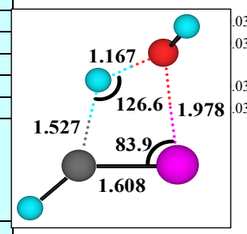
Calculation Level:
G3X ~ QCISD(T,FU)/G3XLarge

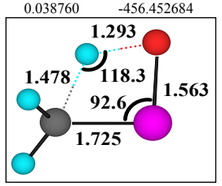
Geometry:
B3LYP/6-311+G(3df,2p)

HCP + H2O

Energy Relative to HCP + H2O

	G3X DH (0 K)	G3X DH (298 K)		G3 DH (0 K)	B3LYP/3+	ZPE	ZPE+H	B3LYP 6-311+G(3df,2p)	MP2 6-31G(d)	MP4 6-31G(d)	QCISD(T) 6-31G(d)	MP2 6-31+G(d)	MP4 6-31+G(d)	MP2 6-31G(2df,p)	MP4 6-31G(2df,p)	MP2=Full G3Large	HF G3Large	HF G3XLagre	Spin-Orbital	Na	Nb	# H	# C	# O	# P	# Cl
H2O	-237.627	-240.513	(kJ/mol)	-237.700	-231.376317	0.021360	0.025139	-76.463325	-76.1967	-76.2071	-76.2077	-76.2096	-76.2201	-76.2672	-76.2819	-76.3618	-76.0568	-76.0568	0.0000	4	4	2		1		
HCP	216.883	215.478		217.112	229.004704	0.014000	0.017519	-380.041461	-379.3445	-379.3741	-379.3729	-379.3483	-379.3782	-379.4044	-379.4396	-379.7826	-379.1494	-379.1495	0.0000	5	5	1	1		1	
HCP + H2O	-20.743			-20.588	-2.372																					
CH2=POH (CPOH-Cis)	-129.816	-140.229	-109.07	-127.763	-124.327	0.039365	0.044332	-456.555183	-455.5814	-455.6226	-455.6234	-455.5958	-455.6375	-455.7142	-455.7651	-456.1866	-455.2574	-455.2583	0.0000	9	9	3	1	1	1	
CH2=POH (CPOH-Trans)	-131.194	-141.577	-110.45	-129.128	-125.216	0.039700	0.044678	-456.555852	-455.5814	-455.6228	-455.6237	-455.5966	-455.6386	-455.7142	-455.7652	-456.1870	-455.2575	-455.2583	0.0000	9	9	3	1	1	1	
CH2=P(=O)H	-91.998	-102.819	-71.25	-90.099	-88.088	0.037899	0.042710	-456.539936	-455.5620	-455.6010	-455.5993	-455.5766	-455.6161	-455.6995	-455.7483	-456.1753	-455.2400	-455.2407	0.0000	9	9	3	1	1	1	
CH3PO (C1 ~ Cs)	-153.944	-163.293	-133.20	-152.333	-147.472	0.038984	0.044356	-456.563623	-455.5983	-455.6397	-455.6376	-455.6106	-455.6528	-455.7267	-455.7784	-456.1973	-455.2645	-455.2652	0.0000	9	9	3	1	1	1	
Transistion States																										
HCP + H2O - H2C=POH (CPOH-Trans)	125.947	115.154	146.69			.033938	0.038760	-456.452684	-455.4769	-455.5186	-455.5199	-455.4927	-455.5350	-455.6127	-455.6643	-456.0827	-455.1291	-455.1297	0.0000	9	9	3	1	1	1	
CH2=POH (CPOH-Cis) - CH3PO	72.339	60.779	93.08			.034053			-455.4994	-455.5398	-455.5369	-455.5133	-455.5544	-455.6366	-455.6864	-456.1090	-455.1504	-455.1511	0.0000	9	9	3	1	1	1	
or																										
CH2POH - CH2=P(=O)H	134.072	124.500	154.82			.033210			-455.4686	-455.5111	-455.5045	-455.4861	-455.5292	-455.6087	-455.6608	-456.0860	-455.1190	-455.1198	0.0000	9	9	3	1	1	1	
CH2=P(=O)H - CH3PO	45.027	33.738	65.77			.034796			-455.5015	-455.5479	-455.5469	-455.5155	-455.5625	-455.6382	-455.6937	-456.1126	-455.1697	-455.1705	0.0000	9	9	3	1	1	1	





Calculations above show that once HCP + H2O gets over the first energy barrier (146.7 kJ/mol) to H2C=POH, the isomerization towards CH3PO will be straight

