Supplementary Information

Co-ordinates for the initial Ins(1,3,4,5)P_4 conformation in the PDB file format

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HEADER
REMARK Ins1345P4
HETATM    1  C1           1       0.000   0.000   0.000                       C
HETATM    2  O1           1       0.000   0.000   1.430                       O
HETATM    3  C2           1       1.452   0.000  -0.513                       C
HETATM    4  O2           1       2.126   1.168  -0.037                       O
HETATM    5  C3           1       1.452   0.000  -2.053                       C
HETATM    6  O3           1       2.800   0.000  -2.530                       O
HETATM    7  C4           1       0.726   1.257  -2.567                       C
HETATM    8  O4           1       0.726   1.257  -3.997                       O
HETATM    9  C5           1      -0.726   1.257  -2.053                       C
HETATM   10  O5           1      -1.400   2.425  -2.530                       O
HETATM   11  C6           1      -0.726   1.257  -0.513                       C
HETATM   12  O6           1      -2.074   1.257  -0.037                       O
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HETATM   14  O1P          1       0.000  -2.874   1.430                       O
HETATM   15  O2P          1       2.489  -1.437   1.430                       O
HETATM   16  O3P          1       0.830  -1.437   3.565                       O
HETATM   17  P3           1       3.630  -1.437  -1.943                       P
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HETATM   22  O7P          1      -0.104   2.694  -6.343                       O
HETATM   23  O8P          1      -1.763   2.694  -3.997                       O
HETATM   24  O9P          1       0.626   3.959  -4.067                       O
HETATM   25  P5           1      -3.059   2.425  -1.943                       P
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HETATM   27  OPG          1      -3.059   2.425  -0.183                       O
HETATM   28  OPH          1      -3.889   0.988  -2.530                       O
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HETATM   30  H2           1       1.956  -0.874  -0.157                       H
HETATM   31  H3           1       1.673   1.951  -0.357                       H
HETATM   32  H4           1       0.948  -0.874  -2.410                       H
HETATM   33  H5           1       1.230   2.131  -2.210                       H
HETATM   34  H6           1      -1.230   0.384  -2.410                       H
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HETATM   36  H8           1      -2.074   1.257   0.923                       H
CONECT    1    2    3   11   29
CONECT    2    1   13
CONECT    3    1    4    5   30
CONECT    4    3   31
CONECT    5    3    6    7   32
CONECT    6    5   17
CONECT    7    5    8    9   33
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CONECT   12   11   36
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CONECT   19   17
CONECT   20   17
CONECT   21    8   22   23   24
CONECT   22   21
CONECT   23   21
CONECT   24   21
CONECT   25   10   26   27   28
CONECT   26   25
CONECT   27   25
CONECT   28   25
CONECT   29    1
CONECT   30    3
CONECT   31    4
CONECT   32    5
CONECT   33    7
CONECT   34    9
CONECT   35   11
CONECT   36   12
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Charge parameters and atom-types for the Ins(1,3,4,5)P_4 isomers optimized using the DFT level of theory in gas phase and in implicit solvent

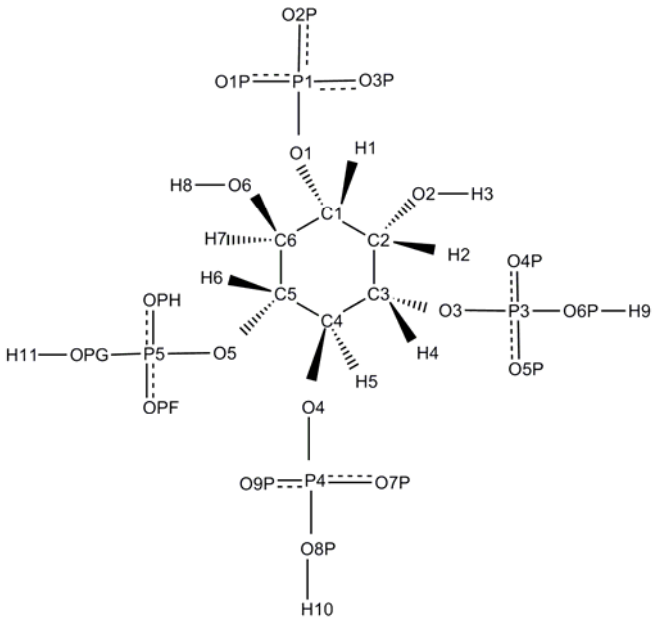

Figure 7: Atomic labelling scheme for the -5 isomer, 1O345H, of Ins(1,3,4,5)P_4.

Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations		Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations
C1	CT	0.064457	0.054532		P4	P	1.259818	1.144515
O1	OS	-0.440653	-0.442010		O7P	O2	-0.851880	-0.799032
C2	CT	0.008829	0.075480		O8P	OH	-0.733737	-0.753892
O2	OH	-0.636875	-0.645566		O9P	O2	-0.823763	-0.816634
C3	CT	0.029218	-0.008141		P5	P	1.206466	1.169697
O3	OS	-0.431196	-0.401554		OPF	O2	-0.847562	-0.834264
C4	CT	0.024091	-0.041055		OPG	OH	-0.759949	-0.728792
O4	OS	-0.430384	-0.390144		OPH	O2	-0.827282	-0.772197
C5	CT	0.002732	0.142454		H1	HC	0.100984	0.101834
O5	OS	-0.433905	-0.431229		H2	HC	0.115432	0.172496
C6	CT	0.051170	0.039379		H3	HO	0.398446	0.379911
O6	OH	-0.646454	-0.615011		H4	HC	0.133396	0.134667
P1	P	1.221593	1.234204		H5	HC	0.134542	0.170174
O1P	O2	-0.889876	-0.929479		H6	HC	0.145124	0.154687
O2P	O2	-0.897616	-0.918606		H7	HC	0.120302	0.077795
O3P	O2	-0.914072	-0.962883		H8	HO	0.485539	0.378535
P3	P	1.250309	1.173772		H9	HY	0.449722	0.462144
O4P	O2	-0.842832	-0.817445		H10	HY	0.427108	0.465369
O5P	O2	-0.878195	-0.854322		H11	HY	0.415118	0.401025
O6P	OH	-0.758166	-0.770411					

Table VII: Atom names, atom-types and charge parameters for the -5 1O345H isomer of Ins(1,3,4,5)P_4. Charge parameters for the 1O345H isomer optimized using the DFT level of theory in both gas phase (Investigation i) and in implicit solvent (Investigation iv), plus assigned atom-types

from the ff99SB force field are provided.

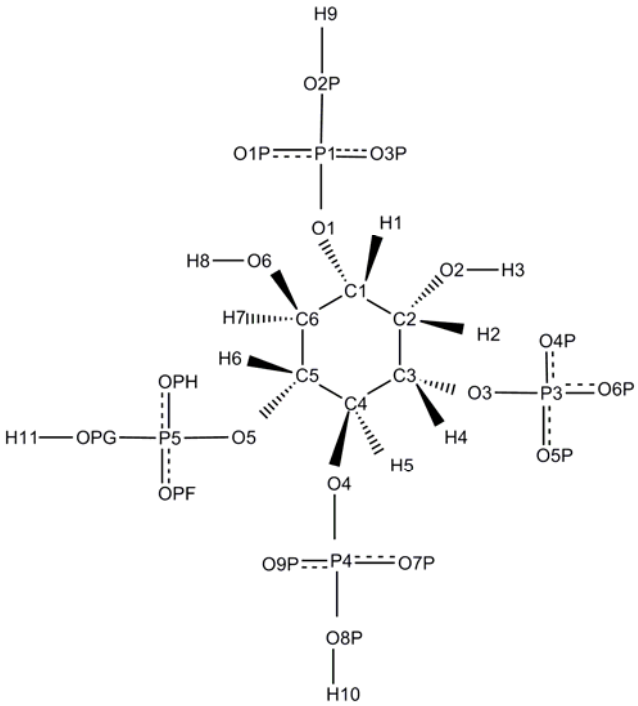

Figure 8: Atomic labelling scheme for the -5 isomer, 3O145H, of Ins(1,3,4,5)P_4.

Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations		Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations
C1	CT	0.025348	0.040405		P4	P	1.188686	1.153536
O1	OS	-0.439751	-0.454266		O7P	O2	-0.832640	-0.814351
C2	CT	0.001280	-0.045884		O8P	OH	-0.716692	-0.803411
O2	OH	-0.630477	-0.638411		O9P	O2	-0.827933	-0.833242
C3	CT	0.024210	-0.023493		P5	P	1.171949	1.190142
O3	OS	-0.377692	-0.313868		OPF	O2	-0.816340	-0.853490
C4	CT	0.007595	-0.060309		OPG	OH	-0.732526	-0.744202
O4	OS	-0.420578	-0.394942		OPH	O2	-0.817281	-0.781105
C5	CT	0.037849	0.025379		H1	HC	0.077313	0.108082
O5	OS	-0.400404	-0.409433		H2	HC	0.147599	0.195950
C6	CT	0.021890	0.039179		H3	HO	0.405027	0.447829
O6	OH	-0.540785	-0.594231		H4	HC	0.099476	0.099343
P1	P	1.182592	1.225168		H5	HC	0.178396	0.209001
O1P	O2	-0.876489	-0.824608		H6	HC	0.143069	0.179736
O2P	OH	-0.861566	-0.722824		H7	HC	0.119300	0.127560
O3P	O2	-0.909832	-0.885626		H8	HO	0.361842	0.358977
P3	P	1.224346	1.161603		H9	HY	0.454961	0.411932
O4P	O2	-0.841628	-0.891608		H10	HY	0.396969	0.505050
O5P	O2	-0.745185	-0.890728		H11	HY	0.372774	0.409618
O6P	O2	-0.854673	-0.908457					

Table VIII: Atom names, atom-types and charge parameters for the -5 3O145H isomer of Ins(1,3,4,5)P_4. Charge parameters for the 3O145H isomer optimized using the DFT level of theory in both gas phase (Investigation i) and in implicit solvent (Investigation iv), plus assigned atom-types

from the ff99SB force field are provided.

