Revised Thermochemical Properties of Phosphinidene (PH), Phosphine (PH_3), Phosphorus Nitride (PN), and Magnesium Phosphate ($Mg_3P_2O_8$)

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Revised thermochemical tables for phosphinidene (PH), phosphine (PH_3), phosphorus nitride (PN), and magnesium orthophosphate ($Mg_3P_2O_8$) are computed. These computations were done because the P reference state was not adjusted to the white P reference state and/or because the tables of these compounds are printed erroneously in the 4th edition of the NIST-JANAF Thermochemical Tables. © *1999 American Institute of Physics and American Chemical Society.* [S0047-2689(99)00406-7]

Key words: phosphinidene, phosphine, phosphorus nitride, magnesium phosphate, enthalpy of formation, thermochemical properties

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1. Introduction

During preparation of the 3rd edition of the JANAF Thermochemical Tables [Chase *et al.* (1985)] the phosphorus reference state was changed to white P from the red-*V* P reference state used in the 2nd edition of the JANAF Tables [Stull and Prophet (1971)]. Somehow five P-bearing compounds [PH (g), PH_2(g), PH_3(g), PN (g), $Mg_3P_2O_8$(s,l)] escaped this update and, thus, the tables for these compounds in the 3rd edition use the enthalpy of formation from red-*V* P instead of that from white P.

Recently, the 4th edition of the NIST-JANAF Thermochemical Tables [Chase (1998)] was released. The preface states that updated thermochemical tables for gaseous PH, PH_2, PH_3, and $Mg_3P_2O_8$(s,l) from the 3rd edition of JANAF are incorporated. However, in the JANAF 3rd and 4th editions the enthalpy of formation has not been adjusted to the white phosphorus reference state for PN (g).

Although the enthalpy of formation for the phosphorus hydrides have been adjusted to the white P reference state, there are still some errors in the printed tables for PH (g) and PH_3(g). In the case of $Mg_3P_2O_8$(s,l) it appears that the same tables were printed in the 3rd and 4th editions, so that the correction for $Mg_3P_2O_8$(s,l) noted in the preface of the 4th edition does not appear in print. Thus, of the five compounds which originally were not adjusted from the red-*V* P to the white P reference state, only PH_2(g) has a corrected table in the 4th edition of the NIST-JANAF Tables.

Sections 2.1–2.4 give updated tables for PH (g), PH_3(g), PN (g), and $Mg_3P_2O_8$(s,l). In all tables, the reference state of P is white P for temperatures from 298.15 to 317.3 K, liquid P from 317.3 to 1180.008 K, and at higher temperatures P_2(g) is used, as is customary in the JANAF Tables. Thermal functions for P (α white, l), P_2(g), H_2(g), N_2(g), O_2(g), and Mg (s, l, g) are taken from the data compiled by Gurvich *et al.* (1989).

The heat capacities for the four compounds are taken from the NIST-JANAF Tables and fitted to polynomial functions (Table 1). The polynomial functions yield good agreement with the C_P data (typically<0.01% deviation) for the gaseous compounds listed in the JANAF Tables. The C_P data for $Mg_3P_2O_8$(s,l) in the JANAF Tables are estimates. The fit coefficients in Table 1 are for the experimental data of Oetting and McDonald (1963). These C_P data are reproduced to within 0.002% by the fits.

The entropies at 298.15 K are taken from the latest NIST-JANAF Tables for all compounds except for $Mg_3P_2O_8$, where the entropy is that used by Oetting and McDonald (1963). A summary of the heats of formation for the four compounds is given in Table 2. Also listed in Table 2 is the

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TABLE 1. Heat capacity functions

