

Table S1. Coefficients for Calculation of  $\Delta G^\circ$  and  $\Delta H^\circ$  for Alkaline-Earth Phosphides
$$\Delta G^\circ = \Delta H^\circ_0 - a T \ln T - (b/2) T^2 - (c/2) T^{-1} \cdot 10^5 + I T$$

$$\Delta H^\circ = \Delta H^\circ_0 + a T + (b/2) T^2 - c T^{-1}$$

Compound	Reference States	Temperature Range (K)	$\Delta H^\circ_0$	<i>a</i>	<i>b</i>	<i>c</i>	<i>I</i>
Ba <sub>3</sub> P <sub>2</sub>	α, red (V)	298-582	-629770	210.44	-0.396	-68.8	1345.3
Ba <sub>3</sub> P <sub>2</sub>	β, red (V)	582-704	-585577	56.813	-0.066	-6.84	396.46
Ba <sub>3</sub> P <sub>2</sub>	β, P <sub>4</sub> (g)	704-768	-651063	56.813	-0.0436	-6.84	497.41
Ba <sub>3</sub> P <sub>2</sub>	γ, P <sub>4</sub> (g)	768-1002	-613959	-45.382	0.0968	-6.84	-175.95
Ba <sub>3</sub> P <sub>2</sub>	l, P <sub>4</sub> (g)	1002-1533	-705009	5.666	0.0684	-316.4	238.01
Ba <sub>3</sub> P <sub>2</sub>	l, P <sub>2</sub> (g)	1533-1814	-819759	5.666	0.0715	-316.4	315.26
Ca <sub>3</sub> P <sub>2</sub>	α, red (V)	298-704	-507358	31.016	-0.045	-1.12	215.13
Ca <sub>3</sub> P <sub>2</sub>	α, P <sub>4</sub> (g)	704-720	-572844	31.016	-0.0225	-1.12	316.08
Ca <sub>3</sub> P <sub>2</sub>	β, P <sub>4</sub> (g)	720-1112	-594696	80.444	-0.0819	6.53	650.93
Ca <sub>3</sub> P <sub>2</sub>	l, P <sub>4</sub> (g)	1112-1533	-597810	-8.758	0.0422	6.53	97.05
Ca <sub>3</sub> P <sub>2</sub>	l, P <sub>2</sub> (g)	1533-1757	-712560	-8.758	0.0454	6.53	174.3

Table S2. Coefficients for Calculation of  $\Delta G^\circ$  and  $\Delta H^\circ$  for Lanthanide and Actinide Phosphides
$$\Delta G^\circ = \Delta H^\circ_0 - a T \ln T - (b/2) T^2 - (c/2) T^{-1} \cdot 10^5 + I T$$

