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Supplementary Material

Hydration States of Cholinium Phosphate-Type Ionic Liquids as the Function of Water Contents

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Elemental analysis of ILs

[Ch][dHp] (C5H16NO5P)
cal : C 29.85, H 8.02, N 6.96 % found: C 29.78, H 8.36, N 7.26 %
[Ch][dBp] 3H2O(C13H38NO8P)
cal: C 42.50, H 10.42, N 3.81% found: C 42.12, H 10.50, N 3.84%.
PC (C5H14NO4P)
cal : C 32.79, H 7.71, N 7.65% found: C 32.22, H 7.383, N 8.01%.

Water contents analyzed with Karl-Fischer titration method

[Ch][dHp]			[Ch][dBp]			PC		
	water ratio (mol/ion-pair)			water ratio (mol/ion-pair)			water ratio (mol/ion-pair)	
water ratio	Exp	Std. error	water ratio	Exp	Std. error	water ratio	Exp	Std. error
1			1	1.36E+00	0.0238	1		
2			2	2.53E+00	0.0685	2		
3	3.02E+00	0.0290	3	2.92E+00	0.0388	3	3.04E+00	0.130257
4	4.51E+00	0.1859	4	3.64E+00	0.0510	4	3.96E+00	0.118077
5	5.35E+00	0.0943	5	4.96E+00	0.2971	5	4.86E+00	0.13596
6	6.18E+00	0.1000	6	6.52E+00	0.5951	6	5.80E+00	0.111341
7	7.02E+00	0.1136	7	6.99E+00	0.3905	7	6.64E+00	0.186194
8	8.19E+00	0.3856	8	8.28E+00	0.3327	8	7.99E+00	0.461706
9	8.82E+00	0.3415	9	9.29E+00	0.4767	9	9.15E+00	0.290416
10	1.01E+01	0.2288	10	1.04E+01	0.1127	10	9.95E+00	0.064552

Details of computational methods

All the C-H bonds were held rigid using the SHAKE algorithm. [A] Reversible RESPA was used for multiple time step integration of equations of motion of atoms. [B,C] The time step size for updating interactions in the Ewald reciprocal space was 8 fs, and that for other interactions was 2 fs. Periodic boundary conditions were employed. The nonbonded forces were truncated at 12 Å, while the Coulomb interactions were computed using the Ewald method. [D] Constant-temperature and -pressure conditions were maintained by using the Nosé-Hoover chain thermostat [E] and Andersen barostat. [F] The time constants for the thermostat and barostat are 0.5 and 2.0 ps, respectively. The force field parameters used for the simulations are summarized in **Table S1** in supporting information. Most of them are taken from OPLS force filed and some parameters were determined based on *ab initio* calculations. Atom types and atomic charges of $[Ch]^+$, $[dHp]^-$, $[dBp]^-$ and PC are shown in **Figures S1**-**S4**. Atomic charges used of the simulations were determined based on atomic charge distributions obtained by electrostatic potential fitting from MP2/6-311G** level *ab initio* calculations. To minimize possible artifacts in the initial configurations, the system was equilibrated at 298 K and 10 MPa started from a low-density condition before the 10 ns equilibrations at 298 K.

The calculated densities and torsional potentials were compared with experimental values and *ab initio* calculations for the validation of the force field. The calculated densities of the mixtures of water with [Ch][dHp], [Ch][dBp] and PC at 298 K are compared with experimental values as shown in **Table S2**. The calculated torsional potentials of $[Ch]^+$ and PC by the force field are compared with those obtained by *ab initio* calculations as shown in **Figures S5-S6**. The calculated densities and torsional potentials using the force field well reproduce the experimental values and *ab initio* calculations.

The geometries of H_2O-$[Ch]^+$ and H_2O-$[dHp]^-$ complexes were optimized from eleven and four initial geometries, respectively. The structures in which oxygen atom of water is close to nitrogen atom of $[Ch]^+$ and those in which water forms hydrogen bonds with $[Ch]^+$ were used as the initial geometries. The structures in which water forms hydrogen bonds with $[dHp]^-$ was used as the initial geometries of the H_2O-$[dHp]^-$ complex.

References:

[A] Ryckaert, J.-P.; Ciccotti, G.; Berendsen, H. J. C., Numerical integration of the cartesian equations of motion of a system with constraints: molecular dynamics of n-alkanes. *J. Comput. Phys.* **1977,** *23* (3), 327-341.

[B] Tuckerman, M.; Berne, B. J.; Martyna, G. J., Reversible multiple time scale molecular dynamics. *J. Chem. Phys.* **1992,** *97* (3), 1990-2001.

[C] Martyna, G. J.; Tuckerman, M. E.; Tobias, D. J.; Klein, M. L., Explicit reversible integrators for extended systems dynamics. *Mol. Phys.* **1996,** *87* (5), 1117-1157.
[D] Allen, M. P.; Tildesley, D. J., *Computer simulation of liquids*. Clarendon Press: 1987.
[E] Martyna, G. J.; Klein, M. L.; Tuckerman, M., Nosé–Hoover chains: The canonical ensemble via continuous dynamics. *J. Chem. Phys.* **1992,** *97* (4), 2635-2643.
[F] Andersen, H. C., Molecular dynamics simulations at constant pressure and/or temperature. *J. Chem. Phys.* **1980,** *72* (4), 2384-2393.

