day 9 pg 1

Ionic

⊕ ⊖ ⊕ ⊖
⊖ ⊕ ⊖ ⊕ (2D)

Attractive

$-\frac{q^2}{p_{ij}R}$ for some p_{ij} (SI: $\frac{1}{4\pi\epsilon_0}\frac{q^2}{r}$ **CGS: $\frac{q^2}{r}$** ✱)

Repulsive

$+\frac{q^2}{p_{ij}R}$ for some other p_{ij}

$\lambda e^{-R/\rho}$ for Pauli exclusion (nearest neighbors)

λ, ρ = empirical parameters

(reference = negative charge)

$$U_{tot} = N\left(z\lambda e^{-R/\rho} - \sum_i' \frac{(\pm) q^2}{p_{ij} R} \right)$$

z ↓ nearest neighbors

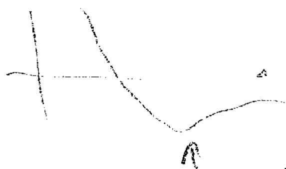
$$-\frac{q^2}{R} \sum_i \frac{(\pm)}{p_{ij}}$$

" " $= \alpha$; Madelung constant

calculate very similar to VdW stuff in last section

NaCl structure: $\alpha = 1.747565$
CsCl $\alpha = 1.762675$
ZnS $\alpha = 1.6381$

$$U_{tot} = N\left(z\lambda e^{-R/\rho} - \frac{\alpha q^2}{R} \right)$$



↑ same deal $\frac{\partial U}{\partial R} = 0$ gives R_0 (transcendental eqn, numerical only)

then $U_{tot}(R=R_0) \rightarrow$ total lattice energy

has analytic:

$$U_{tot} = -\frac{N\alpha q^2}{R_0}\left(1 - \frac{\rho}{R_0}\right)$$

"Madelung" ← repulsive

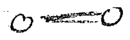
✱ table 7 pg 66 nice agreement!

Cohesive energy a few eV, ~10x larger than VdW noble gases

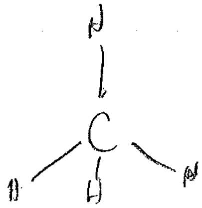
TOPS. 35500

Covalent Crystals

Ex: H_2



one elect ↑ spin
one elect ↓



CH_4

(Newton forbidden 222 diamond problem)

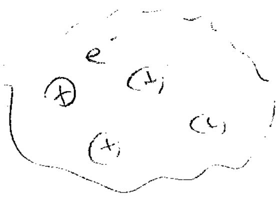
diamond structure (I can't draw)

comes from QM - orbitals (?)

Hard to analyze quantitatively from first principles

Metals

Some electrons free (valence elect of atom → cond. electrons)
↓
but lowered in energy (due to quantum (?))



← some

- weaker binding (ductile, malleable) → still crystalline on microscopic level
- close packed

→ stronger for transition metals though
Table 1 pg 50

→ weaker than ionic
Compare kcal/mol to Table 7 pg 66

Hydrogen bonds

- already discussed in chem

Atomic Radii

- basically, no such thing for universal case

distances between atoms depend strongly on structure

but can get approx <
- vdW
- ionic (modification of vdW)
- covalent
- metallic

Table 9 pg 71
Table 10 pg 72
that's all I'll say