project:
CB – 1

Crystal Binding

Cohesive Energy ≡ Energy required to separate crystal into component atoms

Ne	1.92 kJ/mole	vs	Li	158 kJ/mole
Ar	7.74 kJ/mole		Na	107 kJ/mole

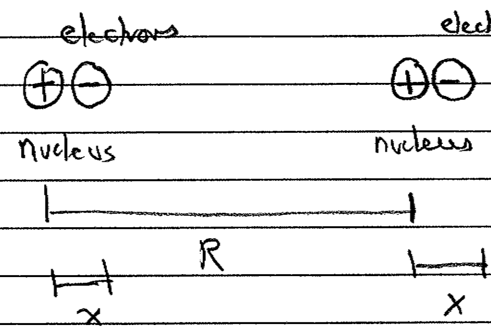
B 561 kJ/mole
C 711 kJ/mole

very small (not surprising : filled shells → weak interactions)

Melting Tempr → Ne 24.6 °K B 2365 °K
(similar point) Ar 83.8 °K

Ne, Ar have **Van der Waals interaction**:
interaction between 2 neutral atoms caused by induced dipole moments

Schematically:



$$U = e^2\left[\frac{+1}{R} + \frac{1}{R} + \frac{-1}{(R-x)} + \frac{-1}{(R+x)}\right]$$

$$= \frac{e^2}{R}\left[2 - \frac{1}{(1-\frac{x}{R})} - \frac{1}{(1+\frac{x}{R})}\right]$$

project: CB-2

$$(1+x)^n = 1 + nx + \frac{n(n-1)}{2}x^2 + \dots$$

$$U = \frac{e^2}{R}\left[2 - \left(1 + \frac{x}{R} + \frac{x^2}{R^2} + \dots\right) - \left(1 - \frac{x}{R} + \frac{x^2}{R^2} \dots\right)\right]$$

$\left(1 - \frac{x}{R}\right)^{-1}$ $\left(1 + \frac{x}{R}\right)^{-1}$

$$U \sim \frac{-2e^2}{R}\frac{x^2}{R^2}$$ ← PE of 2 dipoles $\sim 1/R^3$

vs $1/R$ of 2 charges

But atoms are not permanent dipoles instead they have induced dipoles because of other atom. Interaction is even weaker van der Waals $\sim 1/R^6$

Why? $\vec{p}$ dipole $\sim \vec{E}$ field

$\vec{E} \sim 1/R^2$ charge

$\sim 1/R^3$ dipole ← additional $1/R^3$

~~1/R^3 ... and~~

Why not get closer and closer?

Ultimately, Repulsive force due to Pauli Exclusion principle of overlapping electron clouds. Turns out combination can be very well fit by

$$U(r) = \frac{A}{R^{12}} - \frac{B}{r^6}$$ Lennard-Jones

$\frac{A}{R^{12}}$ ↑ Pauli repulsion; $\frac{B}{r^6}$ ↑ dipole-dipole attraction project:

CB - 3

Ionic crystals NaCl atoms which do have net charge

Binding is due to electrostatic energies of charges $\pm q$

separated by R : $-q^2/R$ Madelung Energy

↑ much much bigger than $\sim 1/R^6$ van der Waals

Again there is ultimately repulsion due to overlap

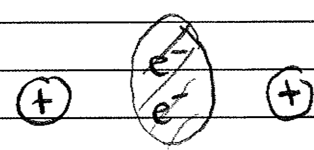
Empirically $+\frac{A}{R^2} - \frac{B}{R}$

↗ Pauli Repulsion (why not $1/R^{12}$ again?! not simple to derive/explain empirical)

↖ $\pm q$ charges

{ A bit like Kepler problem $-1/R$ from gravity and $+1/R^2$ from angular momentum barrier!

Covalent Bond



↑ electrons have opposite spin ↑ ↓ to avoid Pauli repulsion

METALS bonding driven by lowering of energy when electrons delocalize (metal) $KE \sim + \frac{(\Delta p)^2}{2m} \sim + \frac{1}{2m}\left(\hbar/\Delta x\right)^2$

↑ lowest for Δx large

project: CB-4

Finally **Hydrogen Bond**

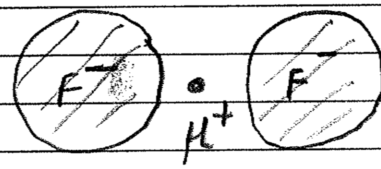
H loses e^- (partially) to atoms like F, O, N

and (approximately) bare H atom (proton)

ρ of e^-

sits between atoms.

HF_2^-



H bond:

Impt in water/ice/DNA