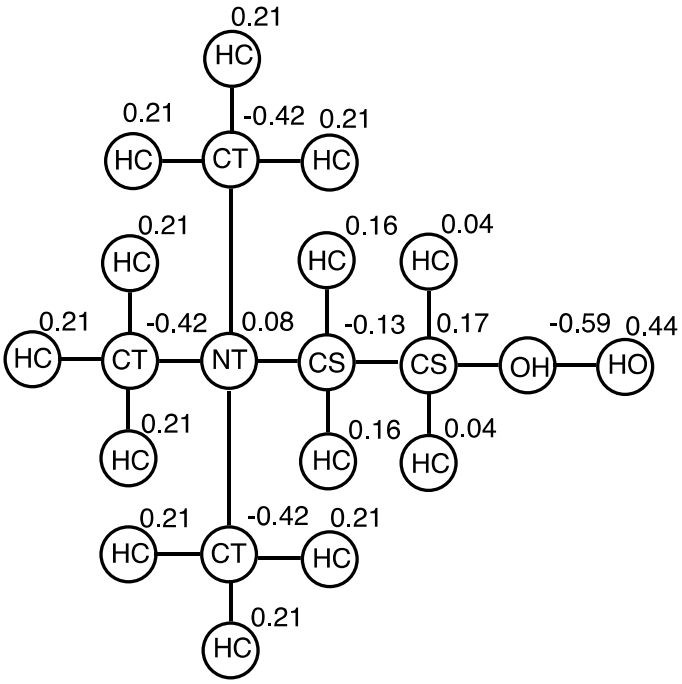

Figure S1. Atom types and atomic charges of cholinium ($[Ch]^+$).

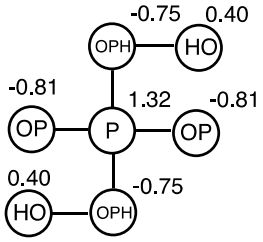

Figure S2. Atom types and atomic charges of dihydrogenphosphate ($[dHp]^-$).

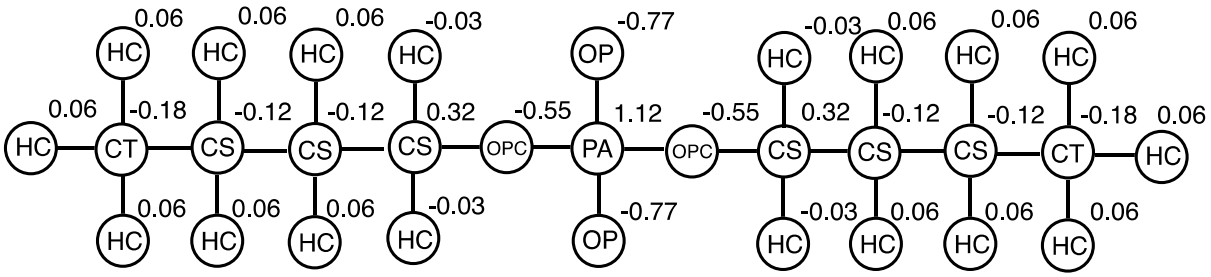

Figure S3. Atom types and atomic charges of dibutylphosphate ($[dBp]^-$).

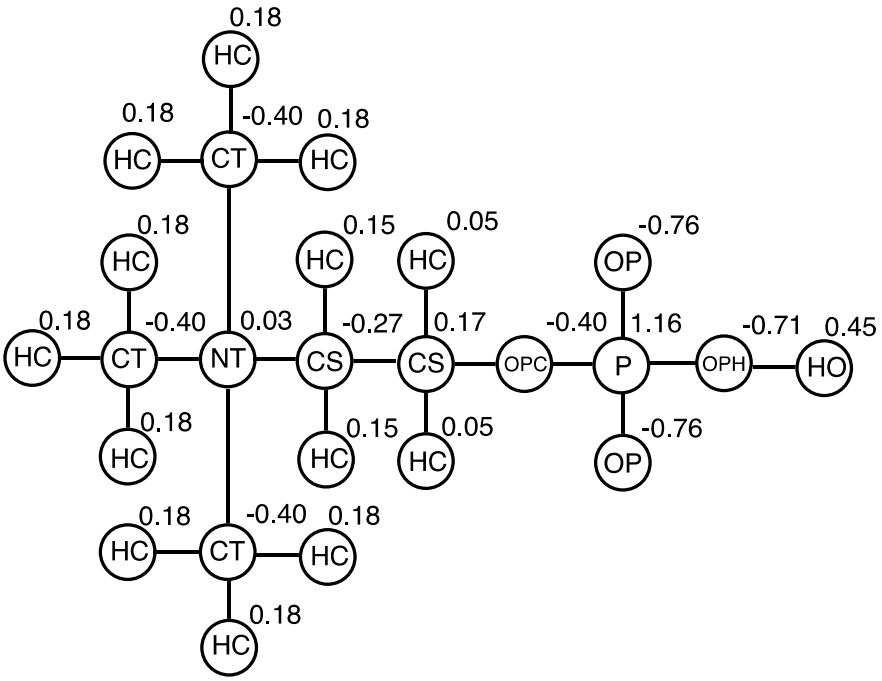

Figure S4. Atom types and atomic charges of phosphocoline (PC).

