Supporting Information for "*Implications of Protonation and Substituent Effects for C-O and O-P Bond Cleavage in Phosphate Monoesters*"

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Reference 55**:**

(55) Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara,

A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Gaussian, Inc.: Wallingford CT, 2004.

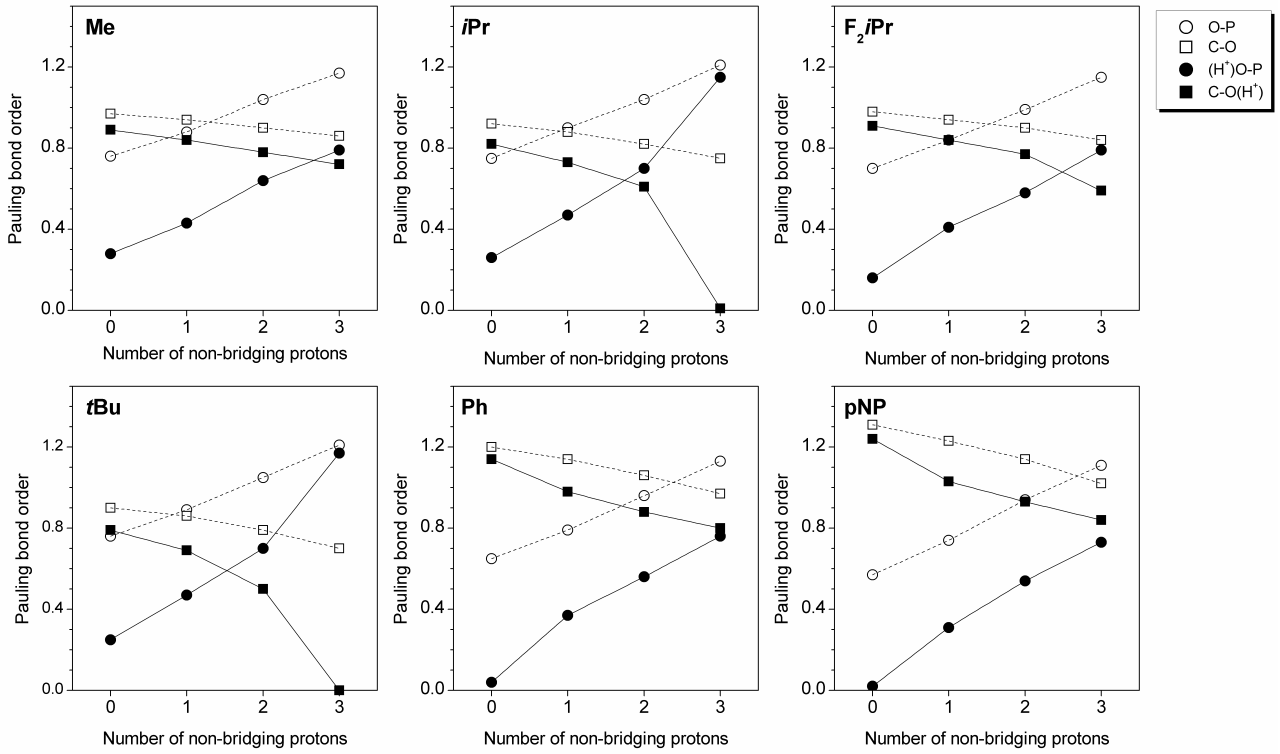

Figure S1. C-O and O-P Pauling bond orders as a function of protonation state and organosubstituent. Bond orders for R-O-P_i (open symbols, dashed lines) and R-O(H^+)-P_i (solid symbols, solid lines) species are shown. The lines are meant as visual aids only. Pauling bond order, n_{ij}, between atoms *i* and *j* is calculated as $n_{ij} = e^{(r_1 - r_{ij})/0.3}$, where r_1 is length of a single bond between atoms *i* and *j*, and r_{ij} is the length of the bond in question: r_1(O-P) = 1.61 Å, r_1(C-O) = 1.41 Å.

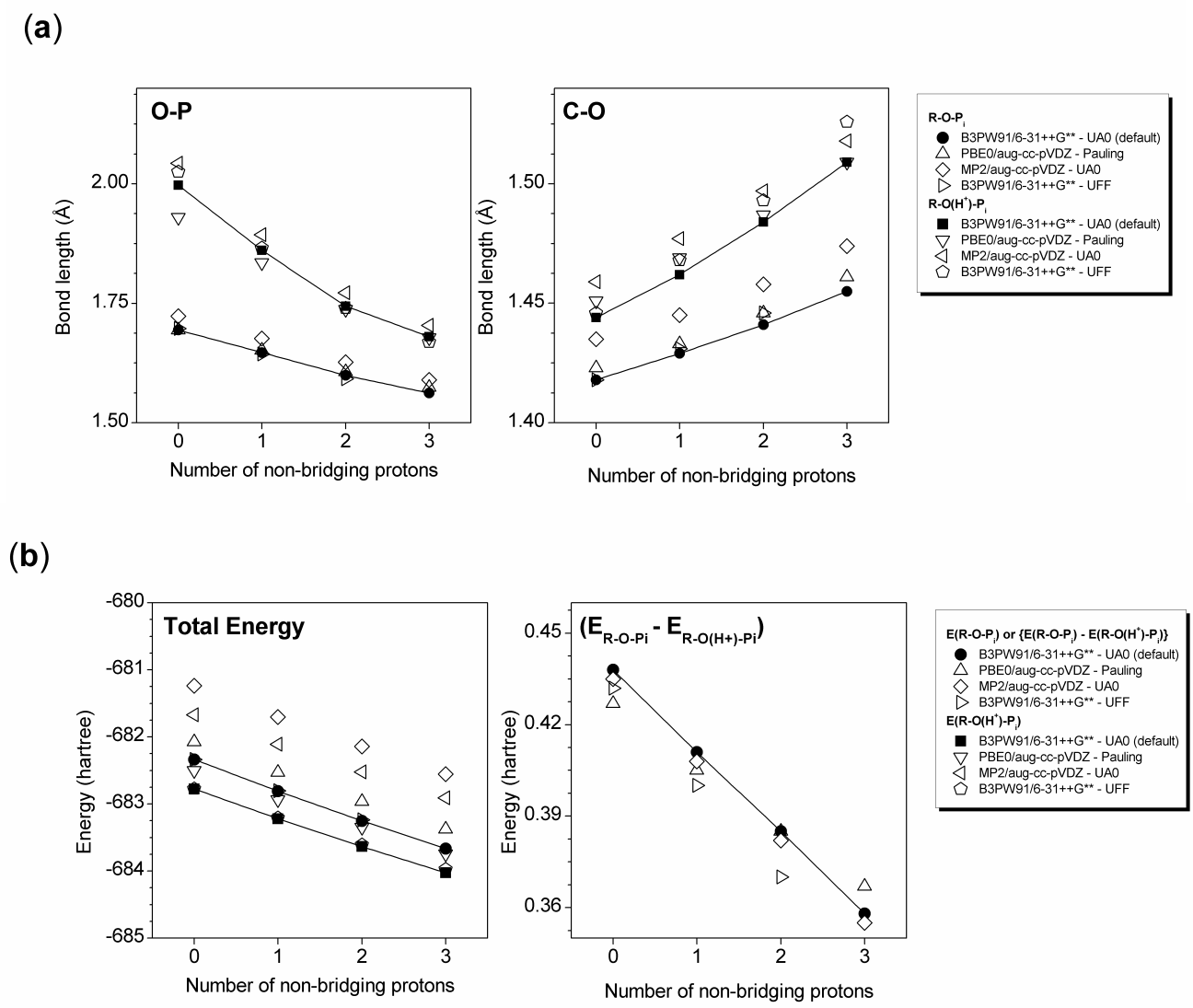

Figure S2. Tests of the computational methods. (**a**) C-O and O-P bond lengths as a function of protonation state of non-bridging oxygens for Me-phosphate with various levels of theory and solvation models. The models were: the default model, B3PW91/6-31++G** with the UA0 method of calculating atomic radii in CPCM solvation, plus PBE0/aug-cc-pVDZ with Pauling radii, MP2/aug-cc-pVDZ with UA0 radii, and the default DFT method with UFF radii. (**b**) Energy versus protonation state of non-bridging oxygens of Me-phosphate. (left) - total energy (right) - energy difference between R-O-P_i and R-O(H^+)-P_i species. The levels of theory are the same as part (a). Energies are the total electronic energies, corrected with the zero point energies taken from the default level of theory.

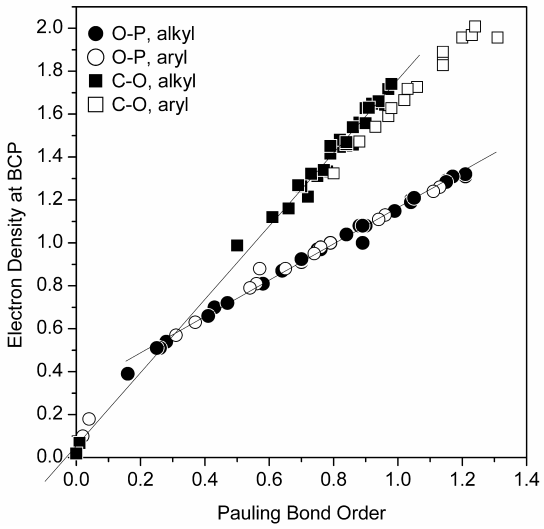

Figure S3. Electron density at the bond critical point (as defined by AIM) versus Pauling bond order for C-O and O-P bonds, including both R-O-P_i and R-O(H^+)-P_i species.

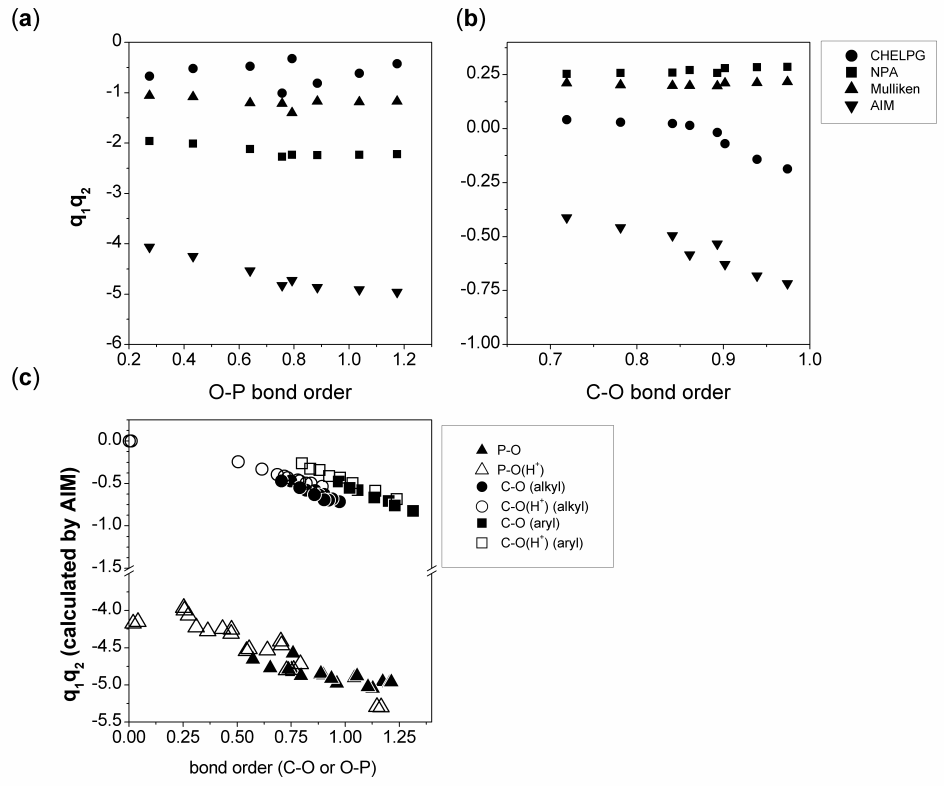

Figure S4. Charge products, q_1q_2, for different phosphate monoesters. Charge products are used instead of Coulombic energy (q_1q_2/r) to avoid the contribution from the distance dependence. (**a**) Charge products for the O-P of all protonation states of Me-O-P_i and Me-O(H^+)-P_i as calculated by four different methods: Charges from electrostatic potential, grid method (CHELPG,

Breneman, C. M.; Wiberg, K. B. *J. Comput. Chem.* **1990,** *11*, 361-373.) natural population analysis (NPA), Mulliken, and atoms in molecules (AIM, Bader, R. F. W., *Atoms in Molecules. A Quantum Theory*. Clarendon Press: Oxford, 1990). (**b**) Same as (a), but for C-O bonds. (**c**) Charge products for all species examined, using AIM charges.