$$\Delta H^\circ = \Delta H^\circ_0 + a T + (b/2) T^2 - c T^{-1}$$

Compound	Reference States	Temperature Range (K)	$\Delta H^\circ_0$	<i>a</i>	<i>b</i>	<i>c</i>	<i>I</i>
ScP	α, red (V)	298-704	-346348	-0.029	-0.0236	-0.15	-0.554
ScP	α, P <sub>4</sub> (g)	704-1533	-379091	-0.029	-0.0123	-0.15	49.921
ScP	α, P <sub>2</sub> (g)	1533-1608	-436466	-0.029	-0.0108	-0.15	88.546
ScP	β, P <sub>2</sub> (g)	1608-1812	-416610	-23.818	0.0004	1.4	-90.395
ScP	l, P <sub>2</sub> (g)	1812-2300	-430705	-23.818	0.0004	1.4	-82.613
YP	α, red (V)	298-704	-372724	-1.233	-0.0211	2.39	-19.355
YP	α, P <sub>4</sub> (g)	704-1533	-405467	-1.233	-0.0099	2.39	31.12
YP	α, P <sub>2</sub> (g)	1533-1752	-462842	-1.233	-0.0083	2.39	69.745
YP	β, P <sub>2</sub> (g)	1752-1799	-460072	-12.287	-0.0007	2.69	-7.752
YP	l, P <sub>2</sub> (g)	1799-2300	-458687	-20.404	-0.0007	2.69	-70.367
LaP	α, red (V)	298-550	-364146	5.128	-0.0108	1.86	42.971
LaP	β, red (V)	550-704	-368242	14.608	-0.0251	-1.85	105.715
LaP	β, P <sub>4</sub> (g)	705-1134	-400985	14.608	-0.0138	-1.85	156.19
LaP	γ, P <sub>4</sub> (g)	1134-1193	-388789	-6.964	0.0008	1.36	2.142
LaP	l, P <sub>4</sub> (g)	1193-1533	-401349	-1.63	0.0008	1.36	50.461
LaP	l, P <sub>2</sub> (g)	1533-2300	-458724	-1.63	0.0024	1.36	89.086
UP	α, red (V)	298-704	-308314	0	0	0	5.436
UP	α, P <sub>4</sub> (g)	704-942	-341057	0	0.0126	0	55.911
UP	β, P <sub>4</sub> (g)	942-1049	-330970	-29.893	0.0466	3.66	-142.66
UP	γ, P <sub>4</sub> (g)	1049-1408	-340580	-25.27	0.0466	3.66	-101.34
UP	l, P <sub>4</sub> (g)	1408-1533	-335112	-35.646	0.0466	3.66	-180.49
UP	l, P <sub>2</sub> (g)	1533-2100	-392487	-35.646	0.0481	3.44	-141.81
U <sub>3</sub> P <sub>4</sub>	α, red (V)	298-704	-1170001	4.66	-0.0055	-11.3	122.45
U <sub>3</sub> P <sub>4</sub>	α, P <sub>4</sub> (g)	704-942	-1300973	4.66	0.0559	-11.3	324.35
U <sub>3</sub> P <sub>4</sub>	β, P <sub>4</sub> (g)	942-1049	-1270712	-85.019	0.1566	-0.32	-271.37
U <sub>3</sub> P <sub>4</sub>	γ, P <sub>4</sub> (g)	1049-1408	-1299542	-71.15	0.1566	-0.32	-147.4
U <sub>3</sub> P <sub>4</sub>	l, P <sub>4</sub> (g)	1408-1533	-1283138	-102.278	0.1566	-0.32	-384.88
U <sub>3</sub> P <sub>4</sub>	l, P <sub>2</sub> (g)	1533-2000	-1512638	-102.278	0.1626	-1.2	-230.18

**Table S3. Coefficients for Calculation of  $\Delta G^\circ$  and  $\Delta H^\circ$  for Chromium Phosphides**

$$\Delta G^\circ = \Delta H^\circ_0 - a T \ln T - (b/2) T^2 - (c/2) T^{-1} \cdot 10^5 + I T$$

$$\Delta H^\circ = \Delta H^\circ_0 + a T + (b/2) T^2 - c T^{-1}$$

Compound	Reference States	Temperature Range (K)	$\Delta H^\circ_0$	<i>a</i>	<i>b</i>	<i>c</i>	<i>I</i>
Cr <sub>3</sub> P	s(1), red (V)	298-311	-177893	101.655	-0.3234	3.27	582.952
Cr <sub>3</sub> P	s(2), red (V)	311-704	-165368	11.7	-0.0152	1.56	73.39
Cr <sub>3</sub> P	s(2), P <sub>4</sub> (g)	704-1533	-198111	11.7	-0.004	1.56	123.865
Cr <sub>3</sub> P	s(2), P <sub>2</sub> (g)	1533-1996	-255486	11.7	-0.0024	1.56	162.49
Cr <sub>12</sub> P <sub>7</sub>	s(1), red (V)	298-311	-1070148	478.126	-1.3971	-3.56	2722.538
Cr <sub>12</sub> P <sub>7</sub>	s(2), red (V)	311-704	-1020048	118.306	-0.1644	-10.39	684.29
Cr <sub>12</sub> P <sub>7</sub>	s(2), P <sub>4</sub> (g)	704-1533	-1249249	118.306	-0.0858	-10.39	1037.615
Cr <sub>12</sub> P <sub>7</sub>	s(2), P <sub>2</sub> (g)	1533-1996	-1650874	118.306	-0.0748	-10.39	1307.99
CrP	s(1), red (V)	298-311	-127171	39.844	-0.1218	-0.3	230.27
CrP	s(2), red (V)	311-704	-122996	9.859	-0.019	-0.866	60.419
CrP	s(2), P <sub>4</sub> (g)	704-1533	-155739	9.859	-0.0078	-0.866	110.89
CrP	s(2), P <sub>2</sub> (g)	1533-1996	-213114	9.859	-0.0062	-0.866	149.52