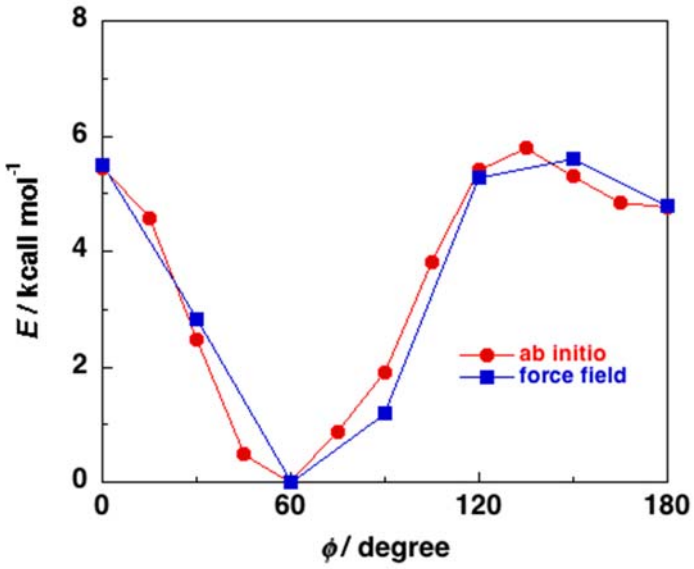

Figure S5. Torsional potential of N-C-C-O bond of cholinium cation ($[Ch]^+$) calculated by MP2/cc-pVTZ//MP2/6-311G** level *ab initio* calculations and that obtained by force field calculations.

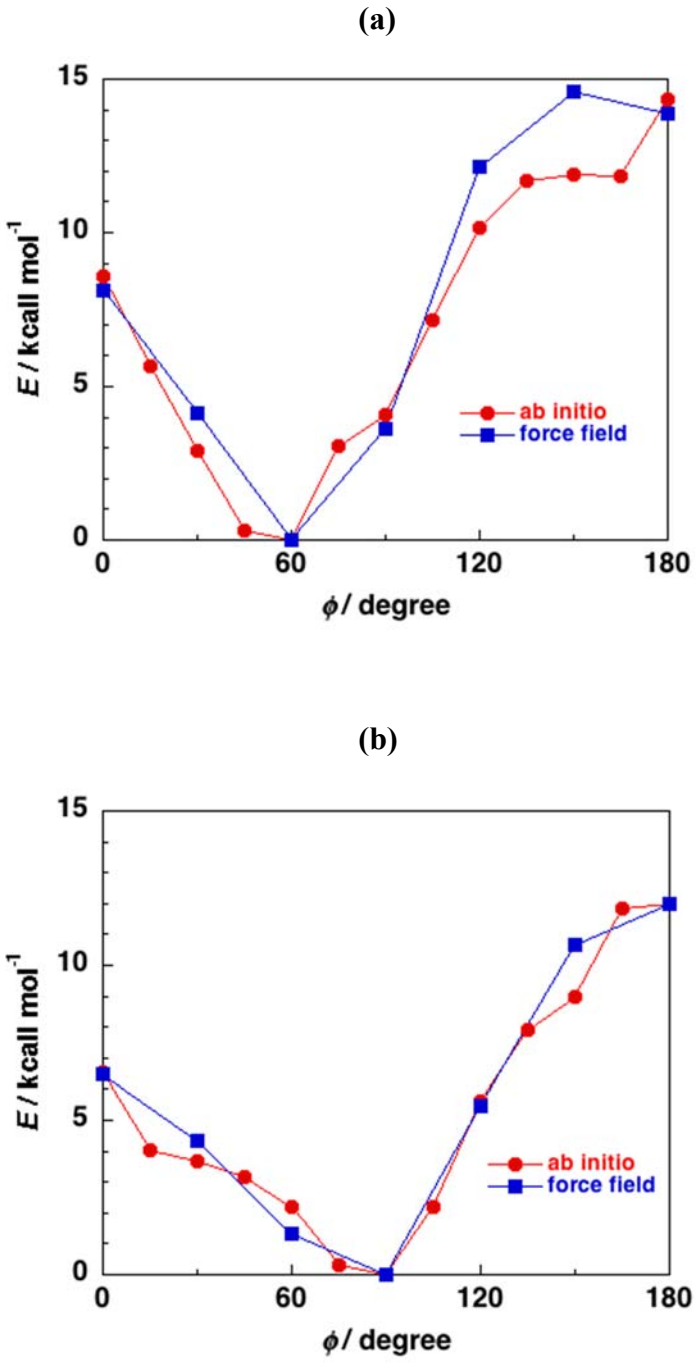

Figure S6. Torsional potentials of (a) N-C-C-O and (b) C-C-O-P bonds of phosphocholine (PC) calculated by MP2/cc-pVTZ//MP2/6-311G** level *ab initio* calculations and that obtained by force field calculations.