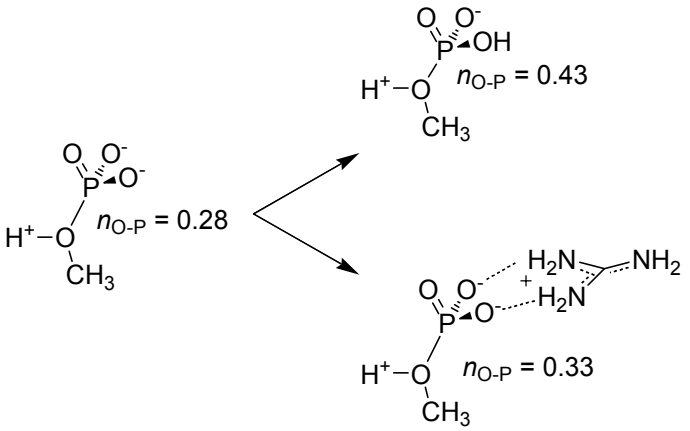

Figure S5. Effect of ionic interactions with bridge-protonated dianion on O-P bond orders.

Table S1. Bond lengths and bond orders for optimized structures.

Species	Number of non-bridging protons	Bond length (Å)		Pauling bond order	
		P-O	C-O	P-O	C-O
Me-O-P_i					
	0	1.694	1.418	0.76	0.97
	1	1.647	1.429	0.88	0.94
	2	1.599	1.441	1.04	0.90
	3	1.562	1.455	1.17	0.86
Me-O(H^+)-P_i					
	0	1.997	1.444	0.28	0.89
	1	1.861	1.462	0.43	0.84
	2	1.744	1.484	0.64	0.78
	3	1.680	1.509	0.79	0.72
*i*Pr-O-P_i					
	0	1.696	1.434	0.75	0.92
	1	1.642	1.449	0.90	0.88
	2	1.598	1.470	1.04	0.82
	3	1.554	1.497	1.21	0.75
*i*Pr-O(H^+)-P_i					
	0	2.018	1.470	0.26	0.82
	1	1.835	1.503	0.47	0.73
	2	1.716	1.556	0.70	0.61

	3	1.569	2.791	1.15	0.01
F_2-*i*Pr-O-P_i					
	0	1.718	1.416	0.70	0.98
	1	1.662	1.428	0.84	0.94
	2	1.613	1.442	0.99	0.90
	3	1.567	1.461	1.15	0.84
F_2-*i*Pr-O(H^+)-P_i					
	0	2.161	1.438	0.16	0.91
	1	1.881	1.463	0.41	0.84
	2	1.773	1.489	0.58	0.77
	3	1.644	1.534	0.89	0.66
*t*Bu-O-P_i					
	0	1.693	1.441	0.76	0.90
	1	1.646	1.456	0.89	0.86
	2	1.594	1.481	1.05	0.79
	3	1.552	1.515	1.21	0.70
*t*Bu-O(H^+)-P_i					
	0	2.022	1.481	0.25	0.79
	1	1.834	1.523	0.47	0.69
	2	1.715	1.615	0.70	0.50
	3	1.564	3.462	1.17	0.00
Ph-O-P_i					
	0	1.738	1.355	0.65	1.20
	1	1.679	1.371	0.79	1.14
	2	1.622	1.393	0.96	1.06
	3	1.574	1.419	1.13	0.97
Ph-O(H^+)-P_i					
	0	2.559	1.371	0.04	1.14
	1	1.912	1.417	0.37	0.98
	2	1.786	1.448	0.56	0.88
	3	1.692	1.477	0.76	0.80
*p*NP-O-P_i					
	0	1.777	1.328	0.57	1.31
	1	1.701	1.348	0.74	1.23
	2	1.630	1.372	0.94	1.14
	3	1.580	1.404	1.11	1.02
*p*NP-O(H^+)-P_i					
	0	2.802	1.346	0.02	1.24
	1	1.960	1.400	0.31	1.03
	2	1.793	1.433	0.54	0.93
	3	1.705	1.463	0.73	0.84

Table S2. Bond lengths and bond orders for Me-phosphate optimized using alternate methods.

Number of non-bridging protons	Me-O-P_i				Me-O(H^+)-P_i			
	Bond length (Å)		Pauling bond order		Bond length (Å)		Pauling bond order	
	P-O	C-O	P-O	C-O	P-O	C-O	P-O	C-O
B3PW91/6-31++G - UA0 (default)**								
0	1.694	1.418	0.76	0.97	1.997	1.444	0.28	0.89
1	1.647	1.429	0.88	0.94	1.861	1.462	0.43	0.84
2	1.599	1.441	1.04	0.90	1.744	1.484	0.64	0.78
3	1.562	1.455	1.17	0.86	1.680	1.509	0.79	0.72
PBE0/aug-cc-pVDZ - Pauling								
0	1.694	1.423	0.76	0.96	1.930	1.451	0.34	0.87
1	1.652	1.433	0.87	0.93	1.835	1.469	0.47	0.82
2	1.607	1.446	1.01	0.89	1.737	1.487	0.65	0.77
3	1.574	1.461	1.13	0.84	1.678	1.509	0.80	0.72
MP2/aug-cc-pVDZ - UA0								
0	1.723	1.435	0.69	0.92	2.043	1.459	0.24	0.85
1	1.676	1.445	0.80	0.89	1.893	1.477	0.39	0.80
2	1.627	1.458	0.94	0.85	1.772	1.497	0.58	0.75
3	1.59	1.474	1.07	0.81	1.704	1.518	0.73	0.70
B3PW91/6-31++G - UFF**								
0	1.697	1.418	0.75	0.97	2.025	1.446	0.25	0.89
1	1.644	1.431	0.89	0.93	1.866	1.468	0.43	0.82
2	1.592	1.446	1.06	0.89	1.740	1.493	0.65	0.76
3					1.669	1.526	0.82	0.68

Table S3. Total energy and energy differences for Me-phosphate optimized using alternate methods.

Number of non-bridging protons	Energy (hartree)[a] Me-O-P_i	Energy (hartree)[a] Me-O(H^+)-P_i	$E_{R\text{-}O\text{-}Pi} - E_{R\text{-}O(H+)\text{-}Pi}$ (hartree)
B3PW91/6-31++G - UA0 (default)**			
0	-682.337	-682.776	0.438
1	-682.809	-683.220	0.411
2	-683.253	-683.637	0.385
3	-683.668	-684.027	0.358
PBE0/aug-cc-pVDZ - Pauling			
0	-682.074	-682.501	0.427
1	-682.530	-682.935	0.405
2	-682.965	-683.351	0.385
3	-683.377	-683.745	0.367
MP2/aug-cc-pVDZ - UA0			
0	-681.238	-681.673	0.435
1	-681.705	-682.113	0.408
2	-682.143	-682.526	0.382
3	-682.554	-682.909	0.355
B3PW91/6-31++G - UFF**			
0	-682.338	-682.770	0.432
1	-682.804	-683.204	0.400
2	-683.237	-683.607	0.370
3	[b]	-683.975	

[a] Total electronic energy, corrected with zero point energies (0.05 to 0.09 hartree) from default method.

[b] Optimization failed.

Table S4. Heterolytic bond dissociation energies for C-O and O-P bonds.

Species	Number of non-bridging protons	Heterolytic bond dissociation energy, ΔH (kcal/mol)	
		P-O	C-O
Me-O-P_i			
	0	45.4	129.4
	1	75.9	115.3
	2	110.7	97.1
	3	147.1	78.5
Me-O(H^+)-P_i			
	0	5.2	94.2
	1	18.6	76.6
	2	37.1	59.2
	3	57.1	41.2
*i*Pr-O-P_i			
	0	36.9	70.3
	1	69.7	58.5
	2	106.4	42.2
	3	146.3	27.0
*i*Pr-O(H^+)-P_i			
	0	2.0	39.7
	1	18.7	25.5
	2	38.6	9.4
	3	64.7	-2.4
F_2-*i*Pr-O-P_i			
	0	32.8	91.5
	1	62.4	76.5
	2	96.7	57.8
	3	135.9	42.0
F_2-*i*Pr-O(H^+)-P_i			
	0	0.6	56.8
	1	11.1	36.4
	2	27.2	16.6
	3	51.3	2.7
*t*Bu-O-P_i			
	0	38.0	60.5
	1	71.0	48.9
	2	108.9	33.8
	3	148.1	18.0
*t*Bu-O(H^+)-P_i			
	0	2.4	30.5
	1	17.1	14.2
	2	38.6	-0.2
	3	76.0	-0.8

Table S5. Coordinates of optimized structures.

```
%NProc=4
%mem=200MB
%chk=cmp-014_f2.chk
#B3PW91/6-31++G** Geom=Check Opt=(ReadFC,MaxCyc=200) Guess(NoSymm,Read)
#SCRF(CPCM,Read,Solvent=water) NoSymm IOP(1/19=7) Output=wfn

Methyl phosphate dianion: Me-O-PO3-2

  -2   1
  C   0.763372275225     -1.083125097487      1.707473856357
  H   0.823046263883     -1.017272742762      2.798512430395
  H   1.780260154503     -1.161291089112      1.300257662966
  H   0.206646576252     -1.990900329392      1.438127695174
  O   0.107930418418      0.083334963729      1.238961254240
  P  -0.168112472417      0.226753308353     -0.426344607491
  O  -0.833216068822      1.615765724573     -0.500600519128
  O  -1.101562424979     -0.941897993459     -0.810338728757
  O   1.218285630417      0.151161695269     -1.101343483144

cmp-014_f2.wfn
RMIN=0.5 OFAC=0.8

--Link1--
%NProc=4
%mem=200MB
%chk=cmp-014_f2.chk
#B3PW91/6-31++G** SCRF(CPCM,Read,Solvent=water) Freq=NoRaman
#Geom=AllCheck Guess=Read SCF=(NoSymm,Tight) NoSymm

RMIN=0.5 OFAC=0.8


  E(RB+HF-PW91) =  -682.390700272     A.U.



Methyl phosphate monoanion: Me-O-PO3H-

 -1     1
  C  -0.001317217189      0.003336715644      0.002595877986
  H   0.019519603184     -0.011672661071      1.098318788331
  H   1.024663047934      0.031344367516     -0.379317585387
  H  -0.539157419379      0.892313847833     -0.334655549135
  O  -0.706289084767     -1.128134630168     -0.510660115558
  P  -0.126716539747     -2.640526087038     -0.210875412439
  O   1.360599383713     -2.694814735793     -0.473015347046
  O  -0.296913508680     -2.792619683386      1.414570847565
  O  -1.081687467740     -3.566475921946     -0.929957049112
  H  -1.245279382866     -2.884553147818      1.665025625457

E(RB+HF-PW91) =  -682.873321659     A.U.



Methyl phosphate: Me-O-PO3H2

  0     1
```

C	1.782923004494	1.263074459489	0.044573030921
H	1.787448844023	1.258268770009	1.137890431501
H	2.806812694347	1.254855448280	-0.330133755656
H	1.256237372827	2.145282584201	-0.328072444025
O	1.165068600439	0.062755817219	-0.460630451778
P	-0.335204700372	-0.333532299159	-0.073895046239
O	-1.145516519204	0.964112478801	-0.527015465367
O	-0.706053143840	-1.633890701205	-0.694220445492
O	-0.461902105291	-0.270902214123	1.523087836521
H	-2.116918408946	0.919106368130	-0.325348251893
H	-0.215822680479	-1.129578485701	1.956879737057

E(RB+HF-PW91) = -683.326775512 A.U.