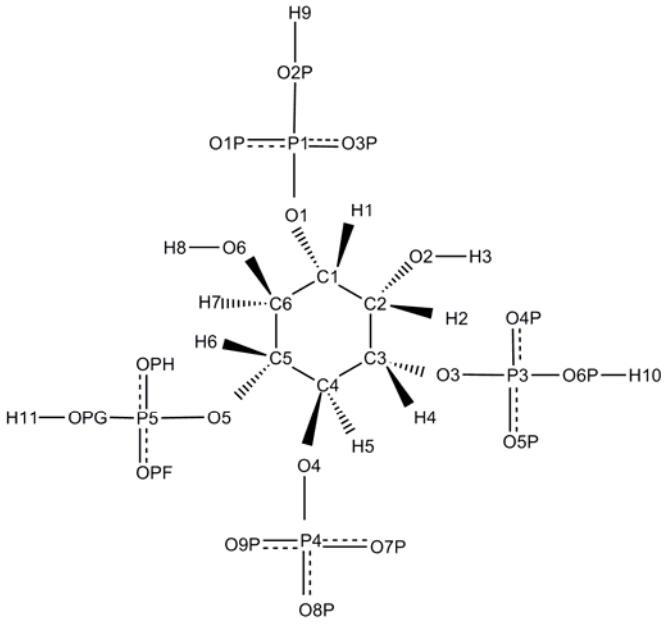

Figure 9: Atomic labelling scheme for the -5 isomer, 4O135H, of Ins(1,3,4,5)P_4.

Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations		Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations
C1	CT	0.067152	0.051815		P4	P	1.154384	1.150013
O1	OS	-0.454090	-0.410885		O7P	O2	-0.757781	-0.790807
C2	CT	0.053995	-0.003845		O8P	O2	-0.830031	-0.817402
O2	OH	-0.600429	-0.646364		O9P	O2	-0.818263	-0.840625
C3	CT	0.029898	-0.013041		P5	P	1.178274	1.173690
O3	OS	-0.429845	-0.373467		OPF	O2	-0.823386	-0.818448
C4	CT	-0.015558	0.001323		OPG	OH	-0.737023	-0.742525
O4	OS	-0.388140	-0.347744		OPH	O2	-0.859649	-0.860035
C5	CT	0.075115	0.032396		H1	HC	0.101603	0.146168
O5	OS	-0.450038	-0.451589		H2	HC	0.102883	0.134737
C6	CT	0.114987	0.057871		H3	HO	0.389414	0.400567
O6	OH	-0.634800	-0.616467		H4	HC	0.112576	0.120579
P1	P	1.281418	1.196497		H5	HC	0.150434	0.199870
O1P	O2	-0.853650	-0.824224		H6	HC	0.126104	0.158223
O2P	OH	-0.745827	-0.721426		H7	HC	0.078517	0.091487
O3P	O2	-0.881105	-0.840392		H8	HO	0.383594	0.389899
P3	P	1.226401	1.176660		H9	HY	0.392764	0.400132
O4P	O2	-0.887978	-0.891130		H10	HY	0.483249	0.499715
O5P	O2	-0.916960	-0.938514		H11	HY	0.457309	0.440110
O6P	OH	-0.875517	-0.872821					

Table IX: Atom names, atom-types and charge parameters for the -5 4O135H isomer of Ins(1,3,4,5)P_4. Charge parameters for the 4O135H isomer optimized using the DFT level of theory in both gas phase (Investigation i) and in implicit solvent (Investigation iv), plus assigned atom-types from the ff99SB force field are provided.

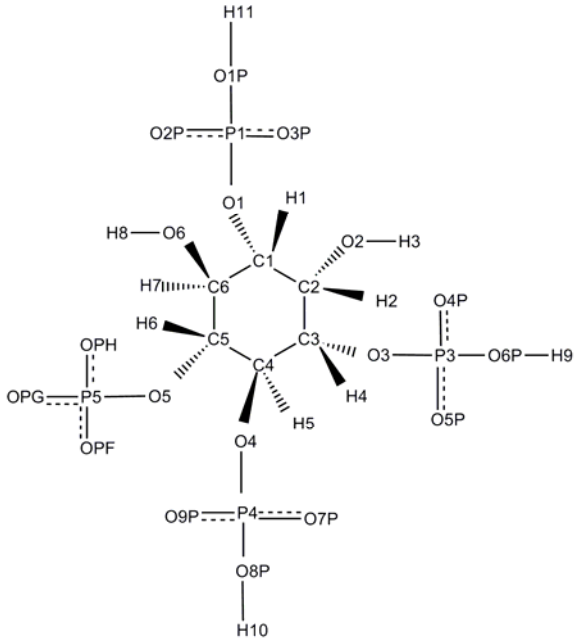

Figure 10: Atomic labelling scheme for the -5 isomer, 5O134H, of Ins(1,3,4,5)P_4.

Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations		Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations
C1	CT	0.123260	0.030379		P4	P	1.289614	1.225117
O1	OS	-0.433811	-0.369027		O7P	O2	-0.860245	-0.859471
C2	CT	0.017893	-0.010909		O8P	OH	-0.762139	-0.813132
O2	OH	-0.647161	-0.670600		O9P	O2	-0.833095	-0.843760
C3	CT	0.065885	-0.000377		P5	P	1.199519	1.253964
O3	OS	-0.432741	-0.433303		OPF	O2	-0.889507	-0.901468
C4	CT	0.064609	-0.036591		OPG	O2	-0.873313	-0.943645
O4	OS	-0.465430	-0.365711		OPH	O2	-0.867124	-0.891553
C5	CT	0.041720	0.010190		H1	HC	0.086896	0.127909
O5	OS	-0.457171	-0.474075		H2	HC	0.099722	0.136338
C6	CT	0.044590	0.164511		H3	HO	0.403981	0.428157
O6	OH	-0.611761	-0.638011		H4	HC	0.112986	0.145792
P1	P	1.207331	1.144348		H5	HC	0.104457	0.174036
O1P	O2	-0.751526	-0.728948		H6	HC	0.111057	0.168703
O2P	OH	-0.849455	-0.816686		H7	HC	0.109183	0.090943
O3P	O2	-0.868837	-0.825319		H8	HO	0.434557	0.390874
P3	P	1.240632	1.190137		H9	HY	0.435962	0.440265
O4P	O2	-0.844004	-0.818523		H10	HY	0.465059	0.524241
O5P	O2	-0.879797	-0.883693		H11	HY	0.411683	0.419305
O6P	OH	-0.743478	-0.740407					

Table X: Atom names, atom-types and charge parameters for the -5 5O134H isomer of Ins(1,3,4,5)P_4. Charge parameters for the 5O134H isomer optimized using the DFT level of theory in both gas phase (Investigation i) and in implicit solvent (Investigation iv), plus assigned atom-types from the ff99SB force field are provided.

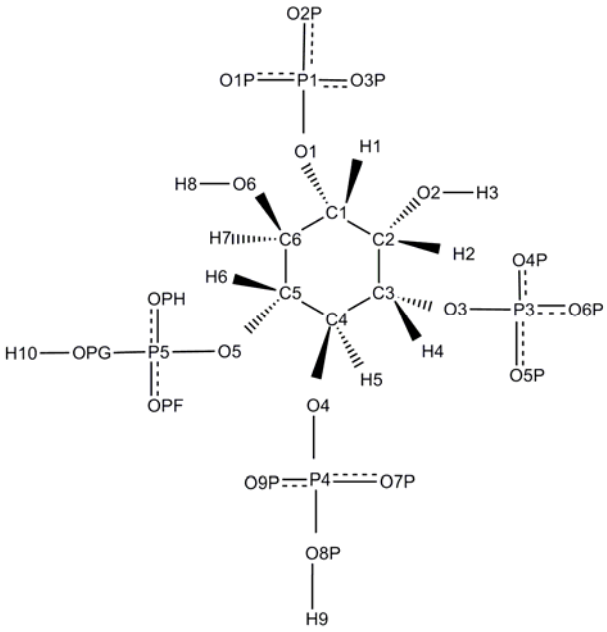

Figure 11: Atomic labelling scheme for the -6 isomer, 13O45H.

Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations		Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations
C1	CT	0.093766	0.040495		P4	P	1.196060	1.179730
O1	OS	-0.439348	-0.447475		O7P	O2	-0.886377	-0.839367
C2	CT	0.007139	-0.013715		O8P	OH	-0.796951	-0.818506
O2	OH	-0.714736	-0.659133		O9P	O2	-0.843762	-0.847359
C3	CT	0.146969	0.016601		P5	P	1.211750	1.229935
O3	OS	-0.477680	-0.354787		OPF	O2	-0.913455	-0.880024
C4	CT	0.270887	-0.010149		OPG	OH	-0.898445	-0.776595
O4	OS	-0.514047	-0.383884		OPH	O2	-0.892259	-0.837850
C5	CT	0.096798	-0.012868		H1	HC	0.089053	0.119010
O5	OS	-0.505482	-0.417740		H2	HC	0.113146	0.185572
C6	CT	0.064200	0.151191		H3	HO	0.478171	0.379343
O6	OH	-0.594670	-0.758614		H4	HC	0.014214	0.107768
P1	P	1.227467	1.212175		H5	HC	0.067743	0.159592
O1P	O2	-0.753984	-0.930290		H6	HC	0.063116	0.132246
O2P	O2	-0.869403	-0.909614		H7	HC	0.115468	0.098671
O3P	O2	-0.896858	-0.945028		H8	HO	0.373761	0.511653
P3	P	1.207054	1.181518		H9	HY	0.508429	0.489190
O4P	O2	-0.910409	-0.906625		H10	HY	0.427991	0.455627
O5P	O2	-0.927561	-0.948150					
O6P	O2	-0.937756	-0.952542					