Compound	a	b	c	d	e	f	T range
PH (g)	+6.2925	−38.9069	−0.934 37	+77.8859	−575.655	+1549.85	298.15–1000
	+28.2596	+7.864 84	−10.3378	−2.530 37	+6.159 02	−6.703 68	1000–3000
	+20.5874	+11.8841	+59.5848	−2.598 99	+2.809 72	−1.147 92	3000–6000
PH_3(g)	+15.8225	+67.1384	+2.110 68	−7.809 28	−178.162	+675.299	298.15–1000
	+36.3827	+51.2889	−39.7398	−24.5454	+56.5439	−51.1261	1000–3000
	+80.0976	+1.537 73	−212.053	−0.337 85	+0.358 26	−0.149 90	3000–6000
PN (g)	+19.5718	+34.2136	+1.722 81	−23.7016	+35.3106	+170.741	298.15–1000
	+34.4731	+3.596 33	−12.5006	−1.688 48	+3.996 03	−3.686 94	1000–3000
	+36.3498	+0.875 69	−12.6166	−0.180 77	+0.225 09	−0.107 87	3000–6000
$Mg_3P_2O_8$(cr)	+229.358	−220.257	−33.0358	+1624.61	−25644.2	+1327 67	298.15–700
	+305.701	−2.065 86	−106.091	+58.5604	−253.528	+446.980	700–1200
	+32 209.2	−60 964.6	−41 195.3	+49 074.1	−186 603	+276 479	1200–1626
$Mg_3P_2O_8$(liq)	+470.700	···	···	···	···	···	1626–4500

The C_p values are fitted to $C_p(T)=a+b\times10^{-3}T+c\times10^{+5}T^{-2}+d\times10^{-6}T^2+e\times10^{-10}T^3+f\times10^{-14}T^4$ (J mol^{-1} K^{-1}). Data are from the NIST-JANAF Tables, except for $Mg_3P_2O_8$, which is from Oetting and McDonald (1963).

TABLE 2. Enthalpy of formation for P-bearing compounds using the red-V or white P reference state and entropies at 298.15 K

Compound	$\Delta_f H°_{298.15\,K}$ $P_{red\text{-}V}$ (kJ mol^{-1})	$\Delta_f H°_{298.15\,K}$ P_{white} kJ mol^{-1}	$S°_{298.15\,K}$ (J mol^{-1} K^{-1})	Reference
P (red)	0	−17.460	22.85±0.08	JANAF Tables
PH (g)	263.65	246.19	196.104	Glushko (1968)
PH (g)	253.55±33.5	236.09±33.5	196.344	JANAF[a,b]
PH (g)	256.72	239.26	···	Huber and Herzberg (1979)
PH (g)	248.212	230.752	196.379	Gurvich *et al.* (1989)
PH (g)	254.81	237.35	195.845	Jordan and Robertson (1994)
PH (g)	253.55±33.5	236.09±33.5	196.344	Adopted value
PH_3(g)	22.90±1.7	5.44±1.7	···	Gunn and Green (1961)
PH_3(g)	22.89	5.44	210.204	Glushko (1968)
PH_3(g)	22.9	5.4	210.23	Wagman *et al.* (1982)
PH_3(g)	22.90±1.7	5.439±1.7	210.243	JANAF[a]
PH_3(g)	22.13	4.67	209.865	Jordan and Robertson (1994)
PH_3(g)	22.90±1.7	5.44±1.7	210.243	Adopted value
PN (g)	117.92±5.0	100.46±5.0	···	Huffman *et al.* (1954)
PN (g)	109.13±5.0	91.67±5.0	211.028	Potter and DiStefano (1961)
PN (g)	116.88	99.42	211.041	Glushko (1968)
PN (g)	72.51±4.2	55.05±4.2	···	Uy *et al.* (1968)
PN (g)	154.53	137.07	211.08	Wagman *et al.* (1968)
PN (g)	189.5±16.7	172.1±16.7	···	Gingerich (1969)
PN (g)	127.33	109.87	211.19	Wagman *et al.* (1982)
PN (g)	104.78±5.0	87.32±5.0	211.137	JANAF[a,c]
PN (g)	188.948±15	171.488±15	211.132	Gurvich *et al.* (1989)
PN (g)	188.948±15	171.488±15	211.137	Adopted value
$Mg_3P_2O_8$(s)	−3745.10±10.5	−3780.02±10.5	189.20	Oetting and McDonald (1963)
$Mg_3P_2O_8$(s)	−3745.8	−3780.7	189.20	Wagman *et al.* (1982)
$Mg_3P_2O_8$(s)	−3745.10±10.5	−3780.02±10.5	188.280	JANAF[a]
$Mg_3P_2O_8$(s)	−3744.78±8	−3779.700±8	189.200	Pandit and Jacob (1995)
$Mg_3P_2O_8$(s)	−3745.0±11	−3780.0±11	189.200	Adopted value

[a]The enthalpy of formation is listed as given in the 2nd edition of the JANAF Tables, where red P is used as the reference state.
[b]The enthalpy of formation for PH (g) from white P is printed erroneously as 233.6±33.5 kJ mol^{-1} in the 4th edition of the NIST-JANAF Tables.
[c]The enthalpy of formation for PN (g) is calculated from the dissociation energy given by Potter and DiStefano (1961). The erroneous NIST-JANAF values are listed here.