Methyl trihydrogen phosphate: Me-O-$PO_3H_3^+$

1	1		
C	-0.002469435641	0.007121904378	0.001293929297
O	0.007077327173	0.002269241919	1.456397419513
H	1.046114135913	-0.035699886648	-0.288673031404
H	-0.460239289051	0.928989095506	-0.363560774193
H	-0.537081205094	-0.870664265491	-0.366027145898
P	-1.305165468491	0.053082803397	2.302725675361
O	-0.738429610109	-0.106243399390	3.748896332135
O	-2.204600337600	-1.121416700990	1.801432048831
O	-2.153952663934	1.356133692326	2.105733823703
H	-1.409390213749	0.018683310770	4.485305346344
H	-3.160711042010	-1.113675385874	2.105941413048
H	-1.753386193568	2.190051336781	2.497310731724

E(RB+HF-PW91) = -683.751080234 A.U.

Methyl phosphate dianion, bridge protonated: Me-O(H^+)-PO_3^{-2}

-1	1		
C	0.007807866248	-0.002281125284	0.001273958479
H	0.054453094156	0.039734028507	1.088928144809
H	1.014209099189	-0.058692440881	-0.420160937109
H	-0.597940286736	-0.852953460580	-0.317458617592
O	-0.648832945215	1.213300723900	-0.420287735626
H	-0.777917164712	1.235623594540	-1.403891223831
P	0.140915324680	2.954459403775	0.154929917309
O	-0.112156437794	2.802081990356	1.639547001855
O	-0.798975099408	3.821420006455	-0.657258583231
O	1.558361774909	2.771518938716	-0.348020000925

E(RB+HF-PW91) = -682.840217411 A.U.

Methyl phosphate monoanion, bridge protonated: Me-O(H^+)-PO_3H^-

0	1		
C	-0.074271530927	0.080909051747	-0.097050314006
H	-0.252956549553	0.391553190643	0.930219756494
H	0.987971124919	0.119860857273	-0.337831698751
H	-0.665751626035	0.669045898806	-0.801066860072

```
  O  -0.475234285550     -1.323394374910     -0.166074396418
  H  -0.232503956348     -1.753463710068     -1.041386849834
  P  -2.204271940821     -1.763565236680      0.361348441983
  O  -3.048555502185     -1.361487475134     -0.801123352022
  O  -1.928004930644     -3.336446705942      0.453686526650
  O  -2.236960588420     -1.150002958484      1.717167190382
  H  -2.151232401461     -3.812079342591     -0.389405818220

E(RB+HF-PW91) =  -683.294772469     A.U.


Methyl phosphate, bridge protonated: Me-O(H+)-PO3H2

  1     1
  P   1.390348020196     -0.000715893683      1.709406956822
  O   0.781283022990     -0.083039935080      3.341519644329
  O   2.345278227588      1.117320601755      1.676019871857
  O   1.873103936536     -1.481831222990      1.513750151711
  H   2.838362693785     -1.630902129852      1.745328368996
  C  -0.267455427569     -1.049523167238      3.752061918809
  H   0.737429864738      0.831907439861      3.794247917378
  H   0.056508107178     -2.015929413077      3.371348801303
  H  -0.268278171061     -1.031364379388      4.840726884866
  H  -1.217593445686     -0.729888070307      3.326335469332
  O  -0.008395384352      0.074336412273      1.003479783672
  H   0.014437595261      0.017518982233      0.001391350151

E(RB+HF-PW91) =  -683.720438727     A.U.



Methyl trihydrogen phosphate, bridge protonated: Me-O(H+)-PO3H3+

  2     1
  C   0.001349777232     -0.000059711889      0.003030477487
  H   0.056515015280      0.036985556972      1.089389006635
  H   0.981982752868     -0.014042038989     -0.471096018470
  H  -0.667480163109     -0.781212132544     -0.349712088248
  O  -0.664723134316      1.300897798875     -0.372330976978
  H  -0.444723911926      2.130101286351      0.227002904543
  P  -1.136914610479      1.674138600983     -1.940927162150
  O  -1.802655749254      0.329694133212     -2.278568032933
  O  -2.039568428787      2.880723799960     -1.632158961067
  O   0.091025060138      1.903179460042     -2.843513058999
  H  -2.151311292241      3.578187514248     -2.365274433540
  H   0.521658180198      2.824837744513     -2.814566181587
  H  -1.933308876367      0.109329113443     -3.263763081462

E(RB+HF-PW91) =  -684.116564456     A.U.


Isopropyl phosphate dianion: iPr-O-PO3-2

 -2     1
  C  -0.032173057691     -0.010636410905      0.016215224061
  C   0.004905163615      0.006070763114      1.541649855670
  H   0.984306657364     -0.056955403155     -0.392215468401
  H  -0.600862519648     -0.877882071891     -0.331586318796
  H  -0.513389607251      0.896413352744     -0.365302060721
```

```
  C   0.730662000090     -1.208932824934      2.109424462038
  H   0.556928648986      0.904073249925      1.859868438849
  O  -1.307054029947      0.204109443140      2.086265077178
  H   1.766050291981     -1.221903599894      1.749913306429
  H   0.240990785784     -2.136446196226      1.797533038123
  H   0.741949584508     -1.180713583199      3.202868689389
  P  -2.495267566267     -0.989118369545      2.285015796019
  O  -3.768996415566     -0.111825125392      2.348612812130
  O  -2.443275426933     -1.923983532715      1.060513304066
  O  -2.188228509024     -1.697111691067      3.622930843965

E(RB+HF-PW91) =  -760.995560202     A.U.


Isopropyl phosphate monoanion: iPr-O-PO3H-

 -1     1
  C   1.644183267569     -0.022094792429     -0.566600518879
  C   2.225572689608     -1.158831314411      0.262548722034
  C   1.840232557926      1.342138859018      0.079275682555
  O   0.263537209188     -0.297054820870     -0.910792480765
  H   1.746112056107     -1.202734209595      1.244501631397
  H   2.076868119861     -2.117847103358     -0.243861929799
  H   2.911972068547      1.542001796421      0.184864358270
  H   1.388873453326      1.377177510657      1.075920037961
  H   1.404168093015      2.135148912111     -0.535109027483
  H   3.302144803941     -1.008068800198      0.400185495615
  P  -1.044223030263     -0.123450929394      0.066030984957
  O  -2.128744291693     -0.919371292509     -0.628305582571
  O  -0.709565142846     -0.377597122438      1.519859416781
  O  -1.434119630147      1.466362771828     -0.119802378796
  H   2.139369411617     -0.013168178500     -1.547205460266
  H  -1.249944548024      1.973231698359      0.701483434818

E(RB+HF-PW91) =  -761.482047144     A.U.



Isopropyl phosphate: iPr-O-PO3H2

  0     1
  C   0.820681455621      1.480793762348     -0.398543633120
  C   0.555374225590      1.966752926701      1.015257415559
  C   2.235476384918      0.968683165159     -0.610404589476
  H   0.623971176116      2.299072747233     -1.101724808332
  O  -0.145593342614      0.468378493026     -0.846722147224
  H   2.943763138092      1.787766960845     -0.446708086887
  H   2.366248604382      0.604459280189     -1.633652330885
  H   2.477663900092      0.162542457408      0.088009612756
  H   1.225556476102      2.806964752688      1.224936390388
  H   0.748857240317      1.186633219894      1.757461276480
  H  -0.474157961539      2.315822741723      1.130443812318
  P  -0.686589951520     -0.824719474825     -0.078718318440
  O   0.510279422156     -1.470721308281      0.763145714366
  O  -1.366046574931     -1.718988646997     -1.059233406643
  O  -1.573374790708     -0.340148169017      1.161510064736
  H  -2.405330401474      0.117629578694      0.875340003739
  H   1.045446475543     -2.110735398773      0.225562841183
```

E(RB+HF-PW91) = -761.938784968 A.U.

Isopropyl trihydrogen phosphate: iPr-O-PO_3H_3

1	1		
P	-0.011614589208	-0.137775556919	0.006729838730
O	0.012358254282	0.032571597745	1.551120276819
C	1.165336989928	-0.009298919741	2.504450588269
O	-1.439905559387	0.279735923432	-0.480528011764
H	-1.760998327866	1.166573623995	-0.139888076016
O	1.158442635287	0.720598507135	-0.581037458074
H	1.277446595221	0.658034539549	-1.575652143906
O	0.215228383126	-1.598636014342	-0.510049091504
H	-0.514973721579	-2.249363298376	-0.288663277375
C	1.781549106794	1.371800778927	2.575276592373
C	2.134894570924	-1.117591004407	2.152602849391
H	0.645661081563	-0.244557711365	3.439783664827
H	2.511371136110	1.387312900418	3.391445747487
H	1.020043532577	2.127900924461	2.784900817412
H	2.890776419636	-1.173809738006	2.942539716218
H	2.298437196674	1.629527615215	1.646727200201
H	1.632680336750	-2.087144207455	2.097597881316
H	2.654679076213	-0.922783890146	1.208905964830

E(RB+HF-PW91) = -762.368454370 A.U.

Isopropyl phosphate dianion, bridge protonated: iPr-O(H^+)-PO_3^{-2}

-1	1		
C	0.108736456597	1.866244279465	-0.108884708005
C	0.119063852284	1.916175374680	1.404760795747
C	1.492731045987	1.891708402687	-0.733513563634
O	-0.625523423706	0.659725814588	-0.514875528703
H	-0.498004522660	2.694420532124	-0.500555048126
H	0.575017440523	2.856731145321	1.728991415461
H	0.700528428284	1.086677210977	1.816767751035
H	-0.897852376456	1.869835887804	1.804257806380
H	2.082403506657	1.041128838463	-0.381676386632
H	1.432170512989	1.853940476885	-1.826666896358
H	2.000983167690	2.821840757966	-0.457875499750
H	-0.771355052119	0.669234211797	-1.493407313868
P	-0.270013704766	-1.264029361252	-0.020847570385
O	-0.635254932753	-1.781480577542	-1.400652452460
O	-1.293492605440	-1.413979151363	1.084242947364
O	1.192161754071	-1.211533208627	0.362372856672

E(RB+HF-PW91) = -761.452469236 A.U.

Isopropyl phosphate monoanion, bridge protonated: iPr-O(H^+)-PO_3H^-

0	1		
C	-0.994992959353	0.508113954111	1.452334945517
C	0.134959995758	0.948055022447	2.358027491386
C	-1.394895853898	-0.942787755961	1.588190591627
O	-0.626901168563	0.754401084057	0.016130361065
H	-1.870430377498	1.158304951265	1.572469563716

H	1.021747670505	0.328489548555	2.205082934544
H	0.393620995785	1.997706777492	2.186697871215
H	-1.772204781026	-1.098444212730	2.603661808091
H	-0.541179651116	-1.607543717907	1.433039342431
H	-2.188810085126	-1.201828412644	0.883401829725
H	-0.192291186368	0.848693032733	3.398308081658
P	0.600570316015	-0.135330537859	-1.017638446374
H	-0.600856409801	1.734482904198	-0.192365801917
O	0.927984578377	0.950095546003	-1.990469350568
O	1.547587040748	-0.767323943479	-0.057920531114
O	-0.381365341337	-1.258694920974	-1.604674893362
H	-0.956165706965	-0.913408050524	-2.335277574364

E(RB+HF-PW91) = -761.912129214 A.U.