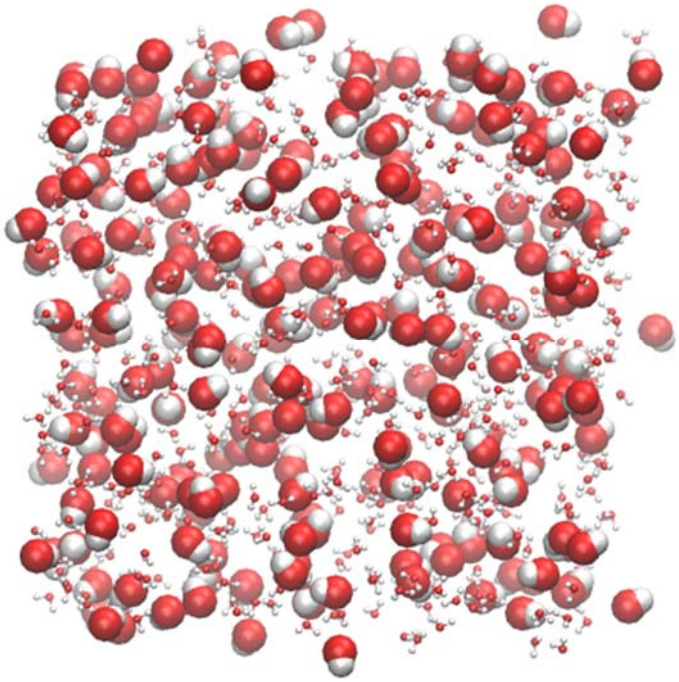

Figure S7. Snapshot of MD simulation of the 2:1 mixtures water and [Ch][dHp]. Water molecules and enhanced hydroxyl groups of $[dHp]^+$ are shown.

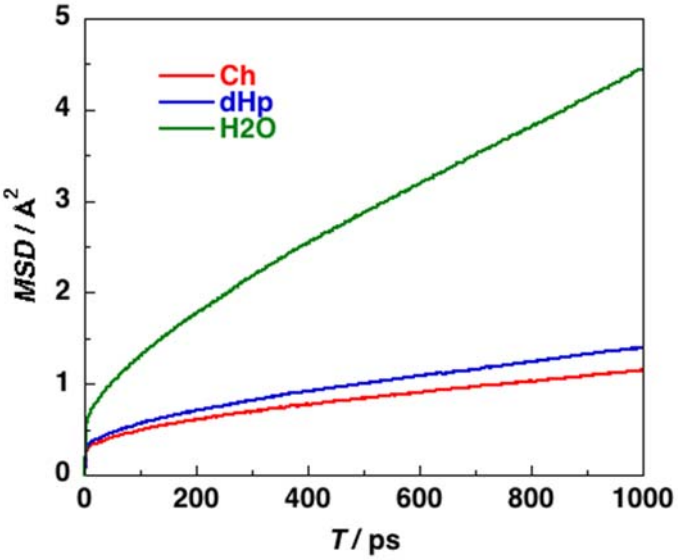

Figure S8. Mean square displacements of $[Ch]^+$, $[dHp]^-$ and water in the 2:1 mixture of water and [Ch][dHp].

Table S1. Force field parameters used for molecular dynamics simulations (Atom types were explained in **Figures S4 and S5**).

Nonbonding parameters

atom	σ (Å)	ε (kJ mol^{-1})
CT	3.5	0.066
CS	3.5	0.066
NT	3.45	0.17
OH	3.12	0.17
HC	2.5	0.03
HO	2.5	0.03
OPC	3.12	0.17
OPH	3.12	0.17
OP	3.12	0.17
P	3.742	0.2
PA	3.742	0.2

$E_{nonbond} = 4\varepsilon [(\sigma/r)^{12} - (\sigma/r)^{6}]$

Bond stretching parameters

bond	k_s (kJ mol^{-1} Å^{-2})	r_0 (Å)
CS-CS	268.0	1.529
CS-CT	268.0	1.529
CS-HC	331.0	1.09
CT-HC	331.0	1.09
CS-NT	382.0	1.48
CT-NT	382.0	1.48
CS-OH	320.0	1.41
OH-HO	553.0	0.945
CS-OPC	570.0	1.408
P-OP	190.0	1.515
P-OPC	190.0	1.705
P-OPH	190.0	1.705
OPH-HO	331.0	0.965

PA-OP	190.0	1.515
PA-OPC	190.0	1.705

$E_{str} = k_s (r - r_0)^2$

Angle bending parameters

angle	k_θ(kJ mol^{-1} rad^{-2})	θ_0 (deg)
CS-CS-CS	100.0	112.0
CS-CS-CT	100.0	112.0
CS-CS-HC	37.43	110.7
CT-CS-HC	37.43	110.7
CS-CT-HC	37.43	110.7
NT-CS-CS	56.2	109.47
NT-CS-HC	35.0	100.0
NT-CT-HC	35.0	100.0
CS-NT-CS	51.8	107.2
CS-NT-CT	51.8	107.2
CT-NT-CT	51.8	107.2
CS-CS-OH	80.0	110.0
OH-CS-HC	35.0	109.5
CS-OH-HO	55.0	106.5
CS-CS-OPC	80.0	104.0
HC-CS-OPC	35.0	109.0
CS-OPC-P	55.0	110.0
OPC-P-OPH	80.0	93.0
OPC-P-OP	80.0	107.0
OP-P-OP	80.0	123.0
OP-P-OPH	80.0	105.0
P-OPH-HO	37.43	110.7
OPH-P-OPH	80.0	101.0
CS-OPC-PA	55.0	110.0
OPC-PA-OP	80.0	107.0
OPC-PA-OPC	80.0	93.0