TABLE 3. Thermodynamic properties of PH (g) at 1 bar

T (K)	$C_p°$	$S°$	$-[G°-H°(298.15\,K)]/T$	$H°-H°(298.15\,K)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
		($J\,mol^{-1}\,K^{-1}$)			($kJ\,mol^{-1}$)		
298.15	29.162	196.344	196.344	0.000	236.090	209.282	−36.665
300	29.163	196.524	196.345	0.054	236.073	209.116	−36.410
400	29.320	204.931	197.490	2.977	234.308	200.463	−26.177
500	29.710	211.511	199.659	5.926	233.184	192.133	−20.072
600	30.302	216.978	202.102	8.925	232.107	184.024	−16.021
700	31.007	221.701	204.572	11.990	231.091	176.092	−13.140
800	31.743	225.889	206.980	15.128	230.140	168.300	−10.989
900	32.452	229.670	209.294	18.338	229.251	160.624	−9.322
1000	33.111	233.123	211.507	21.616	228.416	153.044	−7.994
1100	33.716	236.308	213.619	24.958	227.626	145.546	−6.911
1200	34.261	239.265	215.634	28.358	163.115	139.327	−6.065
1300	34.758	242.028	217.559	31.809	163.148	137.343	−5.519
1400	35.216	244.620	219.401	35.308	163.202	135.357	−5.050
1500	35.643	247.065	221.164	38.851	163.272	133.365	−4.644
1600	36.045	249.378	222.856	42.436	163.363	131.369	−4.289
1700	36.425	251.575	224.481	46.059	163.462	129.366	−3.975
1800	36.787	253.667	226.045	49.720	163.573	127.357	−3.696
1900	37.133	255.666	227.552	53.416	163.695	125.342	−3.446
2000	37.464	257.579	229.006	57.146	163.831	123.320	−3.221
2100	37.783	259.414	230.410	60.909	163.980	121.291	−3.017
2200	38.089	261.179	231.769	64.702	164.143	119.254	−2.831
2300	38.385	262.879	233.085	68.526	164.318	117.210	−2.662
2400	38.671	264.519	234.361	72.379	164.506	115.158	−2.506
2500	38.946	266.103	235.599	76.260	164.706	113.097	−2.363
2600	39.212	267.635	236.802	80.168	164.917	111.029	−2.231
2700	39.467	269.120	237.971	84.102	165.138	108.952	−2.108
2800	39.711	270.560	239.110	88.061	165.368	106.867	−1.994
2900	39.944	271.957	240.218	92.044	165.604	104.773	−1.887
3000	40.165	273.315	241.299	96.049	165.847	102.672	−1.788
3100	40.382	274.636	242.353	100.077	166.095	100.562	−1.694
3200	40.588	275.921	243.382	104.125	166.345	98.444	−1.607
3300	40.785	277.173	244.387	108.194	166.598	96.318	−1.525
3400	40.974	278.394	245.370	112.282	166.851	94.185	−1.447
3500	41.154	279.584	246.330	116.389	167.104	92.044	−1.374
3600	41.328	280.746	247.270	120.513	167.354	89.896	−1.304
3700	41.494	281.881	248.190	124.654	167.601	87.740	−1.239
3800	41.654	282.989	249.092	128.811	167.842	85.579	−1.176
3900	41.808	284.073	249.975	132.984	168.078	83.411	−1.117
4000	41.956	285.134	250.840	137.173	168.306	81.237	−1.061
4100	42.098	286.171	251.690	141.375	168.525	79.058	−1.007
4200	42.237	287.187	252.523	145.592	168.735	76.873	−0.956
4300	42.370	288.183	253.340	149.823	168.933	74.683	−0.907
4400	42.500	289.158	254.143	154.066	169.120	72.489	−0.861
4500	42.627	290.115	254.932	158.323	169.293	70.291	−0.816
4600	42.750	291.053	255.707	162.591	169.452	68.089	−0.773
4700	42.870	291.974	256.469	166.872	169.595	65.884	−0.732
4800	42.988	292.878	257.218	171.165	169.722	63.676	−0.693
4900	43.104	293.765	257.955	175.470	169.832	61.466	−0.655
5000	43.218	294.637	258.680	179.786	169.923	59.253	−0.619
5100	43.331	295.494	259.393	184.114	169.995	57.039	−0.584
5200	43.442	296.337	260.096	188.452	170.048	54.824	−0.551
5300	43.552	297.165	260.788	192.802	170.079	52.608	−0.519
5400	43.661	297.980	261.469	197.163	170.089	50.391	−0.487
5500	43.770	298.782	262.140	201.534	170.076	48.175	−0.458
5600	43.878	299.572	262.801	205.916	170.040	45.958	−0.429
5700	43.985	300.350	263.453	210.310	169.979	43.743	−0.401
5800	44.092	301.116	264.096	214.714	169.894	41.529	−0.374
5900	44.200	301.870	264.730	219.128	169.783	39.317	−0.348
6000	44.306	302.614	265.355	223.553	169.646	37.107	−0.323