Isopropyl phosphate, bridge protonated: iPr-O(H^+)-PO_3H_2

1	1		
C	2.354024163410	-1.066601061913	0.322031596808
C	1.770901893248	0.014364063229	-0.550330543347
H	1.924873025805	-1.049871837313	1.326164373275
H	2.216105544290	-2.056302504765	-0.121542010113
H	3.430943602756	-0.880359814234	0.400709823986
C	1.821537391760	1.413865066766	0.001681207312
H	2.162653793667	-0.025718934456	-1.573635359890
O	0.283596590695	-0.342591446053	-0.837922323612
H	2.879146596659	1.688483219695	0.076695658115
H	0.169321448755	-0.970953154988	-1.627730720787
H	1.386294096291	1.479714498765	1.002099867091
H	1.332160688989	2.128192260499	-0.663832194131
P	-1.165292853890	-0.132998647707	0.057804538595
O	-2.171648544446	-0.996207128646	-0.586617288957
O	-1.384335724836	1.425026031622	0.077054429961
O	-0.572093974812	-0.469319537277	1.473020722759
H	-1.137576402311	-0.167175423215	2.243482806270
H	-1.946163075734	1.762875676415	-0.679501216825

E(RB+HF-PW91) = -762.340213842 A.U.

Isopropyl trihydrogen phosphate, bridge protonated: iPr-O(H^+)-$PO_3H_3^+$

2	1		
C	-0.019152768023	-0.085232501631	0.008288746133
C	0.032501547567	0.008786763032	1.443131592349
H	0.941667618313	-0.233687104482	-0.484843472502
H	-0.663986320392	-0.980221324938	-0.154532227996
H	-0.617611236873	0.724855005580	-0.427020635474
C	1.149325584906	-0.391890505433	2.256609774219
H	-0.895368270114	0.297186375153	1.961972771910
O	0.494000105990	2.745359705045	1.736421099596
H	2.101434062441	-0.474199540119	1.730583885304
H	1.204040134076	0.162696603655	3.200064147031
H	0.833436104295	-1.414477104162	2.577767495596
H	0.341554016256	3.028116645756	2.690050132615
P	0.744246864965	3.935799927574	0.745104486400
O	2.151086030345	4.608419131521	0.876460804914

```
  O  -0.424749447369      4.949554226991      0.980176185865
  O   0.721767231107      3.192037561622     -0.624239642651
  H  -0.302635258423      5.855122217783      0.562486565477
  H   0.962450994534      3.749242015013     -1.424055752626
  H   2.256049295463      5.254650604073      1.638468598322

E(RB+HF-PW91) =  -762.744287040     A.U.


1,3-Difluoro-2-propyl phosphate dianion: F2iPr-O-PO3-2

 -2     1
  C   0.090195067271     -0.005898019522     -0.002507367803
  C   0.013145359592      0.042246480077      1.525533937612
  H   1.011002062353      0.420693885940     -0.403544500768
  H  -0.023499534449     -1.038435731213     -0.342382761799
  C   0.657332347538      1.280786945901      2.139382643076
  H  -1.057628927432      0.062153074699      1.782587645681
  O   0.531731437229     -1.140708117054      2.106141554593
  H   1.696984817019      1.403321967232      1.826395639374
  H   0.597086655573      1.245027437074      3.229820464343
  P   2.210315819455     -1.505453432758      2.131052308199
  O   2.165620361702     -3.031463542233      2.333866457620
  O   2.753679077181     -1.045552162937      0.767052660486
  O   2.784635381389     -0.732702838915      3.333113626851
  F  -0.045313835090      2.432911376196      1.714182032684
  F  -0.988987576479      0.731811585179     -0.552691688754

E(RB+HF-PW91) =  -959.401003992     A.U.


1,3-Difluoro-2-propyl phosphate monoanion: F2iPr-O-PO3H-

 -1     1
  C   0.031298868307      0.089749214264     -0.153945936081
  C  -0.394677972948      0.210788078492      1.305457099664
  C   1.535776620185     -0.091710438074     -0.363866406737
  O  -0.464878760672      1.192444814702     -0.913584558048
  H   0.138913287828      1.010251795771      1.826938103248
  H  -1.474213702107      0.368035140934      1.378859826813
  H   2.141580316013      0.456553585340      0.360438915047
  H   1.803687530762      0.207045035988     -1.381196329837
  P  -0.087823500939      2.781284625481     -0.602430071214
  O   1.298186305326      2.873362478575     -0.014721639475
  O  -0.467159798601      3.505884788379     -1.871817583163
  O  -1.120833366443      3.176623653920      0.605485187208
  H  -0.461104891732     -0.795886190939     -0.580936616580
  H  -2.045714341645      3.258651496462      0.274767844101
  F  -0.094817545925     -0.994457656684      1.970123465527
  F   1.857244842256     -1.460198804762     -0.232591894220

E(RB+HF-PW91) =  -959.882157021     A.U.


1,3-Difluoro-2-propyl phosphate: F2iPr-O-PO3H2

  0     1
  C   0.002657430488      0.022589246170      0.006517168977
  C  -0.152088203716      0.137477762954      1.508272844849
```

```
  C   1.471166110006     -0.076687283720     -0.407544216945
  H  -0.415548096339      0.924640030246     -0.460239451775
  O  -0.784441951490     -1.044034294437     -0.561588276177
  H   1.548881494678     -0.311677696276     -1.472704699179
  H   2.040323922675     -0.801591405524      0.181829121839
  H   0.456089355734      0.972421055298      1.871563405999
  H   0.122598469409     -0.783147238765      2.029895822461
  P  -0.632686126865     -2.640535127100     -0.393258598479
  O   0.878447912391     -3.018173911573     -0.743504764690
  O  -1.702396658310     -3.295538860176     -1.190703720821
  O  -0.577784406321     -2.970889789673      1.166722422020
  H  -1.478507701258     -2.977464885443      1.587357980691
  H   1.035938448559     -3.087792872739     -1.722769224401
  F  -1.490954904920      0.417715488450      1.824795560174
  F   2.055656587259      1.183359581026     -0.199534391284

E(RB+HF-PW91) =  -960.334814385     A.U.


1,3-Difluoro-2-propyl trihydrogen phosphate: F2iPr-O-PO3H3+

  1     1
  P  -0.038381228946     -0.038913233988      0.096787746198
  O  -0.086761732227      0.007820555526      1.655430855850
  H   0.732457752667      0.387100484135      2.096997951037
  O   0.359038276524      1.324338380181     -0.563022536119
  H  -0.079212844920      2.137167182666     -0.165318401285
  O   0.916131178110     -1.110975974724     -0.516806104965
  H   1.892126032232     -0.874315730430     -0.545700067068
  O  -1.497552458837     -0.506617957730     -0.230097845232
  C  -1.971853006063     -0.795782469268     -1.581681172286
  C  -3.210423463281      0.077172394117     -1.747842418027
  C  -2.227097154803     -2.279263726824     -1.702525414235
  H  -1.210937931535     -0.516616877977     -2.327979602700
  H  -2.950901907618      1.135528592194     -1.651483100668
  H  -3.986913504687     -0.192738084118     -1.026354745552
  H  -2.557666956270     -2.511815775533     -2.720277593974
  H  -1.327370595853     -2.852284014525     -1.459145686978
  F  -3.237991099848     -2.673507362030     -0.817076348542
  F  -3.716863067507     -0.132493594413     -3.034140491147

E(RB+HF-PW91) =  -960.763359799     A.U.


1,3-Difluoro-2-isopropyl phosphate dianion, bridge protonated: F2iPr-O(H+)-PO3-2

 -1     1
  C  -0.011333880573     -0.021304866099     -0.022152350897
  C  -0.005291656950      0.027285894759      1.505106099321
  C   1.387030324760     -0.041306066633     -0.589626848826
  O  -0.709784547121      1.114108857597     -0.560210437452
  H  -0.546126352171     -0.927500443865     -0.343966262666
  H   0.687605239864      0.775483189460      1.895784859747
  H  -1.015302206472      0.220919339582      1.879859618294
  H   1.985605370042     -0.806410542637     -0.085618931187
  H   1.868500510087      0.937187219762     -0.502323832868
  P  -0.237531295947      3.200172139615     -0.251058220916
  H  -1.684774741320      1.007551290626     -0.420957925611
  O  -1.696312864768      3.584158390936     -0.157404937916
```

```
  O   0.566081527321      3.046593059473      1.017512114902
  O   0.494184699798      3.420006162359     -1.551841341975
  F   0.394192503009     -1.234917199620      1.982756764075
  F   1.345768241337     -0.370716484143     -1.955454369942

E(RB+HF-PW91) =  -959.851138846     A.U.
```

1,3-Difluoro-2-propyl phosphate monoanion, bridge protonated: $F_2iPr\text{-}O(H^+)\text{-}PO_3H^-$

```
  0     1
  C   0.001658421755     -0.006755806583     -0.017897215297
  C   0.004356510238     -0.035965934871      1.511087620708
  C   1.375435888980      0.050774756965     -0.673218127254
  O  -0.747762263583      1.142972651287     -0.524062263172
  H  -0.545145694770     -0.887014292595     -0.383406026646
  H   0.886919754293      0.439355839725      1.944763246778
  H  -0.904557323527      0.431422634211      1.902613440690
  H   1.953644524073      0.916044420372     -0.335927389304
  H   1.287171837268      0.048087201936     -1.763309093912
  P  -0.328803431285      2.951318340168     -0.217496787244
  H  -1.741945079344      0.986045853836     -0.497025698945
  O  -1.692060480956      3.538494437272     -0.333691024831
  O   0.523106000064      2.880613343475      0.999894040839
  O   0.595552896589      3.149370640025     -1.506084464367
  H   0.070284331226      3.325184499477     -2.331133863426
  F  -0.001032077736     -1.379102534801      1.917801172449
  F   2.068670767805     -1.101066063392     -0.286638331128

E(RB+HF-PW91) =  -960.300805386     A.U.
```

1,3-Difluoro-2-propyl phosphate, bridge protonated: $F_2iPr\text{-}O(H^+)\text{-}PO_3H_2$

```
  1     1
  C  -0.015033286567     -0.017646562636      0.000595729168
  C   0.005779349498     -0.001851313880      1.528712666043
  H   0.985782035803     -0.052445790982     -0.439482007175
  H  -0.623590479061     -0.854138322096     -0.357660667362
  C   1.162982089443      0.744111602066      2.186442070688
  H  -0.952544810742      0.394930137908      1.892085441641
  O  -0.001818682420     -1.411662479920      2.009311326234
  H  -0.698767219996     -1.582879015619      2.736478099454
  H   2.135792386892      0.458051998861      1.774987921247
  H   1.148666340715      0.603788730730      3.271895851678
  P   1.255357407107     -2.660457857481      1.957849698129
  O   0.584589771132     -3.874677201426      2.441502006557
  O   2.436712702183     -1.990072560741      2.736747368630
  O   1.734366654807     -2.469622168226      0.480164121372
  H   1.263198570366     -3.062394178818     -0.181021882202
  H   2.400278059121     -2.121990051974      3.732360536472
  F  -0.622029796672      1.168494836021     -0.417906422974
  F   0.968978756025      2.099364596097      1.916751777106

E(RB+HF-PW91) =  -960.723030163     A.U.
```