Table XI: Atom names, atom-types and charge parameters for the -6 13O45H isomer of Ins(1,3,4,5)P_4. Charge parameters for the 13O45H isomer optimized using the DFT level of theory in both gas phase (Investigation i) and in implicit solvent (Investigation iv), plus assigned atom-types from the ff99SB force field are provided.

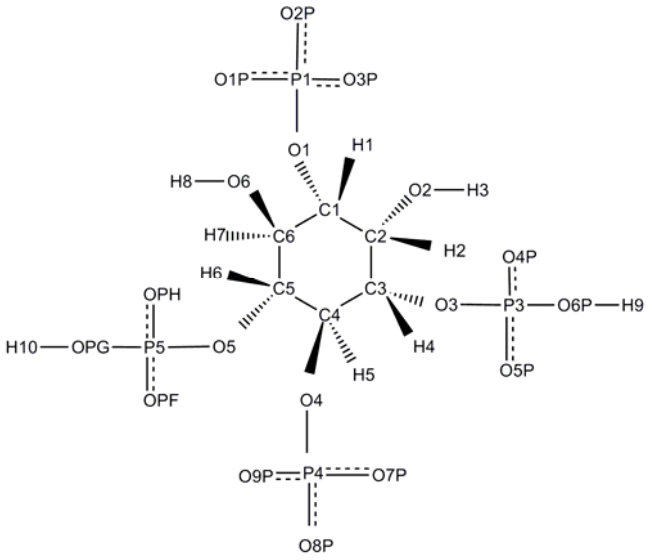

Figure 12: Atomic labelling scheme for the -6 isomer, 14O35H, of Ins(1,3,4,5)P_4.

Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations		Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations
C1	CT	0.087105	0.075569		P4	P	1.197861	1.167154
O1	OS	-0.488174	-0.440517		O7P	O2	-0.937085	-0.953144
C2	CT	-0.090218	0.003380		O8P	O2	-0.934105	-0.883026
O2	OH	-0.563806	-0.660393		O9P	O2	-0.905005	-0.904629
C3	CT	0.083548	-0.025403		P5	P	1.224824	1.276294
O3	OS	-0.491981	-0.394165		OPF	O2	-0.853650	-0.870950
C4	CT	0.447407	-0.009118		OPG	OH	-0.729417	-0.835885
O4	OS	-0.569679	-0.358995		OPH	O2	-0.834759	-0.859487
C5	CT	0.027745	-0.011861		H1	HC	0.111064	0.117419
O5	OS	-0.505153	-0.404841		H2	HC	0.162411	0.103312
C6	CT	0.055585	0.054656		H3	HO	0.378460	0.403045
O6	OH	-0.740504	-0.665474		H4	HC	0.091560	0.140208
P1	P	1.223743	1.224003		H5	HC	0.013005	0.181653
O1P	O2	-0.918376	-0.929374		H6	HC	0.189342	0.153761
O2P	O2	-0.921389	-0.919832		H7	HC	0.130156	0.103834
O3P	O2	-0.946172	-0.951468		H8	HO	0.498909	0.484436
P3	P	1.281248	1.171237		H9	HY	0.393041	0.552291
O4P	O2	-0.889496	-0.847431		H10	HY	0.361793	0.433667
O5P	O2	-0.865293	-0.901082					
O6P	OH	-0.774545	-0.818844					

Table XII: Atom names, atom-types and charge parameters for the -6 14O35H isomer of Ins(1,3,4,5)P_4. Charge parameters for the 14O35H isomer optimized using the DFT level of theory in both gas phase (Investigation i) and in implicit solvent (Investigation iv), plus assigned atom-types from the ff99SB force field are provided.

