

Appendix-F

Table F1: Variation of specific heat, enthalpy, absolute entropy and Gibbs function with temperature at 1 bar for various substances in unit kJ/kmol. [155]

1. At $T_{ref} = 298.15 \text{ K (25}^\circ\text{C)}$, $P_{ref} = 1 \text{ bar}$					
Substance	Formula	$\bar{c}_p^o$	$\bar{h}^o$	$\bar{s}^o$	$\bar{g}^o$
Carbon (graphite)	$C(s)$	8.53	0	5.740	-1711
Sulfur	$S(s)$	22.77	0	32.058	-9558
Nitrogen	$N_2(g)$	28.49	0	191.610	-57128
Oxygen	$O_2(g)$	28.92	0	205.146	-61164
Hydrogen	$H_2(g)$	29.13	0	130.679	-38961
Carbon Monoxide	$CO(g)$	28.54	-110528	197.648	-169457
Carbon dioxide	$CO_2(g)$	35.91	-393521	213.794	-457264
Water	$H_2O(g)$	31.96	-241856	188.824	-298153
Water	$H_2O(l)$	75.79	-285829	69.948	-306685
Methane	$CH_4(g)$	35.05	-74872	186.251	-130403
Sulfur dioxide	$SO_2(g)$	35.59	-296833	284.094	-370803
Hydrogen sulfide	$H_2S(g)$	33.06	-20501	205.757	-81847
Ammonia	$NH_3(g)$	35.59	-46111	192.451	-103491

2. For $298.15 < T \leq T_{max}$, $P_{ref} = 1 \text{ bar}$, with $y = 10^{-3} T$

$$\bar{c}_p^o = a + by + cy^{-2} + dy^2 \quad (F1)$$

$$\bar{h}^o = 10^3 \left[H^+ + ay + \frac{b}{2} y^2 - cy^{-1} + \frac{d}{3} y^3 \right] \quad (F2)$$

$$\bar{s}^o = S^+ a \ln T + by - \frac{c}{2} y^{-2} + \frac{d}{2} y^2 \quad (F3)$$

$$\bar{g}^o = \bar{h}^o - T \bar{s}^o \quad (F4)$$

Table F2: Constants for equation F1 to F4 [155]

Substance	Formula	H^+	S^+	a	b	c	d
Carbon (graphite)	$C(s)$	-2.101	-6.540	0.109	38.940	-0.146	-17.385
Sulfur	$S(s)$	-5.242	-59.014	14.795	24.075	0.071	0
Nitrogen	$N_2(g)$	-9.982	16.203	30.418	2.544	-0.238	0
Oxygen	$O_2(g)$	-9.589	36.116	29.154	6.477	-0.184	-1.017
Hydrogen	$H_2(g)$	-7.823	-22.966	26.882	3.586	0.105	0
Carbon monoxide	$CO(g)$	-120.809	18.937	30.962	2.439	-0.28	0
Carbon dioxide	$CO_2(g)$	-413.886	-87.078	51.128	4.368	-1.469	0
Water	$H_2O(g)$	-253.871	-11.750	34.376	7.841	-0.423	0
Water	$H_2O(l)$	-289.932	-67.147	20.355	109.198	2.033	0
Methane	$CH_4(g)$	-81.242	96.731	11.933	77.647	0.142	-18.414
Sulfur dioxide	$SO_2(g)$	-315.422	-43.725	49.936	4.766	-1.046	0
Hydrogen sulfide	$H_2S(g)$	-32.887	1.142	34.911	10.686	-0.448	0
Ammonia	$NH_3(g)$	-60.244	-29.402	37.321	18.661	-0.649	0