TABLE 4. Thermodynamic properties of PH_3(g) at 1 bar

T (K)	$C_p°$	$S°$	$-[G°-H°(298.15\,K)]/T$	$H°-H°(298.15\,K)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	($J\,mol^{-1}\,K^{-1}$)			($kJ\,mol^{-1}$)			
298.15	37.101	210.243	210.243	0.000	5.440	13.450	−2.356
300	37.180	210.473	210.244	0.069	5.385	13.500	−2.351
400	41.780	221.788	211.755	4.013	1.736	16.833	−2.198
500	46.479	231.619	214.764	8.427	−0.846	20.916	−2.185
600	50.907	240.490	218.324	13.300	−2.980	25.476	−2.218
700	54.934	248.645	222.080	18.595	−4.702	30.360	−2.266
800	58.509	256.219	225.880	24.271	−6.067	35.467	−2.316
900	61.625	263.295	229.648	30.282	−7.131	40.725	−2.364
1000	64.300	269.930	233.348	36.581	−7.949	46.088	−2.407
1100	66.594	276.168	236.960	43.129	−8.571	51.523	−2.447
1200	68.535	282.048	240.475	49.888	−72.801	58.218	−2.534
1300	70.188	287.601	243.888	56.827	−72.401	69.120	−2.777
1400	71.602	292.856	247.200	63.918	−71.919	79.989	−2.984
1500	72.818	297.838	250.411	71.140	−71.377	90.821	−3.163
1600	73.866	302.572	253.525	78.476	−70.784	101.615	−3.317
1700	74.772	307.078	256.543	85.909	−70.171	112.371	−3.453
1800	75.558	311.375	259.471	93.426	−69.542	123.091	−3.572
1900	76.242	315.479	262.312	101.017	−68.901	133.775	−3.678
2000	76.840	319.405	265.069	108.672	−68.254	144.426	−3.772
2100	77.365	323.167	267.747	116.383	−67.605	155.044	−3.857
2200	77.829	326.777	270.348	124.143	−66.955	165.631	−3.933
2300	78.240	330.246	272.878	131.947	−66.310	176.189	−4.001
2400	78.608	333.584	275.338	139.790	−65.671	186.718	−4.064
2500	78.939	336.799	277.732	147.667	−65.042	197.221	−4.121
2600	79.237	339.901	280.064	155.576	−64.424	207.700	−4.173
2700	79.506	342.897	282.336	163.514	−63.820	218.155	−4.220
2800	79.749	345.793	284.551	171.477	−63.232	228.587	−4.264
2900	79.965	348.595	286.711	179.463	−62.662	238.999	−4.305
3000	80.155	351.309	288.820	187.469	−62.112	249.392	−4.342
3100	80.340	353.941	290.878	195.494	−61.583	259.767	−4.377
3200	80.505	356.494	292.889	203.536	−61.077	270.125	−4.409
3300	80.655	358.974	294.854	211.594	60.596	280.467	−4.439
3400	80.794	361.384	296.776	219.667	−60.141	290.796	−4.468
3500	80.921	363.727	298.655	227.753	−59.713	301.111	−4.494
3600	81.038	366.009	300.495	235.851	−59.313	311.414	−4.518
3700	81.147	368.231	302.295	243.960	−58.943	321.707	−4.542
3800	81.247	370.396	304.059	252.080	−58.603	331.990	−4.564
3900	81.340	372.508	305.787	260.209	−58.294	342.265	−4.584
4000	81.427	374.568	307.481	268.348	−58.018	352.532	−4.604
4100	81.507	376.580	309.142	276.495	−57.776	362.793	−4.622
4200	81.582	378.545	310.771	284.649	−57.567	373.048	−4.640
4300	81.652	380.465	312.370	292.811	−57.394	383.298	−4.656
4400	81.718	382.343	313.939	300.979	−57.257	393.546	−4.672
4500	81.779	384.180	315.479	309.154	−57.156	403.790	−4.687
4600	81.836	385.978	316.993	317.335	−57.093	414.033	−4.701
4700	81.890	387.739	318.479	325.521	−57.068	424.274	−4.715
4800	81.941	389.464	319.940	333.713	−57.082	434.516	4.728
4900	81.988	391.154	321.376	341.909	−57.136	444.758	−4.741
5000	82.033	392.810	322.788	350.111	−57.229	455.001	−4.753
5100	82.076	394.435	324.177	358.316	−57.364	465.247	−4.765
5200	82.116	396.029	325.544	366.526	−57.539	475.496	−4.776
5300	82.153	397.594	326.889	374.739	−57.757	485.749	−4.787
5400	82.189	399.130	328.212	382.956	−58.016	496.006	−4.798
5500	82.223	400.638	329.515	391.177	−58.319	506.268	−4.808
5600	82.255	402.120	330.799	399.401	−58.665	516.537	−4.818
5700	82.286	403.576	332.063	407.628	−59.055	526.811	−4.828
5800	82.315	405.008	333.308	415.858	−59.490	537.094	−4.837
5900	82.342	406.415	334.535	424.091	−59.969	547.384	−4.846
6000	82.368	407.799	335.745	432.326	−60.494	557.682	−4.855

