CHEM 548 Exam 1 Reference Sheet

This sheet gives data and formulas you are not asked to memorize. You are responsible for everything taught in lectures 1–10.

Constants and units

- $N_A = 6.022 \times 10^{23}$ mol^{-1}; 1 g $= 6.022 \times 10^{23}$ amu
- $k = 1.381 \times 10^{-23}$ J/K $= 8.617 \times 10^{-5}$ eV/K; $R = 8.314$ J/(K mol); $R = N_A k$
- 1 Å $= 10^{-8}$ cm $= 10^{-10}$ m; 1 mm$^3 = 10^{-9}$ m^3; $1\ \mathrm{meV} = 10^{-3}\ \mathrm{eV}$
- Mass fraction $w_i = n_i M_i / \sum_j n_j M_j$ (wt% axes use w_i; mol% axes use mole fractions)

Geometry and counting

- 2D cell area $ab\sin\gamma$; $|\mathbf{a} \pm \mathbf{b}|^2 = a^2 + b^2 \pm 2ab\cos\gamma$
- Cell volume: cubic a^3; orthorhombic abc; hexagonal $\frac{\sqrt{3}}{2}a^2c$
- Sphere volume $\frac{4}{3}\pi r^3$
- Regular polygon interior angle $(n-2)\,180^\circ/n$
- Binomial count $N!/[n!\,(N-n)!]$
- Density $\rho = ZM/(N_A V)$

Lattices and symmetry

2D crystal systems: oblique (no constraint); rectangular $a \neq b$, $\gamma = 90^\circ$; square $a = b$, $\gamma = 90^\circ$; hexagonal $a = b$, $\gamma = 120^\circ$.

Crystal system	Lattice-parameter constraints
Triclinic	none
Monoclinic	$\alpha = \gamma = 90^\circ$ (b unique)
Orthorhombic	$\alpha = \beta = \gamma = 90^\circ$
Tetragonal	$a = b$; $\alpha = \beta = \gamma = 90^\circ$
Trigonal (rhombohedral axes)	$a = b = c$; $\alpha = \beta = \gamma \neq 90^\circ$
Hexagonal (and trigonal on hexagonal axes)	$a = b$; $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$
Cubic	$a = b = c$; $\alpha = \beta = \gamma = 90^\circ$

- Point coordinates $\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$, fractions written in the order a, b, c
- Coordinate maps of some operations on (x, y, z): $\bar{1}$ $(\bar{x}, \bar{y}, \bar{z})$; 2 along $\mathbf{a}$ $(x, \bar{y}, \bar{z})$; 2 along $\mathbf{b}$ $(\bar{x}, y, \bar{z})$; 2 along $\mathbf{c}$ $(\bar{x}, \bar{y}, z)$; $m \perp \mathbf{a}$ $(\bar{x}, y, z)$; $m \perp \mathbf{b}$ $(x, \bar{y}, z)$; $m \perp \mathbf{c}$ $(x, y, \bar{z})$; 4 along $\mathbf{c}$ $(\bar{y}, x, z)$

Electron counting and formulas

- $\mathrm{VEC}_A = (m\,e_C + n\,e_A)/n$ for C_mA_n
- Generalized 8−N rule: $\mathrm{VEC}_A = 8 + \mathrm{CC}\,(m/n) - \mathrm{AA}$
- Crystal-chemical formula notation: charge as superscript, count as subscript, coordination in brackets with t (tetrahedral), o (octahedral), c (cubic); prefix $^1_\infty$ marks chain dimensionality
- Three balances for C_mA_n with cation charge c, anion charge a, cation coordination N, anion coordination M: electroneutrality $mc = na$; connectivity $mN = nM$; bond valence $c/N = a/M$
- Common ion charges: alkali +1, alkaline earth +2, O^{2-}, N^{3-}, F^-, Cl^-
- Niggli formula $MX_{a/b+c/d}$: numerator = vertices of that kind, denominator = polyhedra sharing each; the numerators sum to the coordination number
- Silicate names: oligo-, cyclo-, catena-, phyllo-, tecto-
- Goldschmidt tolerance factor $t = (r_A + r_O)/[\sqrt{2}\,(r_B + r_O)]$
- Spinel site count $[\mathrm{tet}]_1[\mathrm{oct}]_2\mathrm{O}_4$ on a ccp oxide array

