APPENDIX G
Heat Capacity Equations

Table G.1 Heat Capacity Equations for Organic and Inorganic Compounds (at Low Pressures)*

Forms: (1) $C_p^\circ = a + b(T) + c(T)^2 + d(T)^3$;
(2) $C_p^\circ = a + b(T) + c(T)^{-2}$.
Units of C_p° are J/(g mol)(K or °C).
To convert to cal/(g mol)(K or °C) = Btu/(lb mol)(°R or °F), multiply by 0.2390.

Note: $b \cdot 10^2$ means the value of b is to be multiplied by 10^{-2}, e.g., 20.10×10^{-2} for acetone.

Compound	Formula	Mol. Wt.	State	Form	T	a	$b \cdot 10^2$	$c \cdot 10^5$	$d \cdot 10^9$	Temp. Range (in T)
Acetone	CH_3COCH_3	58.08	g	1	°C	71.96	20.10	–12.78	34.76	0–1200
Acetylene	C_2H_2	26.04	g	1	°C	42.43	6.053	–5.033	18.20	0–1200
Air		29.0	g	1	°C	28.94	0.4147	0.3191	–1.965	0–1500
			g	1	K	28.09	0.1965	0.4799	–1.965	273–1800
Ammonia	NH_3	17.03	g	1	°C	35.15	2.954	0.4421	–6.686	0–1200
Ammonium sulfate	$(NH_4)_2SO_4$	132.15	c	1	K	215.9				275–328
Benzene	C_6H_6	78.11	l	1	K	–7.27329	77.054	–164.82	1897.9	279–350
			g	1	°C	74.06	32.95	–25.20	77.57	0–1200
Isobutane	C_4H_{10}	58.12	g	1	°C	89.46	30.13	–18.91	49.87	0–1200
n-Butane	C_4H_{10}	58.12	g	1	°C	92.30	27.88	–15.47	34.98	0–1200
Isobutene	C_4H_8	56.10	g	1	°C	82.88	25.64	–17.27	50.50	0–1200
Calcium carbide	CaC_2	64.10	c	2	K	68.62	1.19	-8.66×10^{10}	—	298–720
Calcium carbonate	$CaCO_3$	100.09	c	2	K	82.34	4.975	-12.87×10^{10}	—	273–1033
Calcium hydroxide	$Ca(OH)_2$	74.10	c	1	K	89.5				276–373
Calcium oxide	CaO	56.08	c	2	K	41.84	2.03	-4.52×10^{10}		10,273–1173
Carbon	C	12.01	c†	2	K	11.18	1.095	-4.891×10^{10}		273–1373
Carbon dioxide	CO_2	44.01	g	1	°C	36.11	4.233	–2.887	7.464	0–1500
Carbon monoxide	CO	28.01	g	1	°C	28.95	0.4110	0.3548	–2.220	0–1500
Carbon tetrachloride	CCl_4	153.84	l	1	K	12.285	0.01095	–318.26	3425.2	273–343
Chlorine	Cl_2	70.91	g	1	°C	33.60	1.367	–1.607	6.473	0–1200
Copper	Cu	63.54	c	1	K	22.76	0.06117			273–1357
Cumene (Isopropyl benzene)	C_9H_{12}	120.19	g	1	°C	139.2	53.76	–39.79	120.5	0–1200
Cyclohexane	C_6H_{12}	84.16	g	1	°C	94.140	49.62	–31.90	80.63	0–1200