TABLE 5. Thermodynamic properties of PN (g) at 1 bar

T (K)	$C_p°$	$S°$	$-[G°-H°(298.15\,K)]/T$	$H°-H°(298.15\,K)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	(J mol^{-1} K^{-1})			(kJ mol^{-1})			
298.15	29.711	211.137	211.137	0.000	171.488	149.352	−26.166
300	29.726	211.321	211.138	0.055	171.472	149.215	−25.980
400	30.811	220.013	212.315	3.079	169.805	142.117	−18.558
500	31.990	227.016	214.577	6.220	168.865	135.306	−14.135
600	33.030	232.943	217.156	9.472	168.012	128.676	−11.202
700	33.880	238.101	219.788	12.819	167.224	122.183	−9.117
800	34.550	242.671	222.368	16.242	166.479	115.799	−7.561
900	35.073	246.772	224.856	19.724	165.763	109.508	−6.356
1000	35.495	250.490	227.236	23.253	165.062	103.295	−5.396
1100	35.831	253.889	229.507	26.820	164.369	97.152	−4.613
1200	36.103	257.019	231.671	30.417	99.920	92.281	−4.017
1300	36.328	259.918	233.734	34.039	99.985	91.641	−3.682
1400	36.516	262.617	235.701	37.682	100.046	90.997	−3.395
1500	36.675	265.142	237.581	41.342	100.103	90.349	−3.146
1600	36.812	267.513	239.378	45.016	100.158	89.697	−2.928
1700	36.930	269.749	241.100	48.703	100.206	89.041	−2.736
1800	37.033	271.862	242.750	52.402	100.248	88.383	−2.565
1900	37.125	273.867	244.336	56.110	100.286	87.723	−2.412
2000	37.206	275.774	245.861	59.826	100.321	87.061	−2.274
2100	37.279	277.591	247.329	63.550	100.353	86.397	−2.149
2200	37.346	279.326	248.744	67.282	100.384	85.732	−2.036
2300	37.406	280.988	250.110	71.019	100.412	85.065	−1.932
2400	37.462	282.581	251.430	74.763	100.438	84.398	−1.837
2500	37.514	284.111	252.707	78.512	100.461	83.729	−1.749
2600	37.563	285.584	253.943	82.266	100.482	53.059	−1.669
2700	37.609	287.002	255.141	86.024	100.500	82.389	−1.594
2800	37.652	288.371	256.304	89.787	100.514	81.717	−1.524
2900	37.692	289.693	257.433	93.555	100.524	81.046	−1.460
3000	37.730	290.971	258.529	97.326	100.529	80.374	−1.399
3100	37.767	292.209	259.596	101.101	100.529	79.702	−1.343
3200	37.802	293.409	260.634	104.879	100.523	79.031	−1.290
3300	37.836	294.572	261.645	108.661	100.510	78.359	−1.240
3400	37.869	295.702	262.630	112.446	100.490	77.688	−1.194
3500	37.900	296.801	263.591	116.235	100.461	77.018	−1.149
3600	37.931	297.869	264.528	120.026	100.424	76.349	−1.108
3700	37.961	298.908	265.443	123.821	100.376	75.680	−1.068
3800	37.990	299.921	266.337	127.618	100.318	75.014	−1.031
3900	38.018	300.908	267.211	131.419	100.249	74.349	−0.996
4000	38.046	301.871	268.066	135.222	100.167	73.686	−0.962
4100	38.073	302.811	268.902	139.028	100.072	73.025	−0.930
4200	38.099	303.729	269.720	142.836	99.962	72.366	−0.900
4300	38.125	304.626	270.521	146.648	99.838	71.711	−0.871
4400	38.151	305.502	271.306	150.462	99.697	71.058	−0.844
4500	38.176	306.360	272.076	154.278	99.540	70.409	−0.817
4600	38.201	307.199	272.830	158.097	99.364	69.764	−0.792
4700	38.226	308.021	273.570	161.918	99.170	69.122	−0.768
4800	38.250	308.826	274.297	165.742	98.956	68.485	−0.745
4900	38.274	309.615	275.009	169.568	98.721	67.853	−0.723
5000	38.298	310.388	275.709	173.397	98.465	67.225	−0.702
5100	38.321	311.147	276.397	177.228	98.185	66.603	−0.682
5200	38.345	311.892	277.072	181.061	97.882	65.987	−0.663
5300	38.368	312.622	277.736	184.897	97.554	65.377	−0.644
5400	38.391	313.340	278.389	188.735	97.200	64.773	−0.627
5500	38.414	314.044	279.031	192.575	96.820	64.176	−0.609
5600	38.436	314.737	279.662	196.417	96.411	63.589	−0.593
5700	38.459	315.417	280.283	200.262	95.973	63.003	−0.577
5800	38.481	316.086	280.895	204.109	95.506	62.429	−0.562
5900	38.503	316.744	281.497	207.958	95.007	61.863	−0.548
6000	38.525	317.391	282.090	211.810	94.476	61.306	−0.534

