TABLE IIIC-1: CHARACTERISTICS OF GASEOUS MODES

Mode	Molecule	Limit	Z_p	$\frac{\bar{u}_p^*}{\bar{R}}$	$\frac{\bar{c}_{v,p}^*}{\bar{R}}$	p_p	$\frac{\bar{s}_p^*}{\bar{R}}$
Translation	All	$T \gg \Theta_{tr}$	$n\bar{v}\left(\frac{2\pi m^* kT}{h^2}\right)^{3/2}$	$\frac{3}{2}T$	$\frac{3}{2}$	$\frac{\bar{R}T}{\bar{v}}$	$\frac{5}{2} + \ln\left[\frac{(kT)^{5/2}}{p}\left(\frac{2\pi m^*}{h^2}\right)^{3/2}\right]$
Rotation-Nuclear Spin	Monatomic	$T \ll \Theta_{ns}$	1	0	0	0	0
	Non Symmetric Linear	$T \gg \Theta_r$, $T \ll \Theta_{ns}$	$\frac{T}{\Theta_r}$	T	1	0	$1 + \ln\left(\frac{T}{\Theta_r}\right)$
	Symmetric Linear	$T \gg \Theta_r$, $T \ll \Theta_{ns}$	$\frac{T}{2\Theta_r}$	T	1	0	$1 + \ln\left(\frac{T}{2\Theta_r}\right)$
	Non Linear Polyatomic	$T \gg \Theta_r$, $T \ll \Theta_{ns}$	$\frac{\pi^{1/2}}{\sigma}\left(\frac{T}{\Theta_r}\right)^{3/2}$	$\frac{3}{2}T$	$\frac{3}{2}$	0	$\frac{3}{2}\left[1 + \ln\left(\frac{T}{\Theta_r}\right)\right] - \ln\left(\frac{\pi^{1/2}}{\sigma}\right)$
Vibration	Monatomic	None	1	0	0	0	0
	Diatomic	None	$\frac{e^{-\Theta_v/2T}}{(1-e^{-\Theta_v/T})}$	$\Theta_v\left[\frac{1}{2} + \frac{1}{(e^{\Theta_v/T}-1)}\right]$	$\left(\frac{\Theta_v}{T}\right)^2 \frac{e^{\Theta_v/T}}{(e^{\Theta_v/T}-1)^2}$	0	$\frac{\Theta_v/T}{(e^{\Theta_v/T}-1)} - \ln\left(1-e^{-\Theta_v/T}\right)$
	Polyatomic	None	$\prod_{p=1}^{P} \frac{e^{-\Theta_{v,p}/2T}}{(1-e^{-\Theta_{v,p}/T})}$	$\sum_{p=1}^{P} \Theta_{v,p}\left[\frac{1}{2} + \frac{1}{(e^{\Theta_{v,p}/T}-1)}\right]$	$\sum_{p=1}^{P} \left(\frac{\Theta_{v,p}}{T}\right)^2 \frac{e^{\Theta_{v,p}/T}}{(e^{\Theta_{v,p}/T}-1)^2}$	0	$\sum_{p=1}^{P} \frac{\Theta_{v,p}/T}{(e^{\Theta_{v,p}/T}-1)} - \ln\left(1-e^{-\Theta_{v,p}/T}\right)$

TABLE IIIC-2: ROTATIONAL AND VIBRATIONAL TEMPERATURES

Substance	Symbol	Θ_r(K)	σ	Θ_v(K)
Homonuclear Diatomic[a]				
Nitrogen	N_2	2.875	2	3392
Oxygen	O_2	2.079	2	2274
Hydrogen	H_2	87.55	2	6338
Chlorine	Cl_2	0.3465	2	807.3
Fluorine	F_2	1.286	2	1328
Bromine	Br_2	0.1164	2	425.1
Hetronuclear Diatomic[a]				
Carbon Monoxide	CO	2.777	1	3121
Nitric Oxide	NO	2.452	1	2739
Hydrogen Chloride	HCl	15.23	1	4302
Hydrogen Fluoride	HF	30.15	1	5954
Methylidyne	CH	20.80	1	4117
Sodium Chloride	NaCl	0.3121	1	523.2
Symmetric Linear Polyatomic[b]				
Carbon Dioxide	CO_2	0.5631	2	960.1(2) 1932 3380
Methylene	CH_2	11.34	2	1602(2) 3870 4604
Carbon Disulfide	CS_2	0.1568	2	570.9(2) 946.8 2205
Acetylene	C_2H_2	1.693	2	880.0(2) 1049(2) 2840 4722 4854
Nonsymmetric Linear Polyatomic[b]				
Hydrogen Cyanide	HCN	2.137	1	1024(2) 3022 4770
Potassium Cyanide	KCN	0.1570	1	297.8(2) 466.2 3105
Nitrogen Monoxide	N_2O	0.6059	1	847.8(2) 1836.7 3199.5
Nonlinear Polyatomic[b]				
Water	H_2O	0.2246	2	2294 5262 5404
Ammonia	NH_3	0.1233	3	1470 2433(2) 5045 5147(2)
Methane	CH_4	0.07580	12	1879(3) 2207(2) 4196 4343(3)
Carbon Tetrachloride	CCl_4	0.01784	12	313.7(2) 446.0(3) 659.0 1142(3)

Data extracted from JANAF Thermochemical Tables, Second Ed. Issued, June (1971).

[a] Data reported as a wave number. The characteristic temperatures are determined as $\Theta_r = (hc/k) \cdot B_e$ and $\Theta_v = (hc/k) \cdot \omega_e$. (Anharmonic correction parameters are omitted.)

[b] Polyatomic vibrational data is reported as a wave number. Thus $\Theta_{v,p} = (hc/k) \cdot \omega_p$. Polyatomic rotational data given as either a wave number $\Theta_r = (hc/k) \cdot B_o$ or individual or product moments of inertia, $\Theta_r = [h/(8\pi^2 k)] \cdot I^{-1}$ or $\Theta_r = [h/(8\pi^2 k)] \cdot I^{-1/3}$.