**Table S4. Coefficients for Calculation of  $\Delta G^\circ$  and  $\Delta H^\circ$  for Manganese Phosphides**

$$\Delta G^\circ = \Delta H^\circ_0 - a T \ln T - (b/2) T^2 - (c/2) T^{-1} \cdot 10^5 + I T$$

$$\Delta H^\circ = \Delta H^\circ_0 + a T + (b/2) T^2 - c T^{-1}$$

Compound	Reference States	Temperature Range (K)	$\Delta H^\circ_0$	<i>a</i>	<i>b</i>	<i>c</i>	<i>I</i>
Mn <sub>3</sub> P	α, red (V)	298-704	-198514	49.877	-0.0475	-17.75	349.15
Mn <sub>3</sub> P	α, P <sub>4</sub> (g)	704-980	-231257	49.877	-0.0362	-17.75	399.62
Mn <sub>3</sub> P	β, P <sub>4</sub> (g)	980-1360	-225998	22.502	-0.0075	-28.64	219.2
Mn <sub>3</sub> P	γ, P <sub>4</sub> (g)	1360-1378	-225659	25.376	-0.0185	-21.92	232.43
Mn <sub>2</sub> P	α, red (V)	298-704	-160400	11.116	-0.0193	-1.54	65.416
Mn <sub>2</sub> P	α, P <sub>4</sub> (g)	704-980	-193143	11.116	-0.008	-1.54	115.89
Mn <sub>2</sub> P	β, P <sub>4</sub> (g)	980-1360	-189637	-7.134	0.0111	-8.81	-4.393
Mn <sub>2</sub> P	γ, P <sub>4</sub> (g)	1360-1410	-189411	-5.218	0.0038	-4.34	4.427
Mn <sub>2</sub> P	δ, P <sub>4</sub> (g)	1410-1517	-187303	-10.146	0.0049	-4.34	-32.039
Mn <sub>2</sub> P	l, P <sub>4</sub> (g)	1517-1533	-193613	-33.75	0.0205	-4.34	-188.9
Mn <sub>2</sub> P	l, P <sub>2</sub> (g)	1533-1600	-250988	-33.75	0.0221	-4.34	-150.28
Mn <sub>3</sub> P <sub>2</sub>	α, red (V)	298-704	-192687	-8.91	-0.0684	3.07	-165.13
Mn <sub>3</sub> P <sub>2</sub>	α, P <sub>4</sub> (g)	704-980	-258173	-8.91	-0.046	3.07	-64.179
Mn <sub>3</sub> P <sub>2</sub>	β, P <sub>4</sub> (g)	980-1354	-252914	-36.285	-0.0173	-6.7	-244.6
MnP	α, red (V)	298-704	-119342	7.985	-0.0283	4.29	48.439
MnP	α, P <sub>4</sub> (g)	704-980	-152085	7.985	-0.0173	4.29	98.914
MnP	β, P <sub>4</sub> (g)	980-1360	-150332	-1.14	-0.0077	0.66	38.772
MnP	γ, P <sub>4</sub> (g)	1360-1410	-150219	-0.182	-0.0113	2.89	43.182
MnP	δ, P <sub>4</sub> (g)	1410-1424	-149165	-2.646	-0.0108	2.89	24.949
MnP <sub>3</sub>	α, red (V)	298-704	-165087	7.985	-0.051	4.29	60.629
MnP <sub>3</sub>	α, P <sub>4</sub> (g)	704-980	-263316	7.985	-0.0173	4.29	212.05
MnP <sub>3</sub>	β, P <sub>4</sub> (g)	980-1360	-261563	-1.14	-0.0077	0.66	151.91
MnP <sub>3</sub>	γ, P <sub>4</sub> (g)	1360-1410	-261450	-0.182	-0.0113	2.89	156.33
MnP <sub>3</sub>	δ, P <sub>4</sub> (g)	1410-1424	-260396	-2.646	-0.0108	2.89	138.09