1,3-Difluoro-2-propyl trihydrogen phosphate, bridge prot'd: $F_2iPr\text{-}O(H^+)\text{-}PO_3H_3^+$

```
  2     1
  C  -0.044032182822      0.024831831388     -0.027343772489
  C  -0.014565032241     -0.016403869959      1.477041415399
  H   0.951409191273     -0.154554335599     -0.447370685834
  C  -1.300580978106     -0.186201704999      2.238583536521
  H   0.510108279907      0.884923098261      1.834922046399
  O   0.993027740612     -1.112386394093      1.976058096762
  H  -1.128794464487     -0.126300635237      3.317951035064
  H   1.654673509797     -0.720762633671      2.680359531710
  P   0.974039428084     -2.794000319495      1.953344020066
  O   2.397175415921     -3.179874397170      2.398741264339
  O   0.553466597494     -3.002570850073      0.488931706641
  O   0.061906239738     -3.333350809780      3.069583028425
  H   0.252794576476     -3.937948181318      0.222736368844
  H  -0.900317076788     -3.553320124306      2.835055727795
  H   3.153842339573     -2.935882292764      1.765945733253
  H  -0.372789487054      1.039519417130     -0.291012465770
  H  -1.988834734994      0.608406257189      1.923150370254
  F  -1.878800601465     -1.424661288094      1.962840530420
  F  -0.942444182739     -0.871264599469     -0.587491662504

 E(RB+HF-PW91) =  -961.123979843     A.U.
```

t-Butyl phosphate dianion: tBu-O-PO_3^{-2}

```
 -2     1
  C   0.835617842251      1.123435472105     -0.333684314541
  C   0.003012061216      2.278722323034      0.230901886994
  C   2.327304776453      1.426189012171     -0.171152310925
  C   0.509847404678      0.902889987262     -1.812221858194
  O   0.609836498388     -0.062446071295      0.453331049176
  H  -1.059365464611      2.028009823412      0.171289233965
  H   0.262047474713      2.453758038471      1.281281075889
  H   2.932382921786      0.605249979506     -0.570754126634
  H   2.596241977167      2.345962770349     -0.702375234392
  H   2.576646078606      1.554287599528      0.887773590184
  H   0.746156707438      1.805311928077     -2.387444110349
  H  -0.551430304450      0.673261336429     -1.940497464062
  H   1.092142141795      0.068657934425     -2.215320388027
  H   0.190535539415      3.202765144740     -0.328328086243
  P  -0.730918865188     -1.094407841000      0.380951418518
  O  -0.669182193569     -1.739892258602      1.787426119892
  O  -1.989633219511     -0.235589399953      0.146011162740
  O  -0.450785895747     -2.107276144214     -0.751679538870

E(RB+HF-PW91) =  -800.301139796     A.U.
```

t-Butyl phosphate monoanion: tBu-O-PO_3H^-

```
 -1     1
  C  -1.471130675685     -0.012399618786      0.056181762871
  C  -1.531047623763     -0.812849405856     -1.245250424695
  C  -2.431316821557     -0.604374661278      1.086243647887
  C  -1.790704390934      1.461816477326     -0.191258878652
  O  -0.160633665597     -0.112768424624      0.683402561333
  H  -0.856733891954     -0.396446031290     -1.999490849718
  H  -1.257900083279     -1.857931464731     -1.072207736896
```

H	-2.358632593751	-0.060380648488	2.033636408701
H	-3.463226994921	-0.535398566168	0.726642696600
H	-2.197645610709	-1.657731918096	1.271489774831
H	-2.791256261628	1.565268996053	-0.625286561054
H	-1.058981881794	1.898082266061	-0.875759617506
H	-1.764198572352	2.019819504137	0.750694982564
H	-2.548953215759	-0.783788490294	-1.648188838922
P	1.291479447441	-0.031641267107	-0.086715089382
O	1.705115687604	-1.419296183141	-0.540521536679
O	1.340171925554	1.118138692811	-1.067789620203
O	2.210791740670	0.412290547466	1.199158528547
H	2.388991482415	-0.354206803995	1.790140790371

E(RB+HF-PW91) = -800.787707575 A.U.

t-Butyl phosphate: tBu-O-PO_3H_2

0	1		
C	0.071719076124	1.435031349359	0.474446373086
C	-1.110654564801	1.481863477930	1.435639183081
C	1.257850797966	2.223217340535	1.016459669547
C	-0.310695140312	1.910643436737	-0.922677756424
O	0.575853113101	0.043074703921	0.428264360376
H	-1.457116818918	2.515016482233	1.542419361066
H	-1.938429688017	0.872345934519	1.064670387280
H	-0.815783043491	1.113786196935	2.423310652322
H	2.112158328529	2.154408343770	0.336157146161
H	0.983292095214	3.277171836909	1.124511955922
H	-0.606039892131	2.963589046403	-0.873876296862
H	-1.156653307051	1.343529593472	-1.322373968178
H	0.533587579339	1.821858707092	-1.612119768060
H	1.557923759127	1.841548190330	1.997048230355
P	-0.081778341960	-1.187372284122	-0.342207316417
O	0.665498476894	-2.438791108712	0.324759397045
O	-1.571393182903	-1.268629146472	-0.356508443519
O	0.618336065147	-1.116283070043	-1.780687958838
H	0.244274922001	-2.718681389658	1.177888684181
H	0.174370766142	-1.706533641140	-2.442570892126

E(RB+HF-PW91) = -801.246560843 A.U.

