3D shapes of molecules

1 Why do only molecules have shapes?

- only covalent substances have directional electrostatic forces
- bond 只能在特定的方向存在 (bond 定了一个方向, 就只会是那个方向)
- 如何定方向? → Valence Shell Electron Pair Repulsion Theory (VSEPR, out of syllabus)
  - > e^- pairs (in outermost shell of atom, ie b.p. & l.p.) 相斥 → 尽可能离得最远
  - > ↑ Repulsion force
    - l.p. - l.p. : > 90°
    - l.p. - b.p. : 越少 90° 越好
    - b.p. - b.p. : ≥ 90°
  - Reason: l.p. 只被 central atom 吸引; b.p. 被 bond 双方的 atom 吸引 ⇒ l.p. 离 central atom 较近 → 很肥 → repulsion ↑

2 Determining the shape of molecules

STEPS

1. 根据 2D structure 的方法画表
2. 依据 central atom 的 bond pair 与 lone pair 数量, 在下列的表找出 structure 与 shape (其实依据 VSEPR theory)
   - l.p. > b.p. 一定是 linear

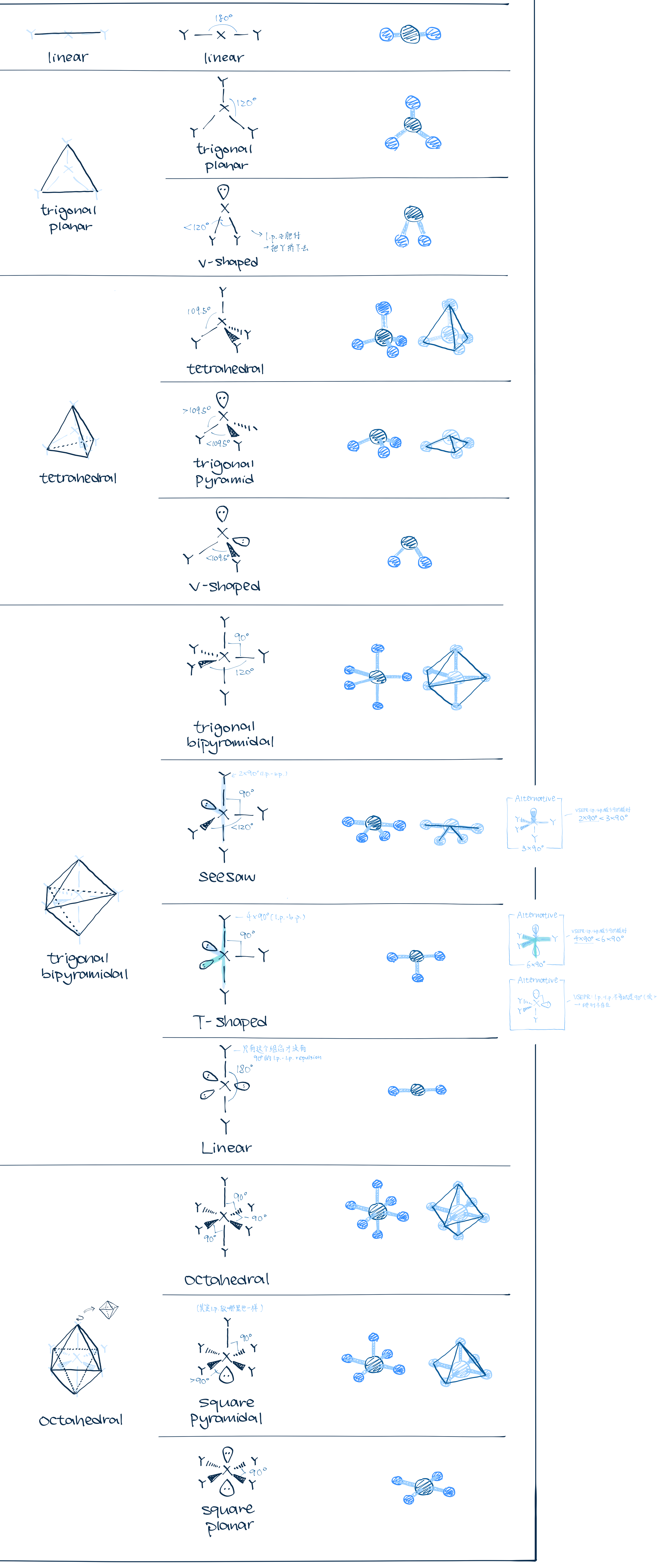
Sum (b.p. + l.p.)	Bond pairs of central atom (包括 single/double... bonds)	Lone pairs of central atom (包括一颗/两颗 e^-)	Arrangement (考虑所有 e^- pairs (b.p. & l.p.) 的形状)	Shape (只考虑 b.p. 的形状)	Model
2	2	0	linear	linear (180°)	
3	3	0	trigonal planar	trigonal planar (120°)	
	2	1		V-shaped (<120°; l.p. 很肥 → 把 Y 挤下去)	
4	4	0	tetrahedral	tetrahedral (109.5°)	
	3	1		trigonal pyramid (>109.5°, <109.5°)	
	2	2		V-shaped (<109.5°)	
5	5	0	trigonal bipyramidal	trigonal bipyramidal (90°, 120°)	
	4 (out of syllabus)	1		seesaw (2×90° (l.p.-b.p.); 90°, <120°)	
	3 (out of syllabus)	2		T-shaped (4×90° (l.p.-b.p.); 90°)	
	2 (out of syllabus)	3		Linear (只有这个组合才没有 90° 的 l.p.-l.p. repulsion; 180°)	
6	6	0	octahedral	octahedral (90°)	
	5 (out of syllabus)	1		square pyramidal (其实 l.p. 放哪里也一样; 90°, >90°)	
	4 (out of syllabus)	2		square planar (90°)	

Seesaw — Alternative: VSEPR: l.p.-b.p. 越少 90° 越好; 2×90° < 3×90°

T-shaped — Alternative: VSEPR: l.p.-b.p. 越少 90° 越好; 4×90° < 6×90°

T-shaped — Alternative: VSEPR: l.p.-l.p. 不能是 90° (须 >) → 排列不存在

没有比 6 更高的组合了.
- 5: 双三角锥 120°
- 6: 双四角锥 90°
- 7: 双五角锥 72°
  → 违反 b.p.-b.p. 之间至少 90° 的规则
  ⇒ 不存在



EXAMPLES