Defects

- Kröger–Vink: species (or v for vacancy), site as subscript (i = interstitial), effective charge as superscript: $\bullet$ = +1, $'$ = −1, $\times$ = 0
- Redox compensation: oxidized = cation vacancy or anion interstitial; reduced = cation interstitial or anion vacancy
- Equilibrium vacancies, with molar ΔH, ΔS (use k per defect):

$$n/N_0 = e^{\Delta S/R}\,e^{-\Delta H/RT}$$

Schottky pairs:

$$n_S/N = e^{\Delta S_S/2k}\,e^{-\Delta H_S/2kT}$$

Frenkel:

$$n_F = (N N_i)^{1/2}\,e^{\Delta S_F/2k}\,e^{-\Delta H_F/2kT}$$

Vacancy formation (SSMC Table 2.1)	Cu	Ag	Au	Al
ΔH_f (kJ/mol)	123	105	91	72
ΔS_f (J/(K mol))	21	12	8.3	18

Phase diagrams

- Phase rule

$$F = C - P + 2$$

at fixed pressure

$$F = C - P + 1$$

- Lever rule: fraction of phase α = $(x_\beta - x_0)/(x_\beta - x_\alpha)$
- Vegard's law $a = x\,a_B + (1-x)\,a_A$; the same linear weighting applies to a band gap
- A compound A_mB_n sits at $x_B = n/(n+m)$ on a binary axis
- Ternary composition: each corner is pure that component; its fraction falls linearly to 0 at the opposite edge, so a line parallel to that edge holds it constant. The three fractions sum to 1. A line from a corner to the opposite edge holds the ratio of the other two components constant.
- Ideal mixing entropy

$$S_{\mathrm{mix}}/Nk = -[x\ln x + (1-x)\ln(1-x)]$$

- Regular-solution consolute temperature $T_c = p\,\varepsilon/2k$

Periodic table (atomic masses, g/mol)

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 **H** 1.008																	2 **He** 4.003
3 **Li** 6.94	4 **Be** 9.012											5 **B** 10.81	6 **C** 12.01	7 **N** 14.01	8 **O** 16.00	9 **F** 19.00	10 **Ne** 20.18
11 **Na** 22.99	12 **Mg** 24.31											13 **Al** 26.98	14 **Si** 28.09	15 **P** 30.97	16 **S** 32.06	17 **Cl** 35.45	18 **Ar** 39.95
19 **K** 39.10	20 **Ca** 40.08	21 **Sc** 44.96	22 **Ti** 47.87	23 **V** 50.94	24 **Cr** 52.00	25 **Mn** 54.94	26 **Fe** 55.85	27 **Co** 58.93	28 **Ni** 58.69	29 **Cu** 63.55	30 **Zn** 65.38	31 **Ga** 69.72	32 **Ge** 72.63	33 **As** 74.92	34 **Se** 78.97	35 **Br** 79.90	36 **Kr** 83.80
37 **Rb** 85.47	38 **Sr** 87.62	39 **Y** 88.91	40 **Zr** 91.22	41 **Nb** 92.91	42 **Mo** 95.95	43 **Tc** (98)	44 **Ru** 101.07	45 **Rh** 102.91	46 **Pd** 106.42	47 **Ag** 107.87	48 **Cd** 112.41	49 **In** 114.82	50 **Sn** 118.71	51 **Sb** 121.76	52 **Te** 127.60	53 **I** 126.90	54 **Xe** 131.29
55 **Cs** 132.91	56 **Ba** 137.33	57 **La** 138.91	72 **Hf** 178.49	73 **Ta** 180.95	74 **W** 183.84	75 **Re** 186.21	76 **Os** 190.23	77 **Ir** 192.22	78 **Pt** 195.08	79 **Au** 196.97	80 **Hg** 200.59	81 **Tl** 204.38	82 **Pb** 207.2	83 **Bi** 208.98	84 **Po** (209)	85 **At** (210)	86 **Rn** (222)
		58–71	58 **Ce** 140.12	59 **Pr** 140.91	60 **Nd** 144.24	61 **Pm** (145)	62 **Sm** 150.36	63 **Eu** 151.96	64 **Gd** 157.25	65 **Tb** 158.93	66 **Dy** 162.50	67 **Ho** 164.93	68 **Er** 167.26	69 **Tm** 168.93	70 **Yb** 173.05	71 **Lu** 174.97	