Table S5. Coefficients for Calculation of  $\Delta G^\circ$  and  $\Delta H^\circ$  for Iron Phosphides

$$\Delta G^\circ = \Delta H^\circ_0 - a T \ln T - (b/2) T^2 - (c/2) T^{-1} \cdot 10^5 + l T$$

$$\Delta H^\circ = \Delta H^\circ_0 + a T + (b/2) T^2 - c T^{-1}$$

Compound	Reference States	Temperature Range (K)	$\Delta H^\circ_0$	<i>a</i>	<i>b</i>	<i>c</i>	<i>l</i>
Fe <sub>3</sub> P	$\alpha$ , red (V)	298-704	-157602	46.047	-0.0871	-14.62	279.49
Fe <sub>3</sub> P	$\alpha$ , P <sub>4</sub> (g)	704-716	-190346	46.047	-0.0759	-14.62	329.97
Fe <sub>3</sub> P	$\alpha$ , P <sub>4</sub> (g)	716-1043	-201425	71.337	-0.1092	-25.41	498.72
Fe <sub>3</sub> P	$\alpha$ , P <sub>4</sub> (g)	1043-1185	94285	-480.69	0.4107	3.27	-3348.84
Fe <sub>3</sub> P	$\gamma$ , P <sub>4</sub> (g)	1185-1493	-202091	-0.534	0.0168	-11.69	65.655
Fe <sub>2</sub> P	$\alpha$ , red (V)	298-704	-149336	51.472	-0.0859	-20.83	317.73
Fe <sub>2</sub> P	$\alpha$ , P <sub>4</sub> (g)	704-1043	-182079	51.472	-0.0747	-20.83	368.20
Fe <sub>2</sub> P	$\alpha$ , P <sub>4</sub> (g)	1043-1185	15061	-316.54	0.2719	-1.71	-2196.834
Fe <sub>2</sub> P	$\gamma$ , P <sub>4</sub> (g)	1185-1493	-182523	3.558	0.0093	-11.67	79.495
FeP	$\alpha$ , red (V)	298-704	-104968	27.857	-0.0449	-10.24	172.04
FeP	$\alpha$ , P <sub>4</sub> (g)	704-1043	-137712	27.857	-0.0337	-10.24	222.52
FeP	$\alpha$ , P <sub>4</sub> (g)	1043-1185	-39142	-156.15	0.1396	-0.68	-1060.00
FeP	$\gamma$ , P <sub>4</sub> (g)	1185-1533	-137934	3.9	0.0083	-6.01	78.17
FeP	$\gamma$ , P <sub>2</sub> (g)	1533-1643	-195308	3.9	0.0072	-5.66	116.79
FeP <sub>2</sub>	$\alpha$ , red (V)	298-704	-162538	27.857	-0.0577	-10.24	193.60
FeP <sub>2</sub>	$\alpha$ , P <sub>4</sub> (g)	704-1043	-228025	27.857	-0.0345	-10.24	294.56
FeP <sub>2</sub>	$\alpha$ , P <sub>4</sub> (g)	1043-1185	-129455	-156.15	0.138	-0.68	-987.96
FeP <sub>2</sub>	$\gamma$ , P <sub>4</sub> (g)	1185-1300	-228427	3.9	0.0067	-6.01	150.20