$E_{bend} = k_\theta(\theta - \theta_0)^2$

Tonsional parameters

dihedral	V_1 (kJ mol^{-1})	V_2 (kJ mol^{-1})	V_3 (kJ mol^{-1})
CS-CS-CS-CT	0.424	0.051	-0.008
CS-CS-CS-HC	0.0	0.0	0.366
CS-CS-CT-HC	0.0	0.0	0.366
CT-CS-CS-HC	0.0	0.0	0.366
HC-CS-CS-HC	0.0	0.0	0.318
HC-CS-CT-HC	0.0	0.0	0.318
CS-NT-CT-HC	0.0	0.0	0.27
CT-NT-CS-CS	0.0	0.0	0.093
CT-NT-CS-HC	0.0	0.0	0.27
NT-CS-CS-OH	-3.6	2.4	0.0
NT-CS-CS-HC	-1.013	0.709	0.473
HC-CS-CS-OH	0.0	0.0	0.366
CS-CS-OH-HO	-1.6	0.0	0.0
NT-CS-CS-OPC	-12.2	3.8	1.8
HC-CS-CS-OPC	0.0	0.0	0.366
CS-CS-OPC-P	-14.0	4.7	0.0
HC-CS-OPC-P	0.0	0.0	0.67
CS-OPC-P-OPH	0.6	3.5	0.0
CS-OPC-P-OP	0.01	0.01	0.01
OPC-P-OPH-HO	0.01	0.01	0.01
OP-P-OPH-HO	0.01	0.01	0.01
OPH-P-OPH-HO	0.01	2.0	0.01
CS-CS-CS-OPC	-1.0	0.0	0.2
CS-CS-OPC-PA	-6.6	-1.0	0.0
HC-CS-OPC-PA	0.0	0.0	0.67
CS-OPC-PA-OPC	-3.0	1.5	0.5
CS-OPC-PA-OP	0.01	0.01	0.01

$E_{torsion} = \Sigma\ V_n/2\ (1 + \cos(n\Phi))$

Table S2. Experimental and calculated densities of the mixtures of water with [Ch][dHp], [Ch][dBp] and PC at 298 K.

Mixtures	d_{exp}[a]	d_{calc}[b]
[Ch][dHp] : water = 1:3	1.28	1.22
[Ch][dHp] : water = 1:7	1.20	1.17
[Ch][dBp] : water = 1:3	1.09	1.07
[Ch][dBp] : water = 1:7	1.04	1.06
PC : water = 1:3	1.27	1.25
PC : water = 1:7	1.19	1.19

[a] Experimental density (g cm^{-3}).

[b] Density calculated by MD simulation (g cm^{-3}).

Cartesian coordinates of optimized geometries in Figure 2

Cholinium cation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.870210	0.022170	0.000000
2	6	0	1.117860	-0.805220	1.225030
3	6	0	1.824700	1.180470	-0.000180
4	6	0	1.117950	-0.805640	-1.224730
5	6	0	-0.530490	0.582070	-0.000100
6	1	0	0.874580	-0.204940	2.102560
7	1	0	0.494610	-1.697060	1.189290
8	1	0	2.170970	-1.088570	1.239530
9	1	0	2.843210	0.790780	-0.000040
10	1	0	1.645300	1.776500	-0.895360
11	1	0	1.645180	1.776870	0.894720
12	1	0	0.874590	-0.205730	-2.102480
13	1	0	2.171090	-1.088890	-1.239140
14	1	0	0.494800	-1.697540	-1.188640
15	6	0	-1.663990	-0.439490	-0.000010
16	1	0	-0.619530	1.211680	0.888620
17	1	0	-0.619470	1.211500	-0.888950
18	8	0	-2.804730	0.388710	-0.000030
19	1	0	-1.620510	-1.074500	-0.893390
20	1	0	-1.620470	-1.074400	0.893450
21	1	0	-3.584150	-0.173710	0.000000

Phosphocholine

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.652740	0.026420	0.000010
2	6	0	-2.777980	-0.827790	-1.222100
3	6	0	-3.748050	1.040880	-0.000210

4	6	0	-2.777780	-0.827020	1.222680
5	6	0	-1.325000	0.758630	-0.000330
6	1	0	-2.605480	-0.200030	-2.096990
7	1	0	-2.032510	-1.619010	-1.182420
8	1	0	-3.783740	-1.250790	-1.244150
9	1	0	-4.709320	0.524380	0.000060
10	1	0	-3.646550	1.657640	0.893160
11	1	0	-3.646740	1.657040	-0.894010
12	1	0	-2.605160	-0.198710	2.097150
13	1	0	-3.783520	-1.250040	1.245150
14	1	0	-2.032280	-1.618240	1.183400
15	6	0	-0.106440	-0.146180	-0.000240
16	1	0	-1.316780	1.389380	-0.892830
17	1	0	-1.316560	1.389810	0.891870
18	8	0	0.960420	0.748360	-0.000490
19	1	0	-0.081860	-0.785040	0.894170
20	1	0	-0.081990	-0.785430	-0.894370
21	15	0	2.421390	-0.142010	0.000090
22	8	0	3.331240	1.221650	-0.000410
23	8	0	2.482170	-0.853570	1.311010
24	8	0	2.482500	-0.854780	-1.310150
25	1	0	4.251680	0.949930	-0.000180

