Lectures: Tuesdays, 1pm – 5pm

16.10.2018	Organization and Overview Methods	Thiele
23.10.2018	Theory of Single Crystal Structure Determination	Thiele
30.10.2018	Theory of Single Crystal Structure Determination	Thiele
06.11.2018	Theory of Single Crystal Structure Determination	Thiele
13.11.2018	Hands-on Session Refinement	Thiele/Steinhauer/Hagenbach
20.11.2018	Hands-on Session Refinement	Thiele/Steinhauer/Hagenbach
04.12.2018	Publication Training	Thiele/Steinhauer/Hagenbach
11.12.2018	Powder Diffraction, Energy Dispersion and X-Ray Fluorescence	Thiele
18.12.2018	Solid State NMR	Steinhauer
08.01.2019	Electrochemical Methods	Sarkar
15.01.2019	Electron Pair Resonance	Sarkar
22.01.2019	Mass spectrometry	Springer
29.01.2019	IR/Raman/Matrix/IMMS	Riedel/Pagel
05.02.2019	UV-Vis/Fluorescence	Kulak

Q&A Session for Installations: 06.11. 4:30 pm

Laptops!

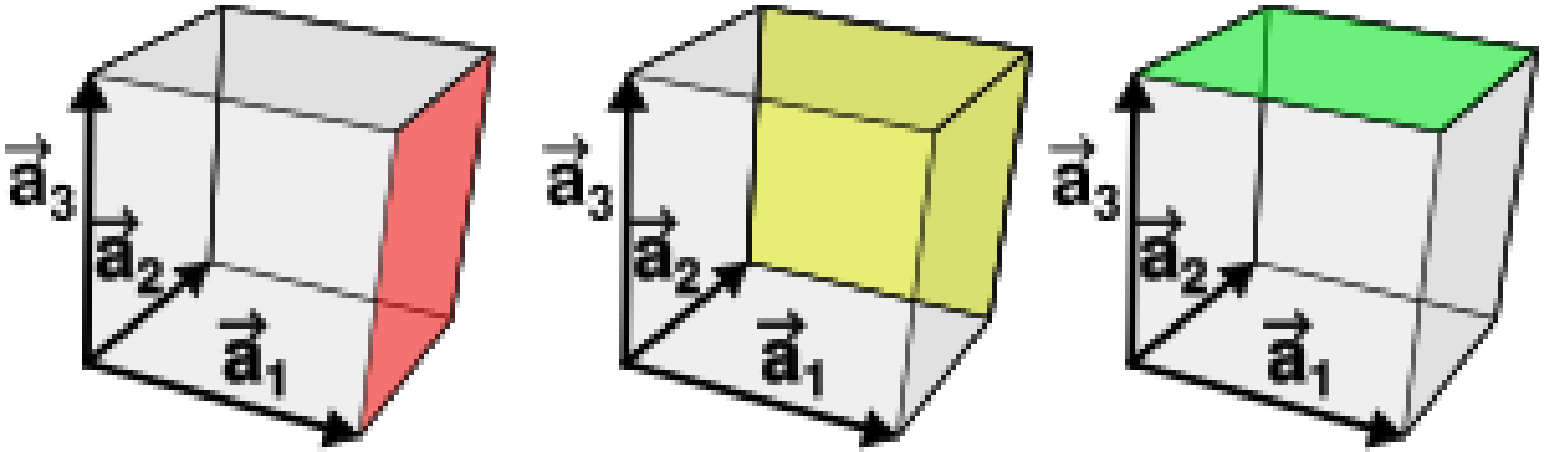
Lectures: Tuesdays, 1pm – 5pm

16.10.2018	Organization and Overview Methods	Thiele
23.10.2018	Theory of Single Crystal Structure Determination	Thiele
30.10.2018	Theory of Single Crystal Structure Determination	Thiele
06.11.2018	Theory of Single Crystal Structure Determination	Thiele
13.11.2018	Hands-on Session Refinement	Thiele/Steinhauer/Hagenbach
20.11.2018	Publication Training & Hands-On	Thiele/Steinhauer/Hagenbach
04.12.2018	**Dies Academicus**	
11.12.2018	Powder Diffraction, Energy Dispersion and X-Ray Fluorescence	Thiele
18.12.2018	Solid State NMR	Steinhauer
08.01.2019	Electrochemical Methods	Sarkar
15.01.2019	Electron Pair Resonance	Sarkar
22.01.2019	Mass spectrometry	Springer
29.01.2019	IR/Raman/Matrix/IMMS	Riedel/Pagel
05.02.2019	UV-Vis/Fluorescence	Kulak