t-Butyl trihydrogen phosphate: tBu-O-$PO_3H_3^+$

1	1		
C	-1.557328238464	-0.008087026814	-0.040902797820
C	-1.925316777271	0.079526555641	1.431283859096
C	-2.441450935251	-0.985694572812	-0.796837350385
C	-1.505464889243	1.352490237681	-0.716539103509
O	-0.194870071866	-0.667001657631	-0.112979177309
P	1.231269898824	-0.068628307959	0.016833159468
H	-1.886260449902	-0.908272285065	1.899298465386
H	-1.259778696293	0.757708475606	1.970834692869
H	-2.947803971512	0.460870443995	1.518295252468
H	-3.473831359981	-0.623250990917	-0.777275969120
H	-2.123662140101	-1.073304462104	-1.839605286899
H	-2.413016429401	-1.974751179207	-0.331023569238
H	-2.513271775960	1.779272961402	-0.709644437967

```
  H  -0.849451562393      2.048966419380     -0.185803604658
  H  -1.179575500380      1.268518483346     -1.757014819569
  O   2.234560789554     -1.270262387759      0.078506313009
  O   1.245285323182      0.854203703913      1.282045391421
  O   1.699255822202      0.825535475590     -1.181322331559
  H   2.005716383284     -1.977920323935      0.750784811722
  H   2.107756926802      1.337545385185      1.450881843634
  H   1.847708207940      0.338700117442     -2.045147497318

E(RB+HF-PW91) =  -801.675288294     A.U.



t-Butyl phosphate dianion, bridge protonated: tBu-O(H+)-PO3-2

 -1     1
  P   1.585707913657     -0.031381456237      0.057769558024
  O  -0.272911670915     -0.112874838102     -0.734176843572
  H  -0.266055675717     -0.927938989181     -1.296038955307
  O   2.148773027564     -1.006513329629     -0.960091129311
  O   1.337532854016     -0.532318280281      1.464325912803
  O   1.866962250327      1.442269541389     -0.136229996751
  C  -1.586881552327      0.039615298338     -0.068797069419
  C  -1.855942494458     -1.193619987594      0.786122234448
  H  -1.070472467028     -1.308361677702      1.536874796344
  H  -1.892224617757     -2.098295950740      0.168413267334
  H  -2.822471147869     -1.091116709358      1.290231231672
  C  -1.494465509016      1.303639501431      0.771345618000
  H  -2.463013005965      1.490672525494      1.244816142136
  H  -0.738288039888      1.197043749195      1.552767291402
  H  -1.238222306015      2.165468068354      0.148613301887
  C  -2.613361404995      0.190074703233     -1.187242553378
  H  -2.386488617615      1.061873545419     -1.808225543130
  H  -2.635398072351     -0.700523529156     -1.825689047255
  H  -3.611930677796      0.319138971757     -0.757498778696

E(RB+HF-PW91) =  -800.759040458     A.U.


t-Butyl phosphate monoanion, bridge protonated: tBu-O(H+)-PO3H-

  0     1
  C  -0.072226644206      0.026310118863     -0.015689680870
  C   0.138200256891     -0.087892407447      1.486566787473
  C   1.245548639758      0.054536956563     -0.765800955053
  C  -0.991612220849      1.176820507469     -0.390767656061
  O  -0.768886114222     -1.272133576334     -0.400550082647
  H  -0.516318927077      2.118609910078     -0.098238197382
  H  -1.176963155647      1.200004808875     -1.466835420987
  H  -1.949693699254      1.104740612677      0.134505024798
  H   0.633193691312      0.820251119544      1.844029942344
  H   0.768373259880     -0.947532865181      1.730349198605
  H  -1.622198807396     -1.405289221229      0.109027250779
  H  -0.815941460675     -0.180473560065      2.016753438652
  H   1.807361331014      0.929341561808     -0.424599367434
  H   1.836141360873     -0.841297840429     -0.561436881031
  H   1.103699716830      0.146253466750     -1.845361510098
  P  -0.929354396747     -2.169490755138     -1.992044182785
  O   0.454550795389     -2.614073972587     -2.319064409612
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  O  -1.441025197141     -0.965167735573     -2.924065590601
  O  -2.070259603288     -3.055776968344     -1.617828200084
  H  -0.755792960694     -0.668115073155     -3.575627333747

E(RB+HF-PW91) =  -801.215634459     A.U.


t-Butyl phosphate, bridge protonated: tBu-O(H+)-PO3H2

  1     1
  C   0.075813097253     -0.115871442728      0.035047420546
  C  -0.002034587633      0.006681485938      1.538723338077
  H   1.110713709723     -0.151403206238     -0.310346997016
  H  -0.450970653876      0.704152661314     -0.462012402530
  H  -0.416150380695     -1.052919542295     -0.248204005223
  C   0.796163877711     -1.031588723448      2.288458918664
  C  -1.404937387984      0.182803245674      2.075294163523
  O   0.680713967851      1.427407014532      1.888460700272
  H  -1.401135827283      0.346783556836      3.155793100556
  H  -1.928203675140      1.006905354620      1.579744429362
  H  -1.959907369547     -0.737755267564      1.866062614211
  H   0.304046745739     -1.993630978825      2.109272300219
  H   1.821835556987     -1.109845491870      1.923124786978
  H   0.795750336231     -0.844367003953      3.364214791277
  P   2.307813179725      1.897098175608      2.161167600451
  H   0.148383138852      2.224390405422      1.549806168577
  O   2.977485701600      1.034967335002      1.029020803555
  O   2.686147018598      1.165233241124      3.502208231688
  O   2.329760250524      3.371432131782      2.114477616700
  H   3.979779959663      1.044666515856      1.037821094702
  H   2.479267945753      1.702045982529      4.321664664806

E(RB+HF-PW91) =  -801.646275867     A.U.


t-Butyl trihydrogen phosphate, bridge protonated: tBu-O(H+)-PO3H3+

  2     1
  P  -0.005475087551      0.113483612535     -0.054092950649
  O   0.076990846090      0.458239952834      1.469026610381
  C   2.866006985401     -0.044913213487      3.457841399287
  H  -0.703260732407      0.979149621626      1.827140070572
  O  -1.391238148486     -0.578343388147     -0.283809993142
  H  -1.659344438689     -0.698097579280     -1.244229467555
  O   0.217192884794      1.330206648580     -1.014937763900
  H  -0.576674819723      1.929168887630     -1.150602969816
  O   1.239681351674     -0.812520932358     -0.216124278392
  H   1.449070604203     -1.088130996917     -1.157571695330
  C   2.908798495139     -1.498440184184      3.342993383629
  C   2.200917926837      0.571388021620      4.600732708343
  C   3.508022765484      0.793458777476      2.455560661674
  H   3.487296518322     -1.871517556437      4.207767612646
  H   1.900452444556     -1.907886708366      3.511719256062
  H   3.340148035792     -1.866352684760      2.412449207277
  H   1.248840180302      0.969736329051      4.199913937571
  H   1.972167091409     -0.121419546079      5.412087251588
  H   2.742616223379      1.460689447010      4.947223087711
  H   3.417382321240      0.377946529720      1.446875103751
  H   3.231668201039      1.847997961388      2.511734100092
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  H   4.589599294214      0.713870824635      2.698366884053

E(RB+HF-PW91) =  -802.065896699     A.U.


Phenyl phosphate dianion: Ph-O-PO3-2

 -2     1
  P   0.006470312757      0.023225038525      0.014366433962
  O  -0.011783120481     -0.066587960009      1.749521034734
  O   1.524449485574     -0.001141049893     -0.219374582298
  O  -0.677616425099      1.352211524771     -0.335251701605
  O  -0.738222442553     -1.231999824488     -0.463538957954
  C  -1.107026067695     -0.015951991682      2.545836715230
  C  -2.428545867710      0.045468673293      2.076077635932
  C  -0.877408940712     -0.034847857181      3.933058626997
  C  -3.489558092223      0.089163832868      2.983789859133
  C  -1.944797850447      0.007639729933      4.828275915026
  H  -2.616537817406      0.059491384051      1.007689135367
  H   0.149753402835     -0.084754841905      4.292432055318
  C  -3.261962765739      0.071145598219      4.361814374983
  H  -4.509467551262      0.137697466542      2.601472821434
  H  -1.743759329450     -0.008376124025      5.899607341344
  H  -4.096016930295      0.105365592148      5.061146638184

E(RB+HF-PW91) =  -874.076481814     A.U.


Phenyl phosphate monoanion: Ph-O-PO3-2

 -1     1
  P   0.003938313995      0.005884306938     -0.001956070944
  O  -0.023705103423     -0.013378428929      1.676273332719
  O   1.442474688873     -0.006752474553     -0.459205648903
  O  -0.665976127615      1.477420240909     -0.189822399238
  O  -0.987167278989     -0.999234387396     -0.531057236068
  C   0.513534143565     -0.999778671335      2.462241412338
  H  -0.025978051686      2.199426712508      0.015913899372
  C   0.897667319534     -2.256718744493      1.982544789125
  C   0.647802503464     -0.698574980786      3.823231684971
  C   1.417588694595     -3.201645396495      2.870980850058
  C   1.164086503071     -1.652284928509      4.699211708355
  H   0.790325990670     -2.500654258808      0.928625145389
  H   0.342632904062      0.284496571166      4.179691431774
  C   1.554747858606     -2.909823034493      4.229186801631
  H   1.715404711800     -4.178041601412      2.488938223785
  H   1.263500530416     -1.407310301362      5.756554896706
  H   1.959737971284     -3.653172899783      4.914315136031

E(RB+HF-PW91) =  -874.554257354     A.U.


Phenyl phosphate: Ph-O-PO3H2

  0     1
  P  -0.065824232097      0.017066928161      0.000333547224
  O  -0.023581809207      0.003016709367      1.621421440290
  O   1.428933224547     -0.192796656464     -0.501023767359
  O  -0.348276151645      1.560223517000     -0.269807182395
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  O  -0.996001771897     -0.961402273926     -0.618454077366
  C   0.338123380324     -1.076355681711      2.424585916519
  H  -1.300749898613      1.813626440781     -0.139876922792
  H   2.090178401286      0.428058917511     -0.093914731112
  C   0.199723778557     -2.405247118426      2.026650063637
  C   0.824454758821     -0.745119817763      3.688972847509
  C   0.566641245244     -3.415589011242      2.920095937291
  C   1.178863439619     -1.765438874982      4.571051579914
  H  -0.192671709604     -2.654503496569      1.044656834227
  H   0.918392072006      0.303306495477      3.968373115469
  C   1.054233826568     -3.104262804784      4.190040286372
  H   0.461767912916     -4.455902527292      2.613491656973
  H   1.558188548569     -1.508730655615      5.559702332166
  H   1.333416520000     -3.899191364583      4.880093595447

E(RB+HF-PW91) =  -875.004620573     A.U.


Phenyl trihydrogen phosphate: Ph-O-PO3H3+

  1     1
  P   0.029049575355     -0.012097275337      0.002624626845
  O  -0.063186902018      0.046373689573      1.558173682393
  O   1.535807527011     -0.167160875498     -0.372106376392
  O  -0.876232851265     -1.218114353524     -0.448086371318
  O  -0.509943697151      1.238339205127     -0.757113322462
  C  -1.115825617418     -1.572114753609     -1.801691871166
  H  -0.992324574673      0.125662556977      1.933149638755
  H   2.040767275162     -0.873443782875      0.134703222948
  H   0.025110906185      2.081041377510     -0.641886273446
  C  -0.247366632819     -2.463086015916     -2.418302182479
  C  -2.251333447753     -1.068668690029     -2.422327494984
  C  -0.530135211087     -2.855454901778     -3.728658260868
  C  -2.517859352999     -1.473321198945     -3.731848423229
  H  -2.910017307124     -0.382447206540     -1.892190344493
  H   0.621537848852     -2.846798599878     -1.885130460359
  C  -1.659521810071     -2.361219386991     -4.385110275844
  H   0.137251175413     -3.553407116223     -4.232890574912
  H  -3.402898196675     -1.091147597606     -4.239308973187
  H  -1.874569313341     -2.672938609715     -5.406466638664

E(RB+HF-PW91) =  -875.429287647     A.U.


Phenyl phosphate dianion, bridge protonated: Ph-O(H+)-PO3-2

 -1     1
  C   0.002164361700      0.003825691029      0.009124339060
  C   0.007170468559      0.006944785933      1.405531620531
  C   1.201828166311     -0.002357475558     -0.706175572338
  H  -0.950928505275      0.008184707372     -0.519333833085
  O   2.760737636790      2.685647689664      3.929437307479
  C   2.414065860053     -0.009280718346     -0.009463912023
  C   1.226706997027     -0.000954579984      2.089142724167
  H   1.193118100844     -0.002992078095     -1.795135360947
  H  -0.928397386657      0.012172154054      1.966529477167
  P   2.359754374218      1.719805953869      5.008882040377
  C   2.433542500745     -0.008459761201      1.385010790913
  H   3.357648719124     -0.014363848078     -0.554779478427
```

```
  O   1.285813346125     -0.010682395607      3.458873934279
  O   1.022517258378      1.865130394013      5.685069932561
  O   3.367293059739      0.746398559073      5.556816363313
  H   3.374037198631     -0.013427031194      1.933173125566
  H   0.373739645267     -0.038338457845      3.835939833913

E(RB+HF-PW91) =  -874.520540335     A.U.


Phenyl phosphate monoanion, bridge protonated: Ph-O(H+)-PO3H-

  0     1
  C   0.010322175237      0.039681781795      0.007919548810
  C   0.018762159729      0.037841348203      1.404039396233
  C   1.210340877384     -0.000677475151     -0.704979446640
  H  -0.942131314382      0.081065316404     -0.519206784953
  C   2.427116006397     -0.056555286984     -0.021261007278
  C   1.245322093407     -0.021773858794      2.051784374750
  H   1.197292500778      0.008042936192     -1.794127958495
  H  -0.908368103825      0.080041902759      1.976636602197
  C   2.455487010814     -0.075388031258      1.374546860385
  H   3.365601478576     -0.095161049834     -0.573122680008
  O   1.285368873946     -0.046320693866      3.468471902733
  H   0.411075199228     -0.354897686318      3.861848597423
  H   3.394582913248     -0.136694778863      1.919063274871
  P   1.961767869394      1.394290415084      4.528983733027
  O   1.266669706905      1.061616962354      5.803725389984
  O   3.495544693297      0.953633676904      4.466792307100
  O   1.744382609899      2.588692156605      3.672494287858
  H   3.710471249968      0.226821364769      5.110088602001

E(RB+HF-PW91) =  -874.971793178     A.U.


Phenyl phosphate, bridge protonated: Ph-O(H+)-PO3H2

  1     1
  P   0.008569139929      0.003785442424      0.003892510179
  O  -0.043053822535     -0.048323707688      1.567220219772
  O   1.278409712519      0.054534670937     -0.737258678591
  O  -1.145660666517     -0.963183274183     -0.420606951861
  O  -0.865893781855      1.545518414239     -0.213956979265
  H   0.761982055463      0.347222607936      2.017711502026
  H  -1.001176140548     -1.400821671761     -1.311754989285
  C  -1.325416987793      1.971524000879     -1.519381919306
  H  -0.466328363254      2.316679461486      0.329392299923
  C  -2.640577453203      1.675263677594     -1.834234114411
  C  -0.448398657932      2.641580296334     -2.356139405098
  C  -3.104079537029      2.082045461714     -3.087213404353
  C  -0.937933959705      3.046314841935     -3.599820974573
  H   0.576356081258      2.847139696694     -2.048211290416
  H  -3.280697971331      1.154169382422     -1.124026060231
  C  -2.256767131784      2.763562024848     -3.964025755912
  H  -4.133676800764      1.867956650746     -3.371075543557
  H  -0.280179210910      3.581252328517     -4.283700851613
  H  -2.628262633810      3.080820002386     -4.937790291084

E(RB+HF-PW91) =  -875.396506208     A.U.
```

Phenyl trihydrogen phosphate, bridge protonated: Ph-O(H^+)-$PO_3H_3^+$

2	1		
P	-0.018820082668	0.014638000203	-0.002121363819
O	-0.031841611522	0.025601507260	1.535249092994
O	1.580786794241	0.017627273646	-0.552052320417
O	-0.453931032459	1.370720932743	-0.578195826104
O	-0.608332643702	-1.290305554837	-0.562579844621
H	1.993095958469	-0.921054848876	-0.767277892734
C	2.571292425173	1.056451399677	-0.205322112640
H	0.072081867144	-0.867791592128	2.011003980798
H	-1.297777113907	1.785967682177	-0.189311751934
H	-0.759966965904	-1.340577610792	-1.569345433617
C	3.297615189403	0.887902231297	0.957822345138
C	2.695813683835	2.102923436829	-1.097399881557
C	4.243218303506	1.875093352564	1.245048551242
C	3.645564819379	3.076634283547	-0.779296535547
H	2.090098341155	2.155935593164	-2.000981893466
H	3.147973091442	0.024340700120	1.605919463066
C	4.411036518711	2.962043178975	0.383696380631
H	4.846243678354	1.786537331651	2.147806338833
H	3.784697416034	3.923303144047	-1.450287989719
H	5.150612460099	3.726491944132	0.619611598322

E(RB+HF-PW91) = -875.793916582 A.U.

P-Nitrophenyl phosphate dianion: pNPh-O-PO_3^{-2}

-2	1		
C	-0.016558589465	0.025659801197	0.005248609503
C	-0.004602814460	0.000963721466	1.406398077394
C	1.177904978554	0.035000420697	-0.693150133574
H	-0.963866470752	0.037320692894	-0.528593406208
C	1.205674709452	-0.014354797027	2.115957284524
C	2.408964707188	0.018826693452	0.002007299995
N	-1.244145416250	-0.008992229899	2.124332850490
H	1.176704377170	0.053267278149	-1.777531977009
C	2.396750440163	-0.005681379069	1.417377391203
O	3.599418678271	0.024304056998	-0.586627304148
O	-2.306029900620	0.002185509897	1.487341107772
O	-1.218125308216	-0.028767533483	3.362378339629
H	1.201017752994	-0.032776473230	3.203049051588
P	3.904753077250	0.073474241598	-2.336425756076
H	3.348078383751	-0.017398691507	1.946997303972
O	5.434693044550	0.064832346258	-2.303067671426
O	3.259726295466	1.386156629206	-2.787014486630
O	3.246394054956	-1.203401287598	-2.863938581000

E(RB+HF-PW91) = -1078.52293125 A.U.