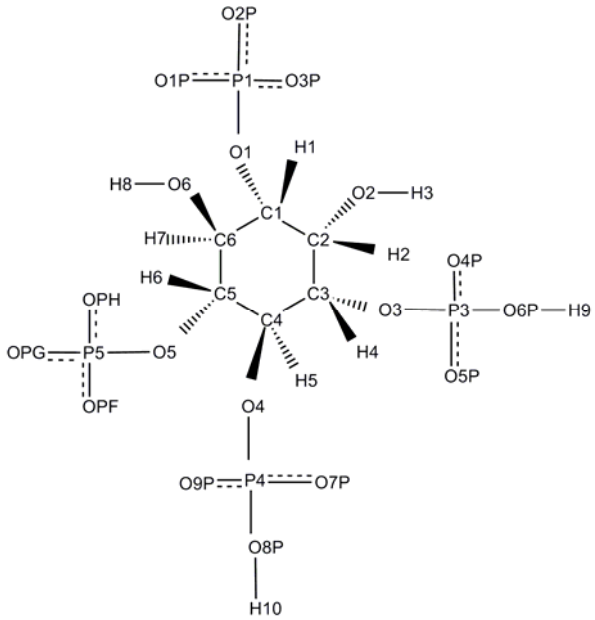

Figure 13: Atomic labelling scheme for the -6 isomer, 15O34H, of Ins(1,3,4,5)P_4.

Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations		Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations
C1	CT	0.089395	0.039687		P4	P	1.248110	1.163037
O1	OS	-0.454519	-0.442716		O7P	O2	-0.891912	-0.894236
C2	CT	0.030986	0.075062		O8P	OH	-0.858599	-0.893942
O2	OH	-0.675099	-0.647495		O9P	O2	-0.808412	-0.885952
C3	CT	0.016353	0.003448		P5	P	1.264643	1.185748
O3	OS	-0.452271	-0.385701		OPF	O2	-0.895760	-0.893543
C4	CT	-0.010827	-0.055839		OPG	O2	-0.854938	-0.849694
O4	OS	-0.429786	-0.373607		OPH	O2	-0.820396	-0.809694
C5	CT	0.044297	0.080212		H1	HC	0.075113	0.110071
O5	OS	-0.479894	-0.414721		H2	HC	0.110894	0.148078
C6	CT	0.164636	0.095682		H3	HO	0.408913	0.365325
O6	OH	-0.669131	-0.641789		H4	HC	0.118709	0.122794
P1	P	1.204602	1.208052		H5	HC	0.156571	0.171731
O1P	O2	-0.915012	-0.928502		H6	HC	0.139567	0.156188
O2P	O2	-0.921008	-0.923910		H7	HC	0.072588	0.062780
O3P	O2	-0.950000	-0.971553		H8	HO	0.432633	0.379792
P3	P	1.242163	1.182467		H9	HY	0.528178	0.498913
O4P	O2	-0.903789	-0.839136		H10	HY	0.496733	0.501294
O5P	O2	-0.944388	-0.898412					
O6P	OH	-0.909340	-0.799919					

Table XIII: Atom names, atom-types and charge parameters for the -6 15O34H isomer of Ins(1,3,4,5)P_4. Charge parameters for the 15O34H isomer optimized using the DFT level of theory in both gas phase (Investigation i) and in implicit solvent (Investigation iv), plus assigned atom-types from the ff99SB force field are provided.

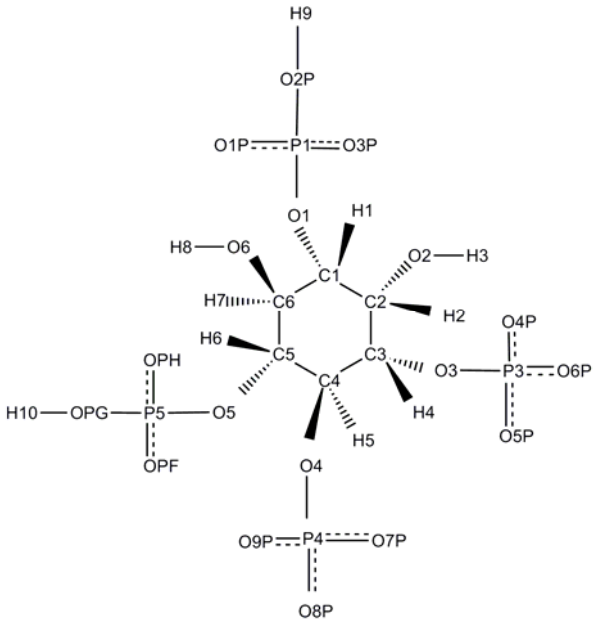

Figure 14: Atomic labelling scheme for the -6 isomer, 34O15H, of Ins(1,3,4,5)P_4.

Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations		Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations
C1	CT	0.350123	0.099150		P4	P	1.207097	1.110517
O1	OS	-0.541851	-0.446383		O7P	O2	-0.960478	-0.928569
C2	CT	-0.048199	-0.055548		O8P	O2	-0.930105	-0.931171
O2	OH	-0.699230	-0.650742		O9P	O2	-0.929292	-0.899224
C3	CT	0.147357	-0.058333		P5	P	1.236009	1.195312
O3	OS	-0.517592	-0.228796		OPF	O2	-0.888834	-0.799040
C4	CT	0.129352	-0.075570		OPG	OH	-0.752439	-0.798958
O4	OS	-0.524221	-0.393788		OPH	O2	-0.873743	-0.871376
C5	CT	0.144544	0.024916		H1	HC	0.065585	0.091548
O5	OS	-0.512323	-0.330904		H2	HC	0.178981	0.196624
C6	CT	0.139986	0.076243		H3	HO	0.481607	0.451336
O6	OH	-0.774836	-0.712871		H4	HC	0.038017	0.068087
P1	P	1.196935	1.210523		H5	HC	0.091567	0.180668
O1P	O2	-0.866932	-0.841187		H6	HC	0.166122	0.141642
O2P	OH	-0.742956	-0.730391		H7	HC	0.086199	0.150563
O3P	O2	-0.891659	-0.900761		H8	HO	0.445868	0.428784
P3	P	1.211382	1.110367		H9	HY	0.434454	0.405697
O4P	O2	-0.925456	-0.897580		H10	HY	0.417632	0.423909
O5P	O2	-0.873079	-0.900964					
O6P	O2	-0.915592	-0.913733					

Table XIV: Atom names, atom-types and charge parameters for the -6 34O15H isomer of Ins(1,3,4,5)P_4. Charge parameters for the 34O15H isomer optimized using the DFT level of theory in both gas phase (Investigation i) and in implicit solvent (Investigation iv), plus assigned atom-types from the ff99SB force field are provided.

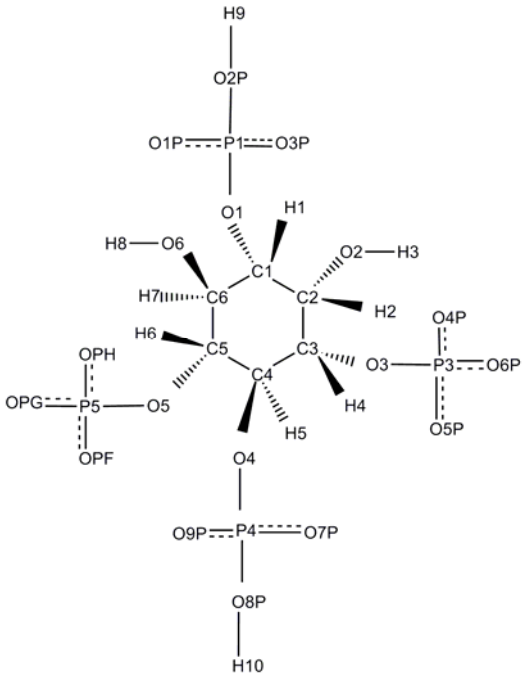

Figure 15: Atomic labelling scheme for the -6 isomer, 35O14H, of Ins(1,3,4,5)P_4.

Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations		Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations
C1	CT	0.088364	0.049933		P4	P	1.117351	1.160362
O1	OS	-0.572709	-0.453692		O7P	O2	-0.873062	-0.867087
C2	CT	0.073581	-0.031240		O8P	OH	-0.718967	-0.841467
O2	OH	-0.568190	-0.654825		O9P	O2	-0.864282	-0.854695
C3	CT	0.079954	-0.014676		P5	P	1.139709	1.223066
O3	OS	-0.500754	-0.314370		OPF	O2	-0.910238	-0.952007
C4	CT	0.374932	-0.051223		OPG	O2	-0.906820	-0.915439
O4	OS	-0.498680	-0.390097		OPH	O2	-0.860828	-0.935988
C5	CT	0.004386	0.025184		H1	HC	0.090050	0.100207
O5	OS	-0.419084	-0.415170		H2	HC	0.169918	0.186514
C6	CT	0.128681	0.061959		H3	HO	0.299892	0.455247
O6	OH	-0.743417	-0.603328		H4	HC	0.035168	0.088403
P1	P	1.299104	1.220359		H5	HC	0.037156	0.189261
O1P	O2	-0.896096	-0.836482		H6	HC	0.200170	0.168737
O2P	OH	-0.741868	-0.738611		H7	HC	0.104527	0.108312
O3P	O2	-0.876369	-0.898820		H8	HO	0.456439	0.346962
P3	P	1.194056	1.153175		H9	HY	0.407503	0.415917
O4P	O2	-0.916010	-0.902317		H10	HY	0.437918	0.547294
O5P	O2	-0.930820	-0.907670					
O6P	O2	-0.940664	-0.921685					

Table XV: Atom names, atom-types and charge parameters for the -6 35O14H isomer of Ins(1,3,4,5)P_4. Charge parameters for the 35O14H isomer optimized using the DFT level of theory in both gas phase (Investigation i) and in implicit solvent (Investigation iv), plus assigned atom-types from the ff99SB force field are provided.