Q&A Session for Installations: 06.11. 4:30 pm

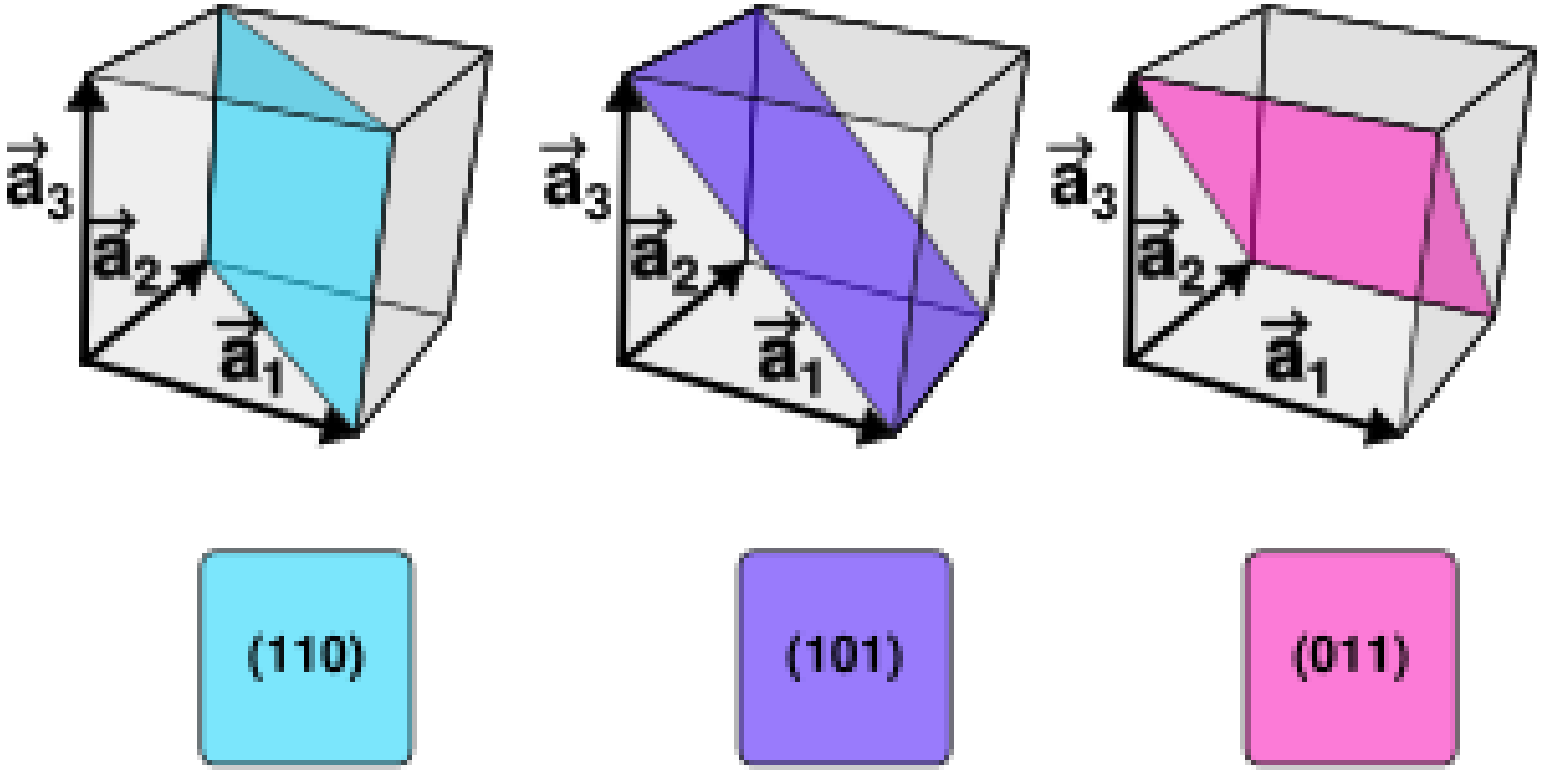
Laptops!

Miller Indices

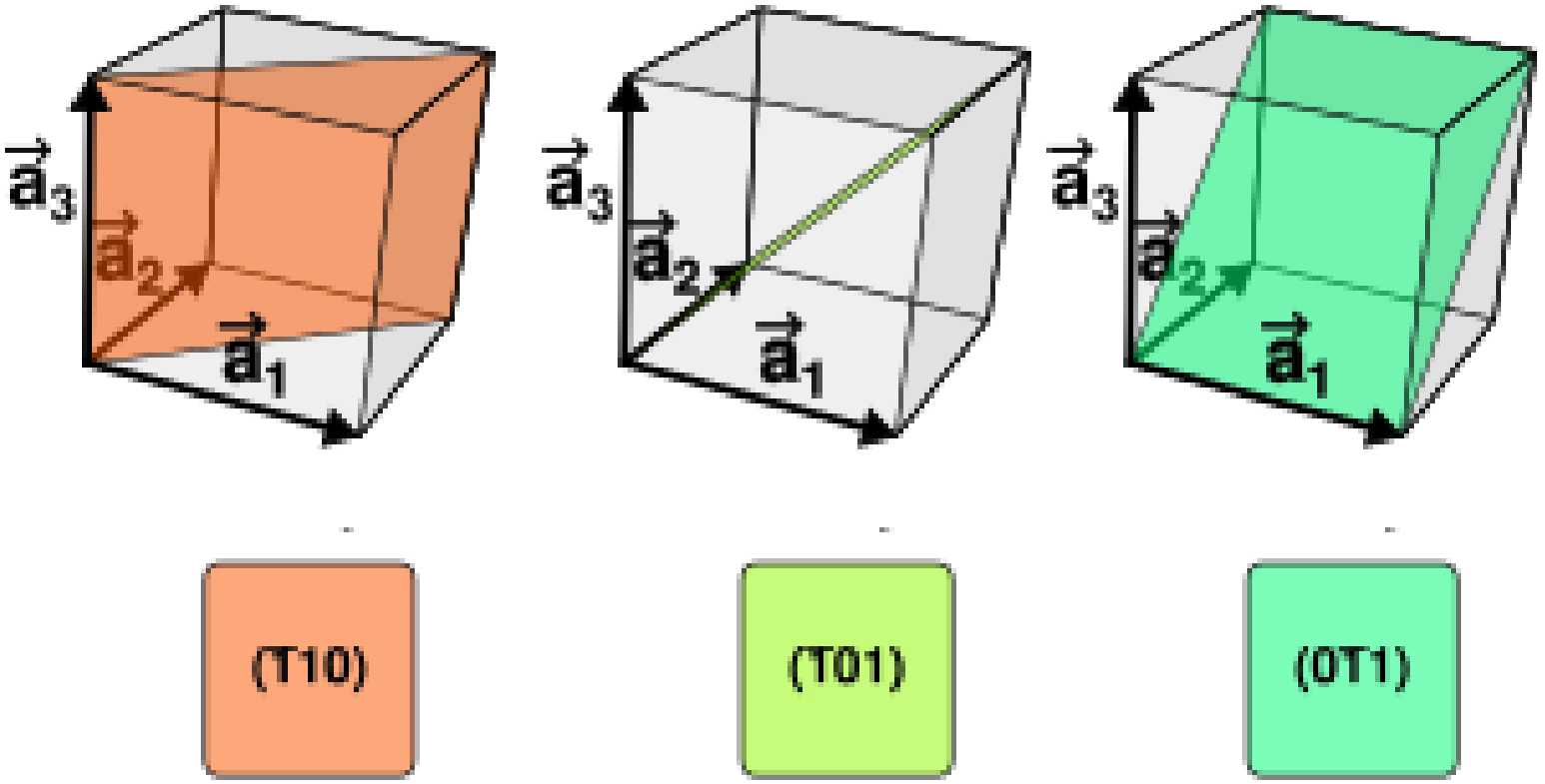


(100) (010) (001)

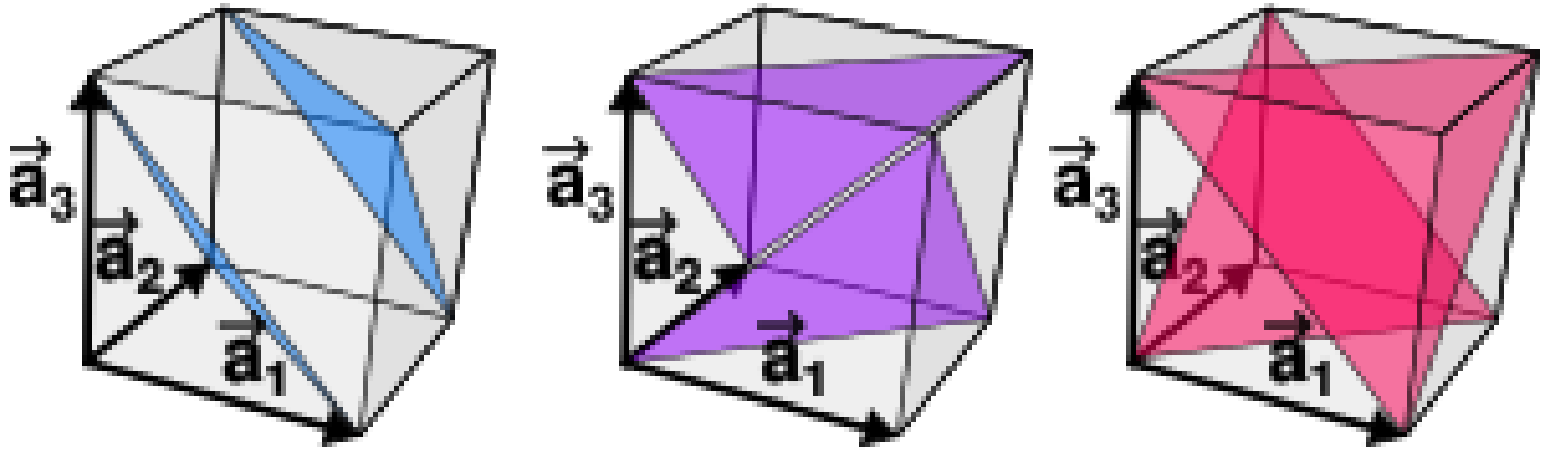
Miller Indices



Miller Indices



Miller Indices

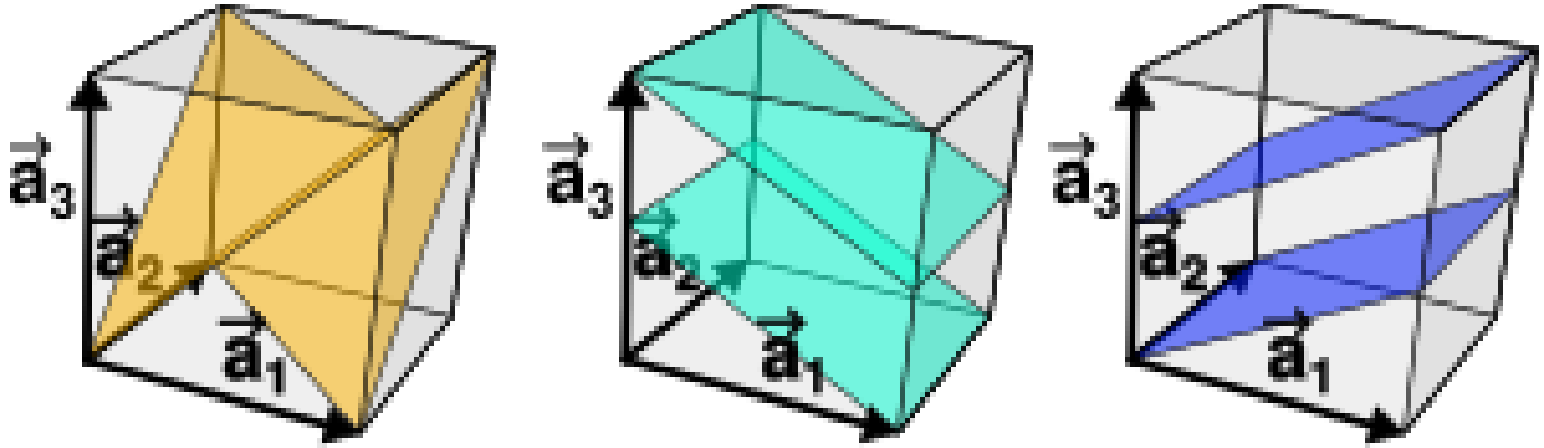


(111)

(T11)

(1T1)

Miller Indices



(11$\bar{1}$)

(102)

($\bar{1}$02)

Monoklin

$$\sin^2\theta = \frac{\lambda^2}{4}\left[\frac{h^2}{a^2\sin^2\beta} + \frac{k^2}{b^2} + \frac{l^2}{c^2\sin^2\beta} - \frac{2hl\cos\beta}{ac\sin^2\beta}\right]$$

Orthorhombisch

$$\sin^2\theta = \frac{\lambda^2}{4}\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]$$

Tetragonal

$$\sin^2\theta = \frac{\lambda^2}{4a^2}\left[h^2 + k^2 + \left(\frac{a}{c}\right)^2 l^2\right]$$

Hexagonal und trigonal

$$\sin^2\theta = \frac{\lambda^2}{4a^2}\left[\frac{4}{3}(h^2 + k^2 + hk) + \left(\frac{a}{c}\right)^2 l^2\right]$$

Kubisch

$$\sin^2\theta = \frac{\lambda^2}{4a^2}\left[h^2 + k^2 + l^2\right]$$

Triklin

$$\sin^2\theta = \frac{\lambda^2}{4}\left[h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2klb^*c^*\cos\alpha^* + 2lhc^*a^*\cos\beta^* + 2hka^*b^*\cos\gamma^*\right]$$

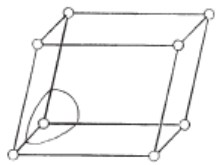
$$a^* = \frac{1}{V}bc\sin\alpha, \qquad \cos\alpha^* = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}$$

$$b^* = \frac{1}{V}ca\sin\beta, \qquad \cos\beta^* = \frac{\cos\gamma\cos\alpha - \cos\beta}{\sin\gamma\sin\alpha}$$

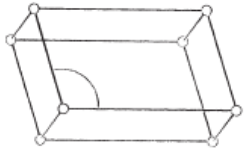
$$c^* = \frac{1}{V}ab\sin\gamma, \qquad \cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}$$

$$\mathrm{V} = abc\sqrt{1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma}$$

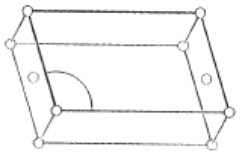
Bravais Lattices



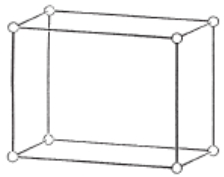
aP



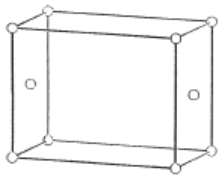
mP



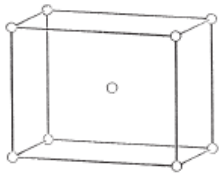
mC



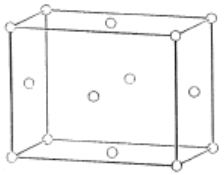
oP



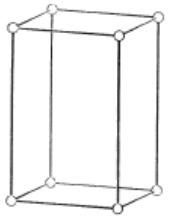
oA



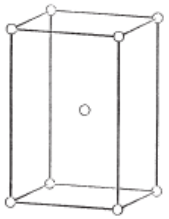
oI



oF



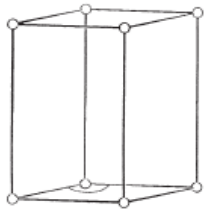
tP



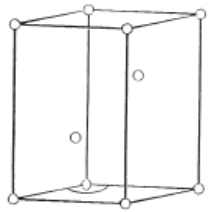
tI

Abb. 9: Die 14 Bravais–Gitter

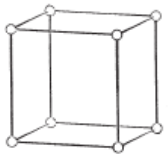
aP triklin; **mP** monoklin primitiv; **mC** monoklin C–zentriert, auch in **mI** transformierbar; **oP** orthorhombisch primitiv; **oA** orthorhombisch A–zentriert, auch **oC** üblich; **oI** orthorhombisch innen– (raum–) zentriert; **oF** orthorhombisch allseits flächenzentriert; **tP** tetragonal primitiv; **tI** tetragonal innen– (raum–)zentriert; **hP** trigonal oder hexagonal primitiv; **hR** rhomboedrisch, hexagonal aufgestellt; **cP** kubisch primitiv; **cI** kubisch innen– (raum–) zentriert; **cF** kubisch allseits flächenzentriert



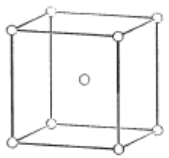
hP



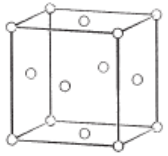
hR