P-Nitrophenyl phosphate monoanion: pNPh-O-PO_3H^-

-1	1		
C	-0.012530288221	0.013394681717	0.002957550053
C	-0.003170863210	0.000867243199	1.400395795216
C	1.189271735001	0.013196441578	-0.688953283185

```
  H  -0.955975537969      0.024253952991     -0.537624469543
  C   1.197863011109     -0.011524604989      2.119587168875
  C   2.403665228996      0.001082480602      0.020016911200
  H   1.181868376390      0.026083852185     -1.775766959012
  N  -1.255513089080      0.001467208728      2.115971314682
  C   2.395447600054     -0.011667538949      1.427436641684
  H   1.186628570211     -0.021708572158      3.206767033761
  O   3.618351507013      0.006884470284     -0.564169934963
  O  -2.307514034192      0.011639749548      1.470027627226
  O  -1.231198036351     -0.008280426141      3.350316038378
  H   3.344942461757     -0.021641372411      1.960204930242
  P   3.907432730063     -0.059462700958     -2.239452289544
  O   5.523940593692      0.009019824718     -2.149992313184
  O   3.427473422132      1.227612526793     -2.851992478733
  O   3.427118326113     -1.400460827953     -2.729770010622
  H   5.917392984288     -0.860578051591     -1.895982244773

E(RB+HF-PW91) =  -1078.99683603     A.U.


p-Nitrophenyl phosphate: pNPh-O-PO3H2

  0     1
  C  -1.846745739127      0.018725347522      0.138502770876
  C  -1.885018222599      0.404807610096      1.478242644160
  C  -0.618593960666     -0.115923641115     -0.496578240025
  H  -2.768439270844     -0.175550279160     -0.404885993443
  C  -0.718080874458      0.662228927652      2.202307674687
  C   0.552831490192      0.139242618796      0.223921895996
  H  -0.588254480086     -0.411409513258     -1.542571570035
  N  -3.170701862320      0.543468625160      2.136586969828
  C   0.506479531164      0.527927046062      1.567754094097
  H  -0.770753508076      0.962119123271      3.246102851642
  O   1.812788832454      0.026035503085     -0.306058156507
  O  -4.190959816600      0.312165461626      1.486788404939
  O  -3.189124793255      0.886803285444      3.319123235740
  H   1.436356811805      0.719339368803      2.100925860597
  P   2.194741681522     -0.350312541707     -1.845742830973
  O   3.780354419107     -0.311259144468     -1.767228196032
  O   1.548457501106      0.502586561868     -2.875483345034
  O   1.859018050119     -1.903956897940     -1.865370050180
  H   4.156482201106      0.594486300867     -1.935748189531
  H   1.771104172998     -2.272211088122     -2.785593678887

E(RB+HF-PW91) =  -1079.44316828     A.U.


p-Nitrophenyl trihydrogen phosphate: pNPh-O-PO3H3+

  1     1
  P  -2.798385872428     -0.012807131466      0.080622900760
  O  -1.585316440349     -0.529559175245     -0.790597825445
  O  -4.088612752113     -0.426313965181     -0.684799656217
  O  -2.863020607547     -0.649052237921      1.501308375325
  O  -2.561687270419      1.515708993081      0.257479202555
  C  -0.230350307433     -0.320817638826     -0.487123458594
  H  -4.154694476187     -0.108577867010     -1.637288288609
  H  -3.100351985070     -1.626426046847      1.534510610423
  H  -3.204177554586      1.994018431923      0.866478347326
```

```
  C   0.453181720160     -1.329706519576      0.183373532299
  C   0.385056996734      0.843925905666     -0.933919388401
  C   1.811138392906     -1.160951647030      0.430389887087
  C   1.742463805704      1.013366605823     -0.685030701649
  H  -0.066131738703     -2.233619639925      0.499451649576
  H  -0.184022214462      1.601121101615     -1.470639025871
  C   2.431257160178      0.009204216091     -0.005536206062
  H   2.378678137595     -1.927761405481      0.952445504785
  H   2.258247200132      1.911197954103     -1.017590203851
  N   3.857658226043      0.187619390459      0.254791624530
  O   4.457459103853     -0.710205686350      0.840910501029
  O   4.391291781755      1.227307332679     -0.124243331099

E(RB+HF-PW91) =  -1079.86310040     A.U.


p-Nitrophenyl phosphate dianion, bridge protonated: pNPh-O(H+)-PO3-2

 -1     1
  C  -0.306049621594     -0.570340251228      0.022322359965
  C  -1.634300622704     -0.958959647560      0.011651735605
  C   0.020536383509      0.795914898461      0.016942324233
  H   0.494239521457     -1.304806425174      0.033879391180
  C  -2.634637074689      0.020690352470     -0.004823173539
  C  -0.990192872556      1.771486586773     -0.000139214295
  H  -1.901196501918     -2.013045618229      0.016084920860
  O   1.327114914989      1.119440315019      0.029717109199
  C  -2.320176173570      1.383798951057     -0.011060494214
  H   1.454977595398      2.100837227280      0.023850339277
  H  -0.723172320849      2.828732911401     -0.004500508910
  N  -4.018430760400     -0.383709832024     -0.015515519099
  P   3.761348093073     -0.266446012065     -0.025996485540
  H  -3.111979641862      2.128977557253     -0.024176645351
  O   4.128232545576      0.414559504351     -1.314523880814
  O  -4.282865191989     -1.589721154764     -0.010073320545
  O   3.086868789602     -1.608579827609     -0.050839635431
  O   4.151069310246      0.354039473914      1.286112453576
  O  -4.891086929043      0.489690074753     -0.029355544650

E(RB+HF-PW91) =  -1078.96200998     A.U.


p-Nitrophenyl phosphate monoanion, bridge protonated: pNPh-O(H+)-PO3H-

  0     1
  C  -1.872546885568      0.707315953489      0.179770806566
  C  -1.822501808880      0.407168086508      1.540993913077
  C  -0.686293480371      0.752555989742     -0.542627919927
  H  -2.823250664106      0.913446191922     -0.306280624668
  C  -0.623195789775      0.149390369363      2.204333289136
  C   0.505709645932      0.483827887117      0.122421699498
  H  -0.684199939744      0.996413757915     -1.602055265589
  N  -3.068367241986      0.364293990834      2.298587951313
  C   0.562367457540      0.182310771795      1.479865513077
  H  -0.616065795580     -0.081836984944      3.266841507906
  O   1.687570592454      0.532125104207     -0.626786053809
  O  -4.120214235009      0.582959350146      1.701422453313
  O  -3.010066203233      0.110876032051      3.499967947601
  H   2.497130828119      0.686087869563     -0.044861070734
```

```
  H   1.517810933189     -0.023312581626      1.963743734527
  P   2.132588385075     -0.746737817876     -2.043240590931
  O   1.865021309261     -2.071629236253     -1.196672308962
  O   3.562752275982     -0.372572710241     -2.199434021055
  O   1.018332685710     -0.508441164355     -2.992858512922
  H   2.652759393591     -2.345475405412     -0.653022573510

E(RB+HF-PW91) =  -1079.40629550     A.U.
```

p-Nitrophenyl phosphate, bridge protonated: pNPh-O(H^+)-PO_3H_2

```
  1     1
  P   0.034350789298      0.099534450518     -0.060796368836
  O  -0.002985434363     -0.000669149280      1.728538476254
  O   1.358697568064      0.670890222661     -0.334966116993
  O  -0.362744188684     -1.350915711809     -0.496767145583
  H   0.416528219937     -1.968039498618     -0.649494509332
  O  -1.243385381744      0.974926332222     -0.248810923358
  H  -2.030918521068      0.525091539213     -0.681050676581
  H   0.924905284446     -0.177432911761      2.132102499882
  C  -1.074812623031     -0.564353242896      2.495107499576
  C  -1.006915161771     -1.900705854616      2.857859064694
  C  -2.116265952965      0.286578729576      2.828983634640
  C  -2.054026472461     -2.419395675659      3.613195753719
  C  -3.167434457096     -0.239880755828      3.574282220523
  H  -2.105864562495      1.332859520002      2.527912594449
  H  -0.158607995485     -2.521455134229      2.568591717783
  C  -3.113658017090     -1.579894603188      3.951313631381
  H  -2.046265085885     -3.460301590567      3.928404445588
  H  -4.008056863819      0.386349630760      3.864294200857
  N  -4.218716711244     -2.130580547695      4.742475914346
  O  -5.150576248513     -1.385428161027      5.027966766431
  O  -4.155674877955     -3.308781471596      5.078758111322

E(RB+HF-PW91) =  -1079.82658224     A.U.
```

p-Nitrophenyl trihydrogen phosphate, bridge protonated: pNPh-O(H^+)-PO_3H_3

```
  2     1
  P  -0.004571404001     -0.109629230513      0.030365050804
  O   0.041663582594      0.290731729125      1.684294134970
  O   1.471449730809     -0.100141471581     -0.392660401080
  H   1.933280182355      0.806156660580     -0.468387805842
  O  -0.640107722334     -1.498963714048     -0.129447789951
  H  -0.032123124036     -2.309958690064     -0.025572545549
  O  -0.952290112113      1.007746098484     -0.427305983848
  H  -1.410087523133      0.883257238418     -1.329414593803
  H   0.915795328216      0.007917017595      2.202760529156
  C  -1.145917349484      0.424666025938      2.527936176568
  C  -1.656891129813     -0.720339806084      3.110501922027
  C  -1.646899715246      1.703763853526      2.678618654362
  C  -2.778344913290     -0.565135656639      3.921544996059
  C  -2.770979120017      1.846359132929      3.488304966669
  H  -1.179579796093      2.560213083083      2.193323187720
  H  -1.199440129028     -1.698060092371      2.955743705551
  C  -3.310522118998      0.711038362659      4.088471884105
  H  -3.227555124799     -1.426034286542      4.412028987279
```

```
  H  -3.213993842148      2.826751727518      3.649732898369
  N  -4.496400490947      0.867400269952      4.942881155863
  O  -4.963584909002      1.992760140888      5.074965633485
  O  -4.954674446527     -0.136132248600      5.476831066672

E(RB+HF-PW91) =  -1080.22200426     A.U.
```