Table S6. Coefficients for Calculation of  $\Delta G^\circ$  and  $\Delta H^\circ$  for Group 11 and 12 Phosphides

$$\Delta G^\circ = \Delta H^\circ_0 - a T \ln T - (b/2) T^2 - (c/2) T^{-1} \cdot 10^5 + l T$$

$$\Delta H^\circ = \Delta H^\circ_0 + a T + (b/2) T^2 - c T^{-1}$$

Compound	Reference States	Temperature Range (K)	$\Delta H^\circ_0$	<i>a</i>	<i>b</i>	<i>c</i>	<i>l</i>
AgP <sub>2</sub>	s, red (V)	298-704	-4190	0	-0.0223	0	-16.607
AgP <sub>2</sub>	s, P <sub>4</sub> (g)	704-826	-69676	0	0	0	84.343
Ag <sub>3</sub> P <sub>11</sub>	s, red (V)	298-704	-35055	0	-0.1238	0	-65.946
Ag <sub>3</sub> P <sub>11</sub>	s, P <sub>4</sub> (g)	704-826	-395228	0	0	0	489.279
Au <sub>2</sub> P <sub>3</sub>	s, red (V)	298-704	-40103	0	-0.0338	0	-9.175
Au <sub>2</sub> P <sub>3</sub>	s, P <sub>4</sub> (g)	704-926	-138332	0	0	0	142.25
Zn <sub>3</sub> P <sub>2</sub>	s, red (V)	298-692	-144613	-1.644	-0.0574	-1.58	-29.163
Zn <sub>3</sub> P <sub>2</sub>	<i>l</i> , red (V)	692-704	-153862	-31.779	-0.0225	0	-200.655
Zn <sub>3</sub> P <sub>2</sub>	<i>l</i> , P <sub>4</sub> (g)	704-1180	-219348	-31.779	0	0	-99.705
Zn <sub>3</sub> P <sub>2</sub>	g, P <sub>4</sub> (g)	1180-1446	-602844	0	0	0	450.06
ZnP <sub>2</sub>	s, red (V)	298-692	-69829	-1.644	-0.034	-1.58	-5.101
ZnP <sub>2</sub>	<i>l</i> , red (V)	692-704	-72912	-31.779	-0.0225	0	-62.265
ZnP <sub>2</sub>	<i>l</i> , P <sub>4</sub> (g)	704-1180	-138399	-31.779	0	0	38.685
ZnP <sub>2</sub>	g, P <sub>4</sub> (g)	1180-1313	-266231	0	0	0	221.94

Table S7. Coefficients for Calculation of  $\Delta G^\circ$  and  $\Delta H^\circ$  for Group 13 and 14 Phosphides

$$\Delta G^\circ = \Delta H^\circ_0 - a T \ln T - (b/2) T^2 - (c/2) T^{-1} \cdot 10^5 + l T$$

$$\Delta H^\circ = \Delta H^\circ_0 + a T + (b/2) T^2 - c T^{-1}$$

Compound	Reference States	Temperature Range (K)	$\Delta H^\circ_0$	$a$	$b$	$c$	$l$
AlP	s, red (V)	298-704	-115575	12.139	-0.0263	-4.36	69.82
AlP	s, P <sub>4</sub> (g)	704-933	-148318	12.139	-0.0151	-4.36	120.3
AlP	l, P <sub>4</sub> (g)	934-1533	-153623	-0.404	-0.0006	-3.63	46.982
AlP	l, P <sub>2</sub> (g)	1533-2000	-210998	-0.404	0.0009	-3.63	85.607
GaP	l, red (V)	298-704	-109068	19.068	-0.0196	-5.87	165.66
GaP	l, P <sub>4</sub> (g)	704-1533	-141811	19.068	-0.0084	-5.87	216.14
GaP	l, P <sub>2</sub> (g)	1533-1730	-199186	19.068	-0.0068	-5.87	254.76
InP	s, red (V)	298-430	-65319	20.787	-0.0484	-5.78	146.53
InP	l, red (V)	430-704	-63813	2.6	-0.0084	-3.09	42.077
InP	l, P <sub>4</sub> (g)	704-1335	-96556	2.6	0.0024	-3.09	92.552
SiP	s, red (V)	298-704	-38344	0	-0.0112	0	-2.001
SiP	l, red (V)	704-1300	-71087	0	0	0	48.474
GeP	s, red (V)	298-704	27816	0	-0.0112	0	-39.435
GeP	l, red (V)	704-1210	-4927	0	0	0	11.04