
P	3.49659100	-0.12645100	0.16427200
C	2.33180900	0.95057200	-0.74795500
H	1.40140300	0.40386600	-0.88037400
H	2.73833400	1.21405700	-1.71990400
C	0.90323800	3.00609500	-0.58273100
H	0.95076700	4.01388800	-0.17377000
H	1.02518900	3.05378300	-1.65947300
C	-0.45053300	2.42318300	-0.23709100
O	-0.44917900	1.64187500	0.80615900
O	-1.42865600	2.73151100	-0.90801500
H	-2.96450600	1.87092800	-0.83727000
N	2.03439400	2.21619100	-0.00362200
H	2.87272300	2.80099500	0.00964000
O	3.51180600	-1.44383000	-0.64037100
O	2.73416400	-0.37237700	1.55157600
H	1.88448300	-0.86445400	1.38317300
O	4.80978400	0.53351600	0.40784100
H	1.81080400	1.99061600	0.97037800

Structure of TS_5 in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54468550 u.a. ; Zero-point correction = 0.268777 u.a. ; G = -1783.326633 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-3.45288600	0.07691100	0.25966400
C	-2.37032300	-1.01851700	-0.73175500
H	-1.46387700	-0.46722400	-0.97334500
H	-2.86869000	-1.31582100	-1.64961700
C	-0.85770100	-3.00760700	-0.62934000
H	-0.88362700	-4.03312100	-0.26677100
H	-0.99719500	-3.00221700	-1.70499600
C	0.47679100	-2.38327800	-0.23584800
O	0.48377800	-1.65129600	0.78711700
O	1.46114400	-2.68126900	-0.96099900
H	2.75833200	-1.90911900	-0.76920900
N	-1.98381300	-2.25888900	0.01058500
H	-2.80101700	-2.86428200	0.09780700
O	-3.72494300	1.27850400	-0.75712200
O	-2.56877500	0.59259700	1.41644800
H	-1.52150100	1.14183800	1.06518100
O	-4.72511500	-0.59955600	0.64558700
H	-1.67232800	-2.00649100	0.95489400
P	3.47332300	-0.07463500	0.21105600
C	2.32044500	0.97830100	-0.73626400
H	1.40291700	0.41598000	-0.89512300
H	2.75514500	1.24156700	-1.69602600
C	0.85089700	3.00204600	-0.61954000
H	0.88248400	4.01923100	-0.23392800
H	0.98295300	3.02286200	-1.69603400
C	-0.49084800	2.39262800	-0.25495000
O	-0.48429300	1.62780900	0.77662300
O	-1.47249200	2.69464800	-0.94476600
H	-2.92434200	1.86680100	-0.83557800
N	1.98521700	2.24144900	-0.00782800
H	2.81354500	2.83897400	0.02464600
O	3.62341300	-1.35688500	-0.68739400
O	2.66162300	-0.46402500	1.51360900
H	1.80347600	-0.95728000	1.27908600
O	4.75980900	0.59643700	0.52414400
H	1.72857900	2.01909700	0.95910700

Structure of TS_6 in aqueous solution at SMD-B3LYP-D3/6-311++G(2d,2p).
E(SCF) = -1783.54259744 u.a. ; Zero-point correction = 0.270085 u.a. ; G = -1783.322785 u.a. at 298,15K.

Charge = 0; Multiplicity = 1

Coordinates (Angstroms)

	X	Y	Z
P	-3.49040200	0.06459200	0.21744700
C	-2.33299800	-1.02029900	-0.70585100
H	-1.42153600	-0.46112900	-0.90452600
H	-2.77326800	-1.34544100	-1.64356200
C	-0.85175100	-3.03358000	-0.51294500
H	-0.87372000	-4.03143200	-0.07861500
H	-1.00613000	-3.10802700	-1.58386100
C	0.49918800	-2.41336700	-0.20530800
O	0.52497600	-1.62935100	0.81124700
O	1.46141700	-2.72767700	-0.91829700
H	2.90336200	-1.87109600	-0.88389400
N	-1.97222400	-2.24231300	0.08234300
H	-2.79864800	-2.83733200	0.16372700
O	-3.73271700	1.24521900	-0.84872000
O	-2.69558400	0.60705600	1.40263900
H	-1.43072300	1.25723500	1.04140100
O	-4.78127700	-0.64301300	0.48729600
H	-1.69857800	-1.96699000	1.03079600
P	3.47179700	-0.08747200	0.20337400
C	2.33802000	1.01900900	-0.71639300
H	1.41783100	0.47306900	-0.91358600
H	2.78516700	1.32842400	-1.65619700
C	0.87937900	3.04998500	-0.52071900
H	0.91378000	4.04962000	-0.09096400
H	1.02149500	3.11946900	-1.59372900
C	-0.47690200	2.45363300	-0.20949700
O	-0.48954700	1.66656100	0.82992000
O	-1.44440200	2.75734700	-0.89748800
H	-2.96074100	1.85896200	-0.87288600
N	2.00157700	2.25264600	0.06512100
H	2.83383700	2.84326600	0.12136300
O	3.69844300	-1.27088400	-0.84360800
O	2.64061100	-0.62301600	1.39068200
H	1.58345000	-1.15509600	1.07468300
O	4.75530600	0.59137500	0.54193300
H	1.75060600	1.99613700	1.02472500