Table S6. Coordinates of structures optimized using alternate computational methods.

```
---------------------------------------------------------------------
MP2/aug-cc-pVDZ optimized geometries with CPCM solvation (RADII=UA0)
---------------------------------------------------------------------

Methyl phosphate dianion Me-O-PO3(-2)

 -2     1
  C   0.751773168006     -1.088816439580      1.702131616391
  H   0.849578636198     -1.034860698336      2.796395634992
  H   1.754754358187     -1.182777078430      1.252442115787
  H   0.154389848638     -1.977015175458      1.435079601829
  O   0.103880577619      0.115512937594      1.267690076335
  P  -0.166306579964      0.227351579223     -0.430604709998
  O  -0.871645488954      1.627161608504     -0.522116442497
  O  -1.085154025644     -0.993712102987     -0.801662304331
  O   1.256073543029      0.165697294559     -1.098615879630

E(MP2) = -681.2915588 A.U.


Methyl Phosphate monoanion Me-O-PO3H(-)

 -1     1
  C    0.000881268060     -0.004149610041      0.001655857436
  H    0.052109893552     -0.075194650882      1.099626570318
  H    1.019679802877      0.025249523907     -0.413372110602
  H   -0.543741335851      0.905586192382     -0.283118926965
  O   -0.739626334999     -1.117434137968     -0.546109484998
  P   -0.123474478899     -2.641048549308     -0.216772338344
  O    1.395658541490     -2.667499319499     -0.457764548282
  O   -0.303881580224     -2.753378027096      1.439417783263
  O   -1.084668825055     -3.605918621529     -0.933803368957
  H   -1.265515536488     -2.858014736194      1.652270647795

E(MP2) = -681.7689316 A.U.


Methyl dihydrogen phosphate Me-O-PO3H2

  0     1
  C    1.760020198136      1.271700279937      0.038727619052
  H    1.665625473601      1.295129213625      1.133555604044
  H    2.817485366081      1.255535324438     -0.248971780408
  H    1.255029014877      2.138048371481     -0.409687804504
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  O    1.190823016831      0.038065534700     -0.489679671538
  P   -0.336206261313     -0.342939076553     -0.076737688717
  O   -1.123243156172      1.012462134900     -0.502417722502
  O   -0.749937940049     -1.653414147421     -0.709676767235
  O   -0.439131214585     -0.268610622117      1.549008930660
  H   -2.096152593744      0.945057527326     -0.284426070638
  H   -0.187100178139     -1.147909168706      1.950351512865

E(MP2) = -682.2174172 A.U.


Methyl trihydrogen phosphate Me-O-PO3H3(+)

  1     1
  C   -0.017622570186      0.001017120271      0.010793916349
  O    0.070133517094     -0.041475696921      1.481974669379
  H    1.021548981902      0.066976472174     -0.326157939717
  H   -0.583480772585      0.889217139111     -0.301684247537
  H   -0.490873441341     -0.921488633539     -0.348401096815
  P   -1.285945910378      0.043076488938      2.308684752738
  O   -0.732406088231     -0.108015577038      3.788500763061
  O   -2.205473365814     -1.139829692130      1.776362228699
  O   -2.131892633225      1.371858254673      2.062849684104
  H   -1.455113341444      0.019042424599      4.484822053656
  H   -3.167735196499     -1.056879518717      2.074513564182
  H   -1.693373175452      2.185132965262      2.474517420361

E(MP2) = -682.6370229 A.U.


Methyl phosphate anionic zwitterion Me-O(H+)-PO3(-2)

 -1     1
  C   0.005456715379      0.006501525531      0.006113499132
  H   0.015385852344      0.035358858156      1.101311109522
  H   1.029887904151      0.031150157202     -0.388477211353
  H  -0.538125975083     -0.877839440912     -0.350837859643
  O  -0.721216140098      1.200505988376     -0.411584439253
  H  -0.786886131876      1.232704501367     -1.405855257169
  P   0.153754013403      2.957483549414      0.155115323504
  O  -0.095964071577      2.790905922816      1.666091093417
  O  -0.796846809923      3.848111908848     -0.669372186946
  O   1.574479868597      2.699328688705     -0.384902147072

E(MP2) = -681.7378559 A.U.


Methyl phosphate anionic zwitterion Me-O(H+)-PO3H(-)

  0     1
  C    -0.090165690435      0.077632351112     -0.105966673963
  H    -0.246866790486      0.417357694399      0.922203508254
  H     0.960538694819      0.171905330674     -0.402223061100
  H    -0.757139229393      0.592162585191     -0.809617611594
  O    -0.404461378947     -1.365965763732     -0.093055850674
  H    -0.198335281128     -1.793119240951     -0.985439573614
  P    -2.196535386924     -1.754289819475      0.375360054275
  O    -2.984559983942     -1.285078859578     -0.834190747344
  O    -1.951546121256     -3.361637891359      0.435861864127
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  O    -2.230926292948     -1.161835087411      1.768808406337
  H    -2.181774726387     -3.776202104211     -0.443257688517

E(MP2) = -682.1877884 A.U.


METHYLPHOSPHATE WITH BRIDGE-OXYGEN PROTONATED Me-O(H+)-PO3H2

  1     1
  O    -0.052458147820      0.013260974529      1.048455273979
  H    -0.016975621917      0.073675924404      0.040048763025
  P     1.402967511758     -0.011439626850      1.705622733133
  O     0.830161750379     -0.091047044220      3.380493550231
  O     2.354966732934      1.139074105713      1.628474576592
  O     1.886940015613     -1.523770804566      1.534915412736
  H     2.862178391237     -1.628178276530      1.776201721563
  C    -0.264599147328     -1.047848905537      3.737529497604
  H     0.705437829568      0.853006610074      3.769531760562
  H     0.052150803673     -2.010475195027      3.324770064282
  H    -0.286261908918     -1.062467885421      4.832054192887
  H    -1.199479169576     -0.685900652061      3.297519572632

E(MP2) = -682.6086452 A.U.


Methyl trihydrogen phosphate with bridge oxygen protonated Me-O(H+)-PO3H3(+)

  2     1
  C     0.082428032273      0.058506294499     -0.044992333494
  H     0.499405425303      0.165493156515      0.960978730981
  H     0.861640281726     -0.051834449130     -0.807195846956
  H    -0.708606429938     -0.695067045645     -0.115446945488
  O    -0.545194125888      1.410535501852     -0.325382003665
  H    -1.234107269751      1.736141353888      0.403894179704
  P    -1.040111507853      1.775235175196     -1.914696294642
  O    -1.865451105060      0.493664676258     -2.275318777039
  O    -1.776331456558      3.113749768699     -1.580610913698
  O     0.268422151796      1.816148903420     -2.774032952835
  H    -2.282858628939      3.526013057939     -2.374948139131
  H     0.773678500387      2.706442453344     -2.699257958566
  H    -1.987186452957      0.345395051219     -3.284464789683

E(MP2) = -682.9989646 A.U.


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PBE0/aug-cc-pVDZ optimized geometries with CPCM solvation (RADII=Pauling)
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Methyl phosphate dianion Me-O-PO3(-2)

 -2     1
  C     0.748770391497     -1.092623444282      1.709230821377
  H     0.859785445543     -0.998317598050      2.795857292581
  H     1.745314949428     -1.206826089162      1.258394293057
  H     0.150447121441     -1.988859474596      1.489880190656
  O     0.102524486355      0.086707468354      1.243088318313
  P    -0.163804629338      0.227958226297     -0.423741604103
  O    -0.870323643609      1.611961135244     -0.491251967418
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  O    -1.069210680629     -0.972837573755     -0.830533888665
  O     1.238122284717      0.190465274288     -1.101726542606

E(RPBE+HF-PBE) = -682.127400169 A.U.


Methyl Phosphate monoanion Me-O-PO3H(-)

 -1     1
  C     0.000043742615      0.003163430226      0.001517572792
  H     0.030320501841     -0.032352081404      1.098617676484
  H     1.021809111958      0.037308953200     -0.396681548278
  H    -0.545833779671      0.896403522871     -0.317406698837
  O    -0.714039584710     -1.123357008755     -0.524068653181
  P    -0.130088804844     -2.635785475033     -0.211754525940
  O     1.376904165821     -2.697372179809     -0.454678468612
  O    -0.304664370975     -2.788743261483      1.424928879317
  O    -1.088613246758     -3.575480720211     -0.942294867033
  H    -1.238416320814     -2.875587115828      1.663850713952

E(RPBE+HF-PBE) = -682.594771062 A.U.


Methyl dihydrogen phosphate Me-O-PO3H2

  0     1
  C     2.180742925940     -0.054475447015      0.018165282512
  H     2.164452205053     -0.105498916666      1.112219588695
  H     2.997099914535     -0.666198500538     -0.372634735586
  H     2.293109157867      0.981858057909     -0.317884757066
  O     0.968069225144     -0.623011218116     -0.526982511250
  P    -0.465948778458     -0.061937859963     -0.066894343559
  O    -0.349510611723      1.505675300283     -0.425981254267
  O    -1.574903218002     -0.845907442082     -0.716265431645
  O    -0.497519855608     -0.019346608816      1.550484424844
  H    -1.169534956810      1.990592431982     -0.245135985187
  H    -0.740133007938     -0.879573796978      1.927408722509

E(RPBE+HF-PBE) = -683.039480925 A.U.


Methyl trihydrogen phosphate Me-O-PO3H3(+)

  1     1
  C    -0.012297000000      0.010555000000      0.020348000000
  O     0.035296000000     -0.045366000000      1.479246000000
  H     1.032759000000      0.041202000000     -0.290501000000
  H    -0.535256000000      0.916393000000     -0.300285000000
  H    -0.505186000000     -0.888826000000     -0.358988000000
  P    -1.295637000000      0.050992000000      2.313147000000
  O    -0.720894000000     -0.053040000000      3.781148000000
  O    -2.228952000000     -1.141666000000      1.859766000000
  O    -2.150339000000      1.362650000000      2.060880000000
  H    -1.392300000000     -0.092292000000      4.482769000000
  H    -3.173374000000     -1.030288000000      2.058950000000
  H    -1.726055000000      2.178319000000      2.380295000000

E(RPBE+HF-PBE) =  -683.460243308 A.U.
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Methyl phosphate anionic zwitterion Me-O(H+)-PO3(-2)

 -1     1
  C    -0.214522795443     -1.893603199017      1.239420671511
  H     0.285230888786     -1.392875825149      2.070832322653
  H     0.507382497436     -2.407753726805      0.598988106509
  H    -0.975628238471     -2.582107438007      1.613418173091
  O    -0.890666713890     -0.852670622554      0.486957371784
  H    -1.462191891106     -1.249060077545     -0.189114076577
  P     0.175176502899      0.528505035541     -0.338989779698
  O     0.602976138801      1.263163889487      0.933253806316
  O    -0.957132703010      1.124406958629     -1.180120647446
  O     1.234658543504     -0.308873395040     -1.060518514213

E(RPBE+HF-PBE) = -682.565179820 A.U.


Methyl phosphate anionic zwitterion Me-O(H+)-PO3H(-)

  0     1
  C    -0.070012371242      0.081351595570     -0.091748585673
  H    -0.260409765530      0.382502398953      0.938147934368
  H     0.996435044640      0.107295366190     -0.318744098230
  H    -0.654256438937      0.669036277330     -0.803964516255
  O    -0.474324269805     -1.328138058412     -0.176116289770
  H    -0.264382340629     -1.682071765771     -1.057863497062
  P    -2.179218574533     -1.764035607839      0.343267712633
  O    -3.047302628523     -1.383386946750     -0.830722027187
  O    -1.900604113744     -3.353244321795      0.452468558066
  O    -2.227127151261     -1.143489089727      1.713424874891
  H    -2.200569390436     -3.824890847749     -0.339667065780

E(RPBE+HF-PBE) =  -683.010440620 A.U.


METHYLPHOSPHATE WITH BRIDGE-OXYGEN PROTONATED Me-O(H+)-PO3H2

  1     1
  O    -0.019950869312      0.007764657257      0.983887174209
  H     0.037383549613      0.055277587545      0.014433811642
  P     1.390449116714     -0.011852007865      1.709939094480
  O     0.792357317215     -0.083846398261      3.339380369872
  O     2.328220867516      1.141382562418      1.644581722118
  O     1.910623582139     -1.499021971295      1.527290334992
  H     2.832831261483     -1.615030324356      1.815541668548
  C    -0.269668536321     -1.038650952432      3.754827774631
  H     0.699065565423      0.797142112063      3.749883325951
  H    -0.004349295387     -1.985480015288      3.284584022879
  H    -0.192990087694     -1.099405553532      4.840208988840
  H    -1.228943431785     -0.650390471747      3.411058831065

E(RPBE+HF-PBE) =  -683.433655748 A.U.


Methyl trihydrogen phosphate with bridge oxygen protonated Me-O(H+)-PO3H3(+)

  2     1
  C     0.115351483184      0.092674275086     -0.021793769012
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  H     0.560968799386      0.296341998734      0.949970702308
  H     0.867499520596      0.003097459188     -0.804859467560
  H    -0.612354022378     -0.717125402919     -0.015000074477
  O    -0.637012101687      1.359089966956     -0.349861767317
  H    -1.276991800600      1.634818216972      0.339178031647
  P    -1.043902690035      1.771853043030     -1.925079149072
  O    -1.961957848906      0.601143759386     -2.385514572891
  O    -1.688602017211      3.159783452991     -1.633569856065
  O     0.293887772364      1.741776796686     -2.723083299287
  H    -2.383900623047      3.434352711967     -2.260756474504
  H     0.835781338834      2.550979651563     -2.649756466111
  H    -2.023041810500      0.471640070359     -3.351346837659

E(RPBE+HF-PBE) = -683.834564544 A.U.
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