Cyclopentane	C_5H_{10}	70.13	g	1	°C	73.39	39.28	–25.54	68.66	0–1200
Ethane	C_2H_6	30.07	g	1	°C	49.37	13.92	–5.816	7.280	0–1200
Ethyl alcohol	C_2H_6O	46.07	l	1	K	–325.137	0.041379	–1403.1	1.7035×10^4	250–400
			g	1	°C	61.34	15.72	–8.749	19.83	0–1200
Ethylene	C_2H_4	28.05	g	1	°C	40.75	11.47	–6.891	17.66	0–1200
Ferric oxide	Fe_2O_3	159.70	c	2	K	103.4	6.711	-17.72×10^{10}	—	273–1097
Formaldehyde	CH_2O	30.03	g	1	°C	34.28	4.268	0.0000	–8.694	0–1200
Helium	He	4.00	g	1	°C	20.8				All
n-Hexane	C_6H_{14}	86.17	l	1	K	31.421	0.97606	–235.37	3092.7	273–400
			g	1	°C	137.44	40.85	–23.92	57.66	0–1200
Hydrogen	H_2	2.016	g	1	°C	28.84	0.00765	0.3288	–0.8698	0–1500
Hydrogen bromide	HBr	80.92	g	1	°C	29.10	–0.0227	0.9887	–4.858	0–1200
Hydrogen chloride	HCl	36.47	g	1	°C	29.13	–0.1341	0.9715	–4.335	0–1200
Hydrogen cyanide	HCN	27.03	g	1	°C	35.3	2.908	1.092		0–1200
Hydrogen sulfide	H_2S	34.08	g	1	°C	33.51	1.547	0.3012	–3.292	0–1500
Magnesium chloride	$MgCl_2$	95.23	c	1	K	72.4	1.58			273–991
Magnesium oxide	MgO	40.32	c	2	K	45.44	0.5008	-8.732×10^{10}		273–2073
Methane	CH_4	16.04	g	1	°C	34.31	5.469	0.3661	–11.00	0–1200
			g	1	K	19.87	5.021	1.268	–11.00	273–1500
Methyl alcohol	CH_3OH	32.04	l	1	K	–259.25	0.03358	–1.1639	1.4052×10^4	273–400
			g	1	°C	42.93	8.301	–1.87	–8.03	0–700
Methyl cyclohexane	C_7H_{14}	98.18	g	1	°C	121.3	56.53	–37.72	100.8	0–1200
Methyl cyclopentane	C_6H_{12}	84.16	g	1	°C	98.83	45.857	–30.44	83.81	0–1200
Nitric acid	HNO_3	63.02	l	1	°C	110.0				25
Nitric oxide	NO	30.01	g	1	°C	29.50	0.8188	–0.2925	0.3652	0–3500
Nitrogen	N_2	28.02	g	1	°C	29.00	0.2199	0.5723	–2.871	0–1500
Nitrogen dioxide	NO_2	46.01	g	1	°C	36.07	3.97	–2.88	7.87	0–1200
Nitrogen tetraoxide	N_2O_4	92.02	g	1	°C	75.7	12.5	–11.3		0–300
Nitrous oxide	N_2O	44.02	g	1	°C	37.66	4.151	–2.694	10.57	0–1200
Oxygen	O_2	32.00	g	1	°C	29.10	1.158	–0.6076	1.311	0–1500

(*Continues*)

Table G.1 Heat Capacity Equations for Organic and Inorganic Compounds (at Low Pressures)* *(Continued)*

Compound	Formula	Mol. Wt.	State	Form	T	a	$b \cdot 10^2$	$c \cdot 10^5$	$d \cdot 10^9$	Temp. Range (in T)
n-Pentane	C_5H_{12}	72.15	l	1	K	33.24	192.41	–236.87	17,944	270–350
			g	1	°C	114.8	34.09	–18.99	42.26	0–1200
Propane	C_3H_8	44.09	g	1	°C	68.032	22.59	–13.11	31.71	0–1200
Propylene	C_3H_6	42.08	g	1	°C	59.580	17.71	–10.17	24.60	0–1200
Sodium carbonate	Na_2CO_3	105.99	c	1	K	121				288–371
Sodium carbonate	$Na_2CO_3 \cdot 10H_2O$	286.15	c	1	K	535.6				298
Sulfur	S	32.07	c‡	1	K	15.2	2.68			273–368
			c§	1	K	18.5	1.84			368–392
Sulfuric acid	H_2SO_4	98.08	l	1	°C	139.1	15.59			10–45
Sulfur dioxide	SO_2	64.07	g	1	°C	38.91	3.904	–3.104	8.606	0–1500
Sulfur trioxide	SO_3	80.07	g	1	°C	48.50	9.188	–8.540	32.40	0–1000
Toluene	C_7H_8	92.13	l	1	K	1.8083	81.222	–151.27	1630	270–370
			g	1	°C	94.18	38.00	–27.86	80.33	0–1200
Water	H_2O	18.016	l	1	K	18.2964	47.212	–133.88	1314.2	273–373
			g	1	°C	33.46	0.6880	0.7604	–3.593	0–1500

*(at 1 atm). †Graphite. ‡Rhombic. §Moinoclinic.