Dihydrogen phosphate anion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.000019	0.000098	-0.174008
2	8	0	-0.961860	-0.853794	0.887000
3	8	0	0.962107	0.852901	0.887600
4	8	0	0.894642	-0.988019	-0.848684
5	8	0	-0.894848	0.988892	-0.847472
6	1	0	-1.733412	-0.293773	0.991023
7	1	0	1.733359	0.292448	0.991541

Dibutylphosphate anion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.000020	-2.002350	-0.000010
2	8	0	1.090180	-0.905750	-0.649280
3	8	0	-1.090230	-0.905790	0.649290
4	8	0	-0.638380	-2.670200	-1.168310
5	8	0	0.638210	-2.670280	1.168310
6	6	0	1.889580	-0.217050	0.290400
7	6	0	-1.889590	-0.217030	-0.290390
8	6	0	2.667200	0.864270	-0.443940
9	1	0	1.264210	0.242680	1.070080
10	1	0	2.580530	-0.909340	0.789730
11	6	0	3.598010	1.648530	0.479550
12	1	0	3.249140	0.392420	-1.245570
13	1	0	1.955570	1.549220	-0.921980
14	6	0	4.375690	2.743210	-0.252650
15	1	0	3.008150	2.096630	1.289370
16	1	0	4.301960	0.953780	0.954890
17	1	0	5.039270	3.293400	0.423420
18	1	0	4.987580	2.310560	-1.051390
19	1	0	3.688170	3.461310	-0.712260
20	6	0	-2.667180	0.864300	0.443950
21	1	0	-1.264170	0.242690	-1.070040
22	1	0	-2.580560	-0.909260	-0.789770
23	6	0	-3.597910	1.648640	-0.479550
24	1	0	-3.249150	0.392460	1.245550
25	1	0	-1.955510	1.549200	0.922030
26	6	0	-4.375560	2.743340	0.252670
27	1	0	-3.008010	2.096740	-1.289330
28	1	0	-4.301890	0.953940	-0.954930
29	1	0	-5.039090	3.293580	-0.423410
30	1	0	-4.987490	2.310700	1.051380
31	1	0	-3.688010	3.461390	0.712320

Cartesian coordinates of optimized geometries in Figure 4

A1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.454680	0.041110	0.012440
2	6	0	1.325250	1.396510	-0.627090
3	6	0	2.835430	-0.476590	-0.249280
4	6	0	1.249760	0.171560	1.489820
5	6	0	0.459330	-0.930880	-0.598370
6	1	0	1.586310	1.296410	-1.681340
7	1	0	0.296050	1.727380	-0.515210
8	1	0	2.023870	2.070000	-0.128680
9	1	0	3.555500	0.272990	0.081130
10	1	0	2.973680	-1.405410	0.305110
11	1	0	2.941930	-0.654360	-1.320150
12	1	0	1.280300	-0.822330	1.938290
13	1	0	2.058360	0.785850	1.887900
14	1	0	0.285800	0.649170	1.658410
15	6	0	-0.949860	-0.845060	-0.034280
16	1	0	0.463150	-0.723120	-1.671160
17	1	0	0.857370	-1.934660	-0.424160
18	8	0	-1.409120	0.481710	-0.110330
19	1	0	-1.553740	-1.531330	-0.641860
20	1	0	-0.965480	-1.226030	0.995710
21	1	0	-2.381870	0.448230	-0.035440
22	8	0	-4.072570	0.065810	0.043150
23	1	0	-4.614180	0.242970	0.815740
24	1	0	-4.655750	0.243170	-0.698650

A2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-0.079810	0.388710	-0.087010
2	6	0	-0.279670	-0.506820	-1.278460
3	6	0	-1.058690	1.521150	-0.191080
4	6	0	-0.367390	-0.389490	1.161110
5	6	0	1.318180	0.971160	-0.074610
6	1	0	-0.143740	0.094950	-2.178040
7	1	0	0.456700	-1.304720	-1.239310
8	1	0	-1.298890	-0.888600	-1.227230
9	1	0	-2.054710	1.091930	-0.300070
10	1	0	-0.991770	2.121210	0.717420
11	1	0	-0.794690	2.123720	-1.061450
12	1	0	-0.168300	0.249170	2.023320
13	1	0	-1.418150	-0.679390	1.127640
14	1	0	0.276720	-1.267710	1.171080
15	6	0	2.404560	0.064720	0.477320
16	1	0	1.538600	1.251400	-1.107680
17	1	0	1.273300	1.875560	0.538800
18	8	0	2.406520	-1.147990	-0.250560
19	1	0	3.341430	0.622680	0.355280
20	1	0	2.254250	-0.105790	1.549960
21	1	0	3.210320	-1.627210	-0.029600
22	8	0	-3.513460	-0.670350	0.161690
23	1	0	-4.203380	-0.330000	0.737340
24	1	0	-3.965510	-1.365790	-0.323120

A3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.112110	0.814810	-0.004710
2	6	0	-1.388570	1.592960	-0.150570
3	6	0	1.022690	1.657010	-0.506400
4	6	0	0.123850	0.505710	1.440690
5	6	0	-0.150880	-0.453510	-0.839010
6	1	0	-1.488220	1.884150	-1.196950
7	1	0	-2.218080	0.958660	0.149660
8	1	0	-1.314350	2.479770	0.480390