TABLE 6. Thermodynamic properties of $Mg_3P_2O_8$(s,l) at 1 bar

T (K)	$C_p°$	$S°$	$-[G°-H°(298.15\,K)]/T$	$H°-H°(298.15\,K)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
		(J mol^{-1} K^{-1})			(kJ mol^{-1})		
298.15	213.468	189.200	189.200	0.000	−3780.000	−3538.019	619.838
300	214.305	190.523	189.204	0.396	−3780.048	−3536.518	615.754
400	250.412	257.492	198.090	23.761	−3782.684	−3454.727	451.135
500	274.596	316.142	215.963	50.089	−3781.812	−3372.804	352.350
600	291.040	367.753	237.050	78.422	−3779.673	−3291.188	286.520
700	303.675	413.582	259.056	108.168	−3776.827	−3209.991	239.529
800	313.800	454.812	280.992	139.056	−3773.500	−3129.238	204.316
900	322.628	492.291	302.419	170.885	−3769.845	−3048.921	176.952
1000	330.703	526.706	323.150	203.557	−3791.708	−2966.884	154.972
1100	338.318	558.586	343.122	237.011	−3787.189	−2884.612	139.977
1200	345.640	588.339	362.330	271.210	−3909.208	−2800.362	121.895
1300	352.665	616.289	380.801	306.134	−3901.289	−2708.273	108.818
1400	359.526	642.674	398.573	341.742	−4279.470	−2606.723	97.257
1500	366.345	667.713	415.688	378.038	−4267.719	−2487.648	86.626
1600	373.081	691.569	432.191	415.006	−4255.406	−2369.375	77.351
1626	375.006	697.598	436.386	424.731		Crystal↔Liquid	
1626	470.700	771.804	436.386	545.391		Transition	
1700	470.700	792.753	451.446	580.222	−4114.953	−2257.536	69.365
1800	470.700	819.657	471.162	627.292	−4092.752	−2148.917	62.359
1900	470.700	845.107	490.179	674.362	−4070.655	−2041.529	56.125
2000	470.700	869.251	508.534	721.432	−4048.659	−1935.302	50.544
2100	470.700	892.216	526.263	768.502	−4026.788	−1830.173	45.522
2200	470.700	914.113	543.398	815.572	−4005.003	−1726.083	40.982
2300	470.700	935.037	559.975	862.642	−3983.303	−1622.983	36.859
2400	470.700	955.069	576.023	909.712	−3961.688	−1520.823	33.099
2500	470.700	974.284	591.571	956.782	−3940.159	−1419.564	29.660
2600	470.700	992.745	606.648	1003.852	−3918.721	−1319.163	26.502
2700	470.700	1010.510	621.279	1050.922	−3897.376	−1219.585	23.594
2800	470.700	1027.628	635.488	1097.992	−3876.129	−1120.797	20.908
2900	470.700	1044.146	649.297	1145.062	−3854.985	−1022.766	18.422
3000	470.700	1060.103	662.726	1192.132	−3833.950	−925.462	16.114
3100	470.700	1075.537	675.795	1239.202	−3813.028	−828.858	13.966
3200	470.700	1090.481	688.521	1286.272	−3792.226	−732.926	11.964
3300	470.700	1104.966	700.922	1333.342	−3771.549	−637.643	10.093
3400	470.700	1119.017	713.014	1380.412	−3751.003	−542.986	8.342
3500	470.700	1132.662	724.810	1427.482	−3730.595	−448.930	6.700