CH3PO + H2O

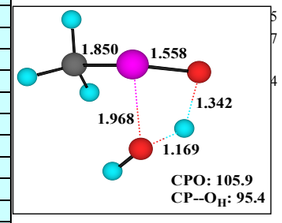
Energy Relative to CH3PO + H2O

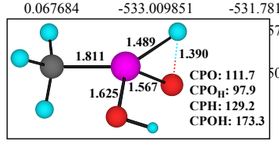
	G3X DH (0 K)	G3X DH (298 K)		G3 DH (0 K)	B3LYP/3+	ZPE	ZPE+H	B3LYP 6-311+G(3df,2p)	MP2 6-31G(d)	MP4 6-31G(d)	QCISD(T) 6-31G(d)	MP2 6-31+G(d)	MP4 6-31+G(d)	MP2 6-31G(2df,p)	MP4 6-31G(2df,p)	MP2=Full G3Large	HF G3Large	HF G3XLagre	Spin-Orbital	Na	Nb	# H	# C	# O	# P	# Cl
H2O	-237.627	-240.513	(kJ/mol)	-237.700	-231.376317	0.021360	0.025139	-76.463325	-76.1967	-76.2071	-76.2077	-76.2096	-76.2201	-76.2672	-76.2819	-76.3618	-76.0568	-76.0568	0.0000	4	4	2		1		
CH3PO (C1)	-153.944	-163.293		-152.333	-147.472	0.038984	0.044356	-456.563623	-455.5983	-455.6397	-455.6376	-455.6106	-455.6528	-455.7267	-455.7784	-456.1973	-455.2645	-455.2652	0.0000	9	9	3	1	1	1	
CH3PO + H2O	-391.570			-390.033	-378.848																					
Three conformers for CH3P(OH)2. The difference is in the dihedral angle of CPOH.																										
CH3P(OH)2 POH-OutOut Cs	-521.850	-540.377	-130.280	-517.797	-497.751	0.066569	0.073324	-533.078370	-531.8478	-531.8964	-531.8972	-531.8703	-531.9204	-532.0522	-532.1154	-532.6144	-531.3797	-531.3813	0.0000	13	13	5	1	2	1	
CH3P(OH)2 POH-InOut C1	-521.851	-540.606	-130.281	-517.845	-498.044	0.066358	0.073026	-533.078274	-531.8487	-531.8974	-531.8983	-531.8703	-531.9204	-532.0525	-532.1157	-532.6141	-531.3803	-531.3819	0.0000	13	13	5	1	2	1	
CH3P(OH)2 POH-InIn Cs	-511.262	-529.809	-119.692	-507.244	-488.199	0.065769	0.072516	-533.073944	-531.8435	-531.8923	-531.8932	-531.8638	-531.9142	-532.0484	-532.1116	-532.6093	-531.3759	-531.3775	0.0000	13	13	5	1	2	1	
CH3P(O)(H)OH HOPO~Cis	-570.288	-589.625	-178.718	-566.482	-540.899	0.065786	0.072232	-533.094033	-531.8651	-531.9104	-531.9094	-531.8842	-531.9310	-532.0724	-532.1326	-532.6367	-531.4026	-531.4041	0.0000	13	13	5	1	2	1	

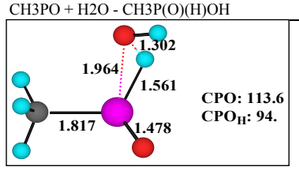
CH3P(O)(H)OH is more stable than CH3P(OH)2. This may imply that the final product from CH3PO + H2O is CH3P(O)(H)OH, instead of CH3P(OH)2.

Transistion States

CH3PO + H2O - CH3P(OH)2	-348.004	-367.701	43.566			5	0.067684	-533.009851	-531.7812	-531.8295	-531.8288	-531.8013	-531.8512	-531.9861	-532.0492	-532.5446	-531.2879	-531.2893	0.0000	13	13	5	1	2	1	
CH3P(OH)2 -- CH3P(O)(H)OH	-312.026	-331.141	79.544			7			578	-531.8055	-531.8017	-531.7822	-531.8314	-531.9672	-532.0297	-532.5342	-531.2674	-531.2692	0.0000	13	13	5	1	2	1	
or directly																										
CH3PO + H2O - CH3P(O)(H)OH	-273.382	-292.047	118.188			4			503	-531.7982	-531.7947	-531.7733	-531.8228	-531.9553	-532.0182	-532.5187	-531.2479	-531.2494	0.0000	13	13	5	1	2	1	







CH3P(O)(OH)2 Cs	-887.563	-907.517		-882.188	-833.811	0.071113	0.078978	-608.396119	-606.9501	-606.9986	-606.9971	-606.9757	-607.0263	-607.2120	-607.2784	-607.8618	-606.3470	-606.3492	0.0000	16	16	5	1	3	1	

Formation of CH3P(O)(OH)2 has to undergo an oxidation process.