9	1	0	0.990100	2.618400	0.007860
10	1	0	1.952480	1.131340	-0.292140
11	1	0	0.894310	1.802220	-1.580020
12	1	0	1.027440	-0.098760	1.515420
13	1	0	0.258530	1.451730	1.966860
14	1	0	-0.748070	-0.019510	1.827800
15	6	0	-0.895030	-1.619870	-0.215060
16	1	0	-0.603740	-0.169510	-1.792150
17	1	0	0.888870	-0.753380	-0.984840
18	8	0	-2.209660	-1.216270	0.120290
19	1	0	-0.886620	-2.410980	-0.975280
20	1	0	-0.350190	-1.993010	0.660260
21	1	0	-2.719640	-2.003810	0.330400
22	8	0	2.944250	-1.038930	0.052420
23	1	0	3.260890	-1.671620	0.702530
24	1	0	3.691970	-0.961550	-0.546340

A4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.020960	0.779330	0.004070
2	6	0	-1.212510	1.679130	-0.062890
3	6	0	1.174550	1.491510	-0.558980
4	6	0	0.271100	0.438020	1.439830
5	6	0	-0.230490	-0.486080	-0.807020
6	1	0	-1.452380	1.870920	-1.109830
7	1	0	-2.043220	1.193130	0.446800
8	1	0	-0.956650	2.613900	0.437380
9	1	0	1.387870	2.352040	0.076590
10	1	0	2.011930	0.792690	-0.557820
11	1	0	0.935850	1.822530	-1.570560
12	1	0	1.174150	-0.171020	1.451220
13	1	0	0.427110	1.373650	1.978760
14	1	0	-0.573060	-0.115780	1.841220
15	6	0	-1.616630	-1.099590	-0.715710
16	1	0	-0.038660	-0.218480	-1.850250

17	1	0	0.539990	-1.180740	-0.467620
18	8	0	-1.926150	-1.347350	0.642410
19	1	0	-2.360900	-0.446340	-1.187090
20	1	0	-1.565200	-2.024620	-1.303710
21	1	0	-2.712520	-1.899880	0.672820
22	8	0	2.947120	-1.210500	0.018900
23	1	0	3.614240	-1.280610	0.706870
24	1	0	3.274350	-1.811900	-0.655080

A5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.591995	-0.068136	0.010556
2	6	0	-1.538282	-1.012081	-1.150600
3	6	0	-2.716231	0.900691	-0.201165
4	6	0	-1.852438	-0.835366	1.270831
5	6	0	-0.308612	0.721869	0.115993
6	1	0	-1.262394	-0.447702	-2.042221
7	1	0	-0.799646	-1.786218	-0.947889
8	1	0	-2.524786	-1.460516	-1.275507
9	1	0	-3.654670	0.345542	-0.229157
10	1	0	-2.719163	1.611890	0.625317
11	1	0	-2.553242	1.419994	-1.145810
12	1	0	-1.885355	-0.130533	2.102222
13	1	0	-2.810386	-1.346943	1.168964
14	1	0	-1.055642	-1.560870	1.421240
15	6	0	0.980706	-0.091193	0.194889
16	1	0	-0.269436	1.377192	-0.757178
17	1	0	-0.389548	1.337652	1.015315
18	8	0	1.949197	0.886093	0.463120
19	1	0	0.925335	-0.844241	0.993790
20	1	0	1.170572	-0.607585	-0.754156
21	1	0	2.806889	0.515908	0.188294
22	8	0	4.197185	-0.361632	-0.429777
23	1	0	4.730468	0.042728	-1.118338
24	1	0	4.844435	-0.703032	0.191948

A6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.360460	-0.878250	-0.027810
2	6	0	0.267850	-2.235370	-0.026160
3	6	0	-1.513780	-0.869040	-0.989770
4	6	0	-0.882000	-0.553830	1.341090
5	6	0	0.616860	0.172240	-0.488980
6	1	0	0.701700	-2.418860	-1.010110
7	1	0	1.038030	-2.275170	0.743000
8	1	0	-0.507520	-2.971950	0.188120
9	1	0	-2.245600	-1.604930	-0.653940
10	1	0	-1.938300	0.135070	-0.989370
11	1	0	-1.137700	-1.134940	-1.978290
12	1	0	-1.294980	0.454780	1.308890
13	1	0	-1.653930	-1.283920	1.588520
14	1	0	-0.067220	-0.623560	2.059650
15	6	0	1.904930	0.290190	0.318450
16	1	0	0.864000	-0.060280	-1.527660
17	1	0	0.082210	1.122370	-0.451380
18	8	0	2.524140	1.415140	-0.269470
19	1	0	1.694000	0.455780	1.381960
20	1	0	2.516870	-0.613540	0.212100
21	1	0	3.413220	1.485670	0.088000
22	8	0	-2.093920	2.227460	0.046870
23	1	0	-3.009960	2.423330	0.261050
24	1	0	-1.736470	3.091960	-0.172890