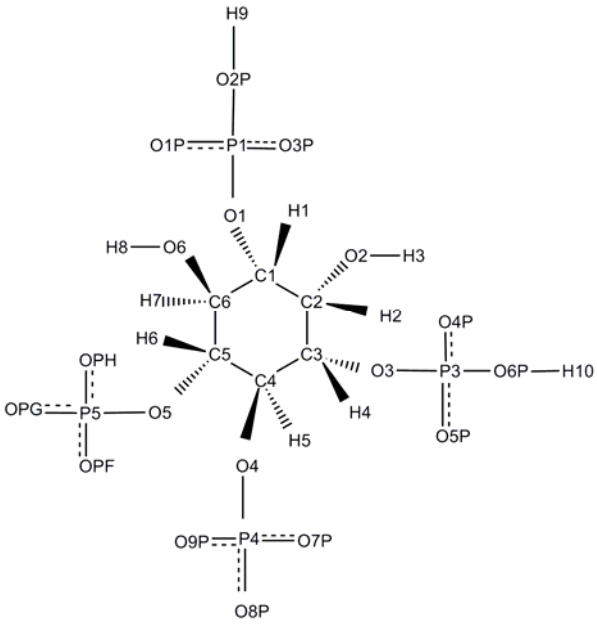

Figure 16: Atomic labelling scheme for the -6 isomer, 45O13H, of Ins(1,3,4,5)P_4.

Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations		Atom	ff99SB atom-type	Charge from gas phase calculations	Charge from implicit solvent calculations
C1	CT	0.093976	0.040394		P4	P	1.232417	1.235426
O1	OS	-0.469224	-0.369916		O7P	O2	-0.899018	-0.855161
C2	CT	0.039703	-0.001886		O8P	O2	-0.859343	-0.868003
O2	OH	-0.672906	-0.662217		O9P	O2	-0.791452	-0.872161
C3	CT	0.030880	-0.046226		P5	P	1.183591	1.138666
O3	OS	-0.471469	-0.395765		OPF	O2	-0.924377	-0.894970
C4	CT	0.234846	-0.022232		OPG	O2	-0.887561	-0.974276
O4	OS	-0.552305	-0.383125		OPH	O2	-0.919193	-0.911625
C5	CT	0.312545	0.072067		H1	HC	0.123491	0.138234
O5	OS	-0.545313	-0.402341		H2	HC	0.222211	0.153541
C6	CT	0.052825	0.045002		H3	HO	0.356090	0.409705
O6	OH	-0.718797	-0.563247		H4	HC	0.072579	0.127197
P1	P	1.210851	1.179642		H5	HC	0.060597	0.167795
O1P	O2	-0.858163	-0.837686		H6	HC	0.034403	0.145398
O2P	OH	-0.744083	-0.731502		H7	HC	0.120220	0.085253
O3P	O2	-0.884459	-0.859626		H8	HO	0.422779	0.331953
P3	P	1.188794	1.193307		H9	HY	0.422007	0.414980
O4P	O2	-0.888018	-0.920389		H10	HY	0.505325	0.526224
O5P	O2	-0.928440	-0.936265					
O6P	OH	-0.906012	-0.896165					

Table XVI: Atom names, atom-types and charge parameters for the -6 45O13H isomer of Ins(1,3,4,5)P_4. Charge parameters for the 45O13H isomer optimized using the DFT level of theory in both gas phase (Investigation i) and in implicit solvent (Investigation iv), plus assigned atom-types from the ff99SB force field are provided.

Absolute energy values

Method	Charge of isomer	Isomer	Absolute energy
QM geometry optimization using DFT level of theory in gas phase	-4	1345H	-2955.51054203 Hartree
	-5	5O134H	-2954.58116343 Hartree
	-6	13O45H	-2953.52631124 Hartree
MM energy minimization in gas phase, with ff99SB atom types	-4	1345H	-11.0011 kcal mol^{-1}
	-5	5O134H	2.38092 kcal mol^{-1}
	-6	13O45H	20.4906 kcal mol^{-1}
QM geometry optimization using MP2 level of theory in gas phase	-4	1345H	-2944.74699756 Hartree
	-5	1O345H	-2943.81328454 Hartree
	-6	13O45H	-2942.76737024 Hartree
MM energy minimization in gas phase, with GAFF atom types	-4	1345H	3.4857 kcal mol^{-1}
	-5	4O135H	12.8553 kcal mol^{-1}
	-6	45O13H	25.3140 kcal mol^{-1}
QM geometry optimization using DFT level of theory in a solvent reaction field	-4	1345H	-2956.29182024Hartree
	-5	4O135H	-2955.78091556 Hartree
	-6	15O34H	-2955.27682553 Hartree
MM energy minimization in implicit solvent	-4	1345H	-705.72 kcal mol^{-1}
	-5	5O134H	-803.51 kcal mol^{-1}
	-6	14O35H	-904.07 kcal mol^{-1}

Table XVII: The absolute energies for the lowest energy isomers, of each charge subset, for each method. Exact digits are given to facilitate the exact reproduction of the calculation.