Calculation Level: **G3X ~ QCISD(T,FU)/G3XLarge**

Geometry: **B3LYP/6-311+G(3df,2p)**

HCP + H2O

Energy Relative to HCP + H2O

	G3X DH (0 K)	G3X DH (298 K)		G3 DH (0 K)	B3LYP/3+	ZPE	ZPE+H	B3LYP 6-311+G(3df,2p)	MP2 6-31G(d)	MP4 6-31G(d)	QCISD(T) 6-31G(d)	MP2 6-31+G(d)	MP4 6-31+G(d)	MP2 6-31G(2df,p)	MP4 6-31G(2df,p)	MP2=Full G3Large	HF G3Large	HF G3XLagre	Spin-Orbital	Na	Nb	# H	# C	# O	# P	# Cl
H2O	-237.627	-240.513	(kJ/mol)	-237.700	-231.376317	0.021360	0.025139	-76.463325	-76.1967	-76.2071	-76.2077	-76.2096	-76.2201	-76.2672	-76.2819	-76.3618	-76.0568	-76.0568	0.0000	4	4	2		1		
HCP	216.883	215.478		217.112	229.004704	0.014000	0.017519	-380.041461	-379.3445	-379.3741	-379.3729	-379.3483	-379.3782	-379.4044	-379.4396	-379.7826	-379.1494	-379.1495	0.0000	5	5	1	1		1	
HCP + H2O	-20.743			-20.588	-2.372																					
CH2=POH (CPOH-Cis)	-129.816	-140.229	-109.07	-127.763	-124.327	0.039365	0.044332	-456.555183	-455.5814	-455.6226	-455.6234	-455.5958	-455.6375	-455.7142	-455.7651	-456.1866	-455.2574	-455.2583	0.0000	9	9	3	1	1	1	
CH2=POH (CPOH-Trans)	-131.194	-141.577	-110.45	-129.128	-125.216	0.039700	0.044678	-456.555852	-455.5814	-455.6228	-455.6237	-455.5966	-455.6386	-455.7142	-455.7652	-456.1870	-455.2575	-455.2583	0.0000	9	9	3	1	1	1	
CH2=P(=O)H	-91.998	-102.819	-71.25	-90.099	-88.088	0.037899	0.042710	-456.539936	-455.5620	-455.6010	-455.5993	-455.5766	-455.6161	-455.6995	-455.7483	-456.1753	-455.2400	-455.2407	0.0000	9	9	3	1	1	1	
CH3PO (C1 ~ Cs)	-153.944	-163.293	-133.20	-152.333	-147.472	0.038984	0.044356	-456.563623	-455.5983	-455.6397	-455.6376	-455.6106	-455.6528	-455.7267	-455.7784	-456.1973	-455.2645	-455.2652	0.0000	9	9	3	1	1	1	
Transistion States																										
HCP + H2O - H2C=POH (CPOH-Trans)	125.947	115.154	146.69	127.574	130.745	0.033938	0.038760	-456.452684	-455.4769	-455.5186	-455.5199	-455.4927	-455.5350	-455.6127	-455.6643	-456.0827	-455.1291	-455.1297	0.0000	9	9	3	1	1	1	
CH2=POH (CPOH-Cis) - CH3PO	72.339	60.779	93.08	74.101	75.590	0.034053	0.038583	-456.473805	-455.4994	-455.5398	-455.5369	-455.5133	-455.5544	-455.6366	-455.6864	-456.1090	-455.1504	-455.1511	0.0000	9	9	3	1	1	1	
or																										
CH2POH - CH2=P(=O)H	134.072	124.500	154.82	136.084	133.961	0.033210	0.038497	-456.450742	-455.4686	-455.5111	-455.5045	-455.4861	-455.5292	-455.6087	-455.6608	-456.0860	-455.1190	-455.1198	0.0000	9	9	3	1	1	1	
CH2=P(=O)H - CH3PO	45.027	33.738	65.77	46.925	49.283	0.034796	0.039429	-456.484557	-455.5015	-455.5479	-455.5469	-455.5155	-455.5625	-455.6382	-455.6937	-456.1126	-455.1697	-455.1705	0.0000	9	9	3	1	1	1	

Calculations above show that once HCP + H2O gets over the first energy barrier (146.7 kJ/mol) to H2C=POH, the isomerization towards CH3PO will be straight

CH3PO + H2O

Energy Relative to CH3PO + H2O

	G3X DH (0 K)	G3X DH (298 K)		G3 DH (0 K)	B3LYP/3+	ZPE	ZPE+H	B3LYP 6-311+G(3df,2p)	MP2 6-31G(d)	MP4 6-31G(d)	QCISD(T) 6-31G(d)	MP2 6-31+G(d)	MP4 6-31+G(d)	MP2 6-31G(2df,p)	MP4 6-31G(2df,p)	MP2=Full G3Large	HF G3Large	HF G3XLagre	Spin-Orbital	Na	Nb	# H	# C	# O	# P	# Cl
H2O	-237.627	-240.513	(kJ/mol)	-237.700	-231.376317	0.021360	0.025139	-76.463325	-76.1967	-76.2071	-76.2077	-76.2096	-76.2201	-76.2672	-76.2819	-76.3618	-76.0568	-76.0568	0.0000	4	4	2		1		
CH3PO (C1)	-153.944	-163.293		-152.333	-147.472	0.038984	0.044356	-456.563623	-455.5983	-455.6397	-455.6376	-455.6106	-455.6528	-455.7267	-455.7784	-456.1973	-455.2645	-455.2652	0.0000	9	9	3	1	1	1	
CH3PO + H2O	-391.570			-390.033	-378.848																					
Three conformers for CH3P(OH)2. The difference is in the dihedral angle of CPOH.																										
CH3P(OH)2 POH-OutOut Cs	-521.850	-540.377	-130.280	-517.797	-497.751	0.066569	0.073324	-533.078370	-531.8478	-531.8964	-531.8972	-531.8703	-531.9204	-532.0522	-532.1154	-532.6144	-531.3797	-531.3813	0.0000	13	13	5	1	2	1	
CH3P(OH)2 POH-InOut C1	-521.851	-540.606	-130.281	-517.845	-498.044	0.066358	0.073026	-533.078274	-531.8487	-531.8974	-531.8983	-531.8703	-531.9204	-532.0525	-532.1157	-532.6141	-531.3803	-531.3819	0.0000	13	13	5	1	2	1	
CH3P(OH)2 POH-InIn Cs	-511.262	-529.809	-119.692	-507.244	-488.199	0.065769	0.072516	-533.073944	-531.8435	-531.8923	-531.8932	-531.8638	-531.9142	-532.0484	-532.1116	-532.6093	-531.3759	-531.3775	0.0000	13	13	5	1	2	1	
CH3P(O)(H)OH HOPO~Cis	-570.288	-589.625	-178.718	-566.482	-540.899	0.065786	0.072232	-533.094033	-531.8651	-531.9104	-531.9094	-531.8842	-531.9310	-532.0724	-532.1326	-532.6367	-531.4026	-531.4041	0.0000	13	13	5	1	2	1	
CH3P(O)(H)OH is more stable than CH3P(OH)2. This may imply that the final product from CH3PO + H2O is CH3P(O)(H)OH, instead of CH3P(OH)2.																										
Transistion States																										
CH3PO + H2O - CH3P(OH)2	-348.004	-367.701	43.566	-344.475	-331.290	0.061375	0.067684	-533.009851	-531.7812	-531.8295	-531.8288	-531.8013	-531.8512	-531.9861	-532.0492	-532.5446	-531.2879	-531.2893	0.0000	13	13	5	1	2	1	
CH3P(OH)2 -- CH3P(O)(H)OH	-312.026	-331.141	79.544	-307.598	-290.510	0.061357	0.067888	-532.994301	-531.7578	-531.8055	-531.8017	-531.7822	-531.8314	-531.9672	-532.0297	-532.5342	-531.2674	-531.2692	0.0000	13	13	5	1	2	1	
or directly																										
CH3PO + H2O - CH3P(O)(H)OH	-273.382	-292.047	118.188	-269.722	-262.528	0.060844	0.067546	-532.983137	-531.7503	-531.7982	-531.7947	-531.7733	-531.8228	-531.9553	-532.0182	-532.5187	-531.2479	-531.2494	0.0000	13	13	5	1	2	1	
CH3P(O)(OH)2 Cs	-887.563	-907.517		-882.188	-833.811	0.071113	0.078978	-608.396119	-606.9501	-606.9986	-606.9971	-606.9757	-607.0263	-607.2120	-607.2784	-607.8618	-606.3470	-606.3492	0.0000	16	16	5	1	3	1	
Formation of CH3P(O)(OH)2 has to undergo an oxidation process.																										