A7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.200510	0.275400	0.000990

2	6	0	-0.611340	-0.492500	-1.220350
3	6	0	-0.923920	1.589550	-0.001630
4	6	0	-0.607400	-0.484890	1.228280
5	6	0	1.277230	0.560470	-0.002250
6	1	0	-0.262140	0.051070	-2.099420
7	1	0	-0.160820	-1.483320	-1.185680
8	1	0	-1.699110	-0.567560	-1.211100
9	1	0	-1.993280	1.382730	0.001840
10	1	0	-0.633240	2.144970	0.890690
11	1	0	-0.637570	2.139080	-0.898990
12	1	0	-0.253660	0.062890	2.102920
13	1	0	-1.695300	-0.557670	1.224270
14	1	0	-0.159130	-1.476840	1.197320
15	6	0	2.196580	-0.656460	0.000290
16	1	0	1.483430	1.158880	-0.893230
17	1	0	1.486300	1.164630	0.884170
18	8	0	3.477390	-0.063470	-0.003140
19	1	0	2.034380	-1.268620	0.895720
20	1	0	2.032110	-1.274080	-0.890960
21	1	0	4.131380	-0.767620	-0.002040
22	8	0	-3.691500	-0.492180	-0.002470
23	1	0	-4.461920	0.081840	-0.021860
24	1	0	-4.081830	-1.370060	0.018270

A8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.074720	-0.012520	0.000000
2	6	0	0.868350	0.830110	-1.224140
3	6	0	2.477630	-0.539440	0.000010
4	6	0	0.868280	0.829930	1.224250
5	6	0	0.144160	-1.196400	-0.000090
6	1	0	0.931410	0.183000	-2.100140
7	1	0	-0.102860	1.318350	-1.156690
8	1	0	1.661820	1.578480	-1.253220
9	1	0	3.165650	0.306500	0.000190

10	1	0	2.621260	-1.145510	0.895090
11	1	0	2.621390	-1.145230	-0.895240
12	1	0	0.931500	0.182720	2.100170
13	1	0	1.661630	1.578430	1.253380
14	1	0	-0.103010	1.318020	1.156920
15	6	0	-1.347080	-0.879240	-0.000390
16	1	0	0.381750	-1.786760	-0.888590
17	1	0	0.381380	-1.786530	0.888670
18	8	0	-1.920840	-2.170090	0.000350
19	1	0	-1.625100	-0.305010	0.890570
20	1	0	-1.624940	-0.306090	-0.892100
21	1	0	-2.876380	-2.071920	-0.000530
22	8	0	-1.740910	2.440460	0.000080
23	1	0	-2.696470	2.341910	0.000320
24	1	0	-1.626090	3.394630	-0.000100

A9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.179710	0.048950	-0.023090
2	6	0	-2.030730	-1.089410	0.442580
3	6	0	-1.906090	0.797880	-1.100330
4	6	0	-0.917420	0.992930	1.118040
5	6	0	0.112020	-0.453110	-0.617760
6	1	0	-2.246190	-1.734800	-0.410090
7	1	0	-1.494750	-1.643250	1.212770
8	1	0	-2.955780	-0.683610	0.854470
9	1	0	-2.878630	1.105250	-0.714260
10	1	0	-1.309790	1.669710	-1.370990
11	1	0	-2.029330	0.139110	-1.960530
12	1	0	-0.102970	1.658680	0.830210
13	1	0	-1.838260	1.542350	1.316880
14	1	0	-0.637180	0.417080	1.998390
15	6	0	1.060600	-1.142180	0.359660
16	1	0	-0.155280	-1.130760	-1.432200
17	1	0	0.621420	0.423690	-1.018250

18	8	0	2.295470	-1.147490	-0.343130
19	1	0	1.152330	-0.576070	1.291230
20	1	0	0.725340	-2.160370	0.584130
21	1	0	2.846000	-1.844400	0.024820
22	8	0	2.112420	1.703190	0.069170
23	1	0	2.670680	0.944190	-0.134370
24	1	0	2.717030	2.448300	0.067860

B1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.407950	-0.000010	-0.000020
2	8	0	-1.450380	-0.949820	0.869640
3	8	0	-1.450450	0.949860	-0.869510
4	8	0	0.295420	0.906050	0.963500
5	8	0	0.295260	-0.906080	-0.963610
6	1	0	-1.501520	-1.762070	0.361710
7	1	0	-1.501480	1.762120	-0.361580
8	8	0	2.887940	0.000030	0.000050
9	1	0	2.249630	0.472210	0.551410
10	1	0	2.250260	-0.472460	-0.551750

B2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.570880	-0.004460	-0.168360
2	8	0	-0.282400	0.935830	0.920050
3	8	0	1.578790	-0.841880	0.844290
4	8	0	-0.411220	-1.004430	-0.702470
5	8	0	1.399580	0.931500	-0.978290
6	1	0	0.169310	1.782100	0.909280
7	1	0	1.105670	-1.655280	1.030660
8	8	0	-2.938120	-0.033070	-0.022100

9	1	0	-2.201420	-0.524360	-0.423660
10	1	0	-2.409640	0.560920	0.517240

B3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.592940	-0.054120	-0.145830
2	8	0	-0.146180	-0.801640	1.088990
3	8	0	1.318870	1.193360	0.603120
4	8	0	1.647370	-0.937390	-0.652190
5	8	0	-0.477930	0.518530	-0.991340
6	1	0	-1.029470	-0.484120	1.186690
7	1	0	2.192400	0.936950	0.837760
8	8	0	-2.945420	0.109640	0.060960
9	1	0	-2.164990	0.440950	-0.392420
10	1	0	-3.065620	-0.742000	-0.320910
