Supporting Information:

Table S-1. Fitted and structural parameters of aminomethanephosphine

	values	σ[a]	D[b]	units
Fitted parameters				
$\mu_{NH2}\mu_{PH2}$	11.0	1.77	0.88	Å^3 kcal/mol
$\mu_{NH2}q_{PH2}$	-76.9	3.53	0.78	Å^4 kcal/mol
$\mu_{PH2}q_{NH2}$	-28.1	7.17	0.69	
v_1	0.4458	0.07	0.66	kcal/mol
v_2	1.211	0.07	0.61	
v_3	2.596	0.06	0.58	
v_4	-0.0128	0.07	0.72	
v_5	0.3142	0.07	0.66	
v_6	2.338	0.06	0.63	
V_0	-0.051	0.07	0.89	
Structural parameters				
r	2.77			Å
θ_{dPH_2}	112.5			degrees
θ_{dNH_2}	70.0			
θ_{qPH_2}	115.2			
θ_{qNH_2}	105.7			
α_{PH_2}	150.8			
α_{NH_2}	38.5			

[a]Standard errors of the fitted parameters.

[b]Dependence = $1 - \frac{(\text{variance of the parameter, other parameters constant})}{(\text{variance of the parameter, other parameters changing})}$

Table S-2: Fitted and structural parameters of hydroxymethanephosphine

	values	σ[a]	D[b]	units
Fitted parameters				
$\mu_{PH2}\mu_{OH}$	12.6	1.082	0.71	Å^3 kcal/mol
$\mu_{PH2}q_{OH}$	24.9	1.925	0.53	Å^4 kcal/mol
$\mu_{OH}q_{PH2}$	-79.0	4.565	0.67	
v_1	0.5267	0.05	0.63	kcal/mol
v_2	1.768	0.05	0.61	
v_3	2.413	0.05	0.48	
v_4	-0.0177	0.06	0.74	
v_5	-0.2363	0.05	0.65	
v_6	1.186	0.05	0.63	
V_0	0.3783	0.05	0.88	
Structural parameters				
r	2.71			Å
θ_{dOH}	82.8			degrees
θ_{dPH_2}	103.9			
θ_{qOH}	62.5			
θ_{qPH_2}	115.2			
α_{PH_2}	150.6			
α_{OH}	39.9			

[a]Standard errors of the fitted parameters.

[b]Dependence = $1 - \frac{(\text{variance of the parameter, other parameters constant})}{(\text{variance of the parameter, other parameters changing})}$

Table S-3: Fitted and structural parameters of mercaptomethanephosphine

	values	σ[a]	D[b]	units
Fitted parameters				
$\mu_{PH2}\mu_{SH}$	2.99	1.15	0.98	Å^3 kcal/mol
$\mu_{PH2}q_{SH}$	30.5	8.86	0.95	Å^4 kcal/mol
$\mu_{PH}q_{SH2}$	-29.6	8.14	0.94	
v_1	0.462	0.07	0.67	kcal/mol
v_2	0.289	0.06	0.62	
v_3	2.594	0.06	0.58	
v_4	-0.394	0.07	0.69	
v_5	0.086	0.06	0.66	
v_6	1.434	0.06	0.63	
V_0	0.494	0.07	0.89	
Structural parameters				
r	3.07			Å
θ_{dSH}	99.4			degrees
θ_{dPH_2}	95.2			
θ_{qSH}	73.3			
θ_{qPH_2}	115.2			
α_{PH_2}	147.0			
α_{SH}	33.9			

[a]Standard errors of the fitted parameters.

[b]Dependence = 1 - $\frac{(\text{variance of the parameter, other parameters constant})}{(\text{variance of the parameter, other parameters changing})}$

Table S-4: Fitted and structural parameters of hydroxymethanethiol

	values	σ[a]	D[b]	units
Fitted parameters				
$\mu_{SH}\mu_{OH}$	17.3	2.56	0.97	Å^3 kcal/mol
$\mu_{SH}q_{OH}$	140.0	4.63	0.57	Å^4 kcal/mol
$\mu_{OH}q_{SH}$	38.7	5.79	0.95	
v_1	-2.230	0.07	0.82	kcal/mol
v_2	-1.295	0.06	0.73	
v_3	1.255	0.05	0.56	
v_4	-0.796	0.08	0.82	
v_5	-2.876	0.05	0.67	
v_6	1.459	0.05	0.65	
V_0	6.020	0.08	0.94	
θ_{qSH}	79.0	2.74	0.94	
Structural parameters				
r	2.66			Å
θ_{dSH}	99.1			degrees
θ_{dOH}	81.6			
θ_{qOH}	62.5			
α_{OH}	140.6			
α_{SH}	29.6			

[a]Standard errors of the fitted parameters.

[b]Dependence = $1 - \frac{(\text{variance of the parameter, other parameters constant})}{(\text{variance of the parameter, other parameters changing})}$