3600	470.700	1145.922	736.324	1474.552	−3710.330	−355.454	5.157
3700	470.700	1158.818	747.569	1521.622	−3690.215	−262.541	3.706
3800	470.700	1171.371	758.557	1568.692	−3670.255	−170.169	2.339
3900	470.700	1183.598	769.300	1615.762	−3650.456	−78.319	1.049
4000	470.700	1195.515	779.807	1662.832	−3630.824	130.230	−0.170
4100	470.700	1207.138	790.088	1709.902	−3611.364	103.878	−1.323
4200	470.700	1218.481	800.154	1756.972	−3592.082	194.260	−2.416
4300	470.700	1229.556	810.012	1804.042	−3572.983	284.185	−3.452
4400	470.700	1240.378	819.670	1851.112	−3554.073	373.668	−4.436
4500	470.700	1250.955	829.137	1898.182	−3535.356	462.724	−5.371

enthalpy of formation of red-V P from white P. This value is needed to convert the enthalpy of formation of P-bearing compounds from the red-V P reference state to the white P reference state. For a P-bearing compound the enthalpy of formation from white P is $\Delta_f H°(298.15) = \Delta_f H°$ (298.15, from P red-V) $-17.460 \times n$ (kJ/mol), where n designates the number of P atoms in the compound's formula. Table 2 lists the enthalpy of formation for the red-

V and white P reference state as appropriate.

2. Thermodynamic Data Tables

2.1. PH (g)

The enthalpy of formation of PH (g) is $\Delta_f H°(298.15) = 253.55 \pm 33.5$ kJ/mol in the 2nd edition of the JANAF Tables for the formation from red P. This value was not adjusted to the white P reference state in the 3rd edition. The enthalpy of formation $\Delta_f H°(298.15) = 236.09 \pm 33.5$ kJ/mol results when white P is used as the reference state. The 4th edition of the NIST-JANAF Tables lists $\Delta_f H°(298.15) = 233.6 \pm 33.5$ kJ/mol. This datum appears to be a typographical error of the value for the enthalpy of formation from red-V P, since the description in the text mentions 60.6 ± 8 kcal/mol, which is the value used in the 2nd edition of the JANAF Tables where red-V P was used as the reference state. The enthalpy of formation of PH (g) printed in the 4th edition of NIST-JANAF is close to the value for the formation of PH (g) from white P, and thus, the erroneous datum may have been overlooked.

The enthalpy of formation selected in the 2nd edition of the JANAF Tables is based on the estimated dissociation energy of $D°(0\text{ K}) = 294.6$ kJ/mol by Jordan (1964). Huber and Herzberg (1979) also selected a theoretical dissociation energy of $D°(0\text{ K}) = 291.4$ kJ/mol, which gives $\Delta_f H°(298.15) = 239.3$ kJ/mol for the formation of PH (g) (from white P).

Other data compilations select values of the enthalpy of formation close to that used in the JANAF Tables when adjusted to the appropriate P reference state (See Table 2). The JANAF datum is between the data selected by Glushko (1968) and by Gurvich *et al.* (1989) and the corrected enthalpy of formation from the JANAF Tables is adopted in the computation of the thermodynamic functions of PH (g) listed in Table 3.

2.2. PH_3(g)

Essentially all thermochemical compilations use the enthalpy of formation $\Delta_f H°(298.15) = 5.44 \pm 1.7$ kJ/mol for PH_3 (from white P) determined by Gunn and Green (1961). The 4th edition of the NIST-JANAF Tables uses this enthalpy of formation for white P as the reference state. A more recent determination of the enthalpy of formation of phosphine was given by Jordan and Robertson (1994), who used experimental data of Berkowitz (1988) to obtain $\Delta_f H°(298.15) = 4.67$ kJ/mol for PH_3(g) from white P. This value is close to the enthalpy of formation previously determined and the older value of $\Delta_f H°(298.15) = 5.44 \pm 1.7$ has been selected here.

While the adjustment to the white P reference state is done appropriately in the 4th edition of the NIST-JANAF Tables, the computations of $\Delta_f H°$, $\Delta_f G°$, and log K_f are incorrect (except for $\Delta_f H°$ at 298.15 K). The reasons for these errors in the JANAF Tables are not easy to trace. The recalculated thermochemical data are given in Table 4.

2.3. PN (g)

As mentioned in Sec. 1, the enthalpy of formation of PN (g) is not adjusted to the white P reference state in either the 3rd or 4th edition of the JANAF Tables. The selected value of $\Delta_f H°(298.15) = 104.8 \pm 5.0$ kJ/mol for formation from red-V P in the 2nd edition of the JANAF Tables is based on the data of Potter and DiStefano (1961). Adjustment to the white P reference state gives $\Delta_f H°(298.15) = 87.3 \pm 5.0$ kJ/mol. However, the enthalpy of formation was also calculated incorrectly in the 2nd edition of the JANAF Tables from the dissociation energy of $D°(0\text{ K}) = 693.85$ kJ/mol given by Potter and DiStefano (1961). It seems that the dissociation energy was taken to be for 298.15 K instead of 0 K, so that the enthalpy increments $(H_0 - H_{298.15})$ are missing in the calculated enthalpy of formation for PN (g) in the JANAF Tables. The enthalpy of formation obtained from the dissociation energy reported by Potter and DiStefano (1961) is $\Delta_f H°(298.15) = 91.67$ kJ/mol.

The enthalpy of formation of PN (g) is rather uncertain (Table 2) and other compilations select the enthalpy of formation as $\Delta_f H°(298.15) = 99.4$ kJ/mol [Glushko (1968), primarily based on data of Huffman *et al.* (1954)] and $\Delta_f H°(298.15) = 171.5 \pm 15$ kJ/mol [Gurvich *et al.* (1989)]. Gurvich *et al.* (1989) review available data and gave preference to the experimental data of Gingerich *et al.* (1969), which were not included in the evaluation of the enthalpy of formation of PN (g) in the JANAF Tables. Here, the value given by Gurvich *et al.* (1989) is adopted for computing the thermochemical data for PN (g) listed in Table 5.

2.4. $Mg_3P_2O_8$(s,l)

It seems that the same tables for $Mg_3P_2O_8$(s,l) were printed in the 3rd and 4th editions, so that the adjustment of the enthalpy of formation of $Mg_3P_2O_8$(s,l) for the white P reference state does not appear in print, although an update is noted in the preface of the 4th edition. This missing adjustment was previously noted by Pandit and Jacob (1995). The enthalpy of formation of $Mg_3P_2O_8$(s) from white P is $\Delta_f H°(298.15) = -3780.02$ kJ/mol from the selected value of $\Delta_f H°(298.15) = -3745.10$ kJ/mol from red-V P in the 2nd edition of the JANAF Tables and is essentially identical to those values selected by Oetting and McDonald (1963), Wagman *et al.* (1982), or Pandit and Jacob (1995). The value $\Delta_f H°(298.15) = -3780.0$ kJ/mol was used for the revised computed thermodynamic functions for $Mg_3P_2O_8$(s,l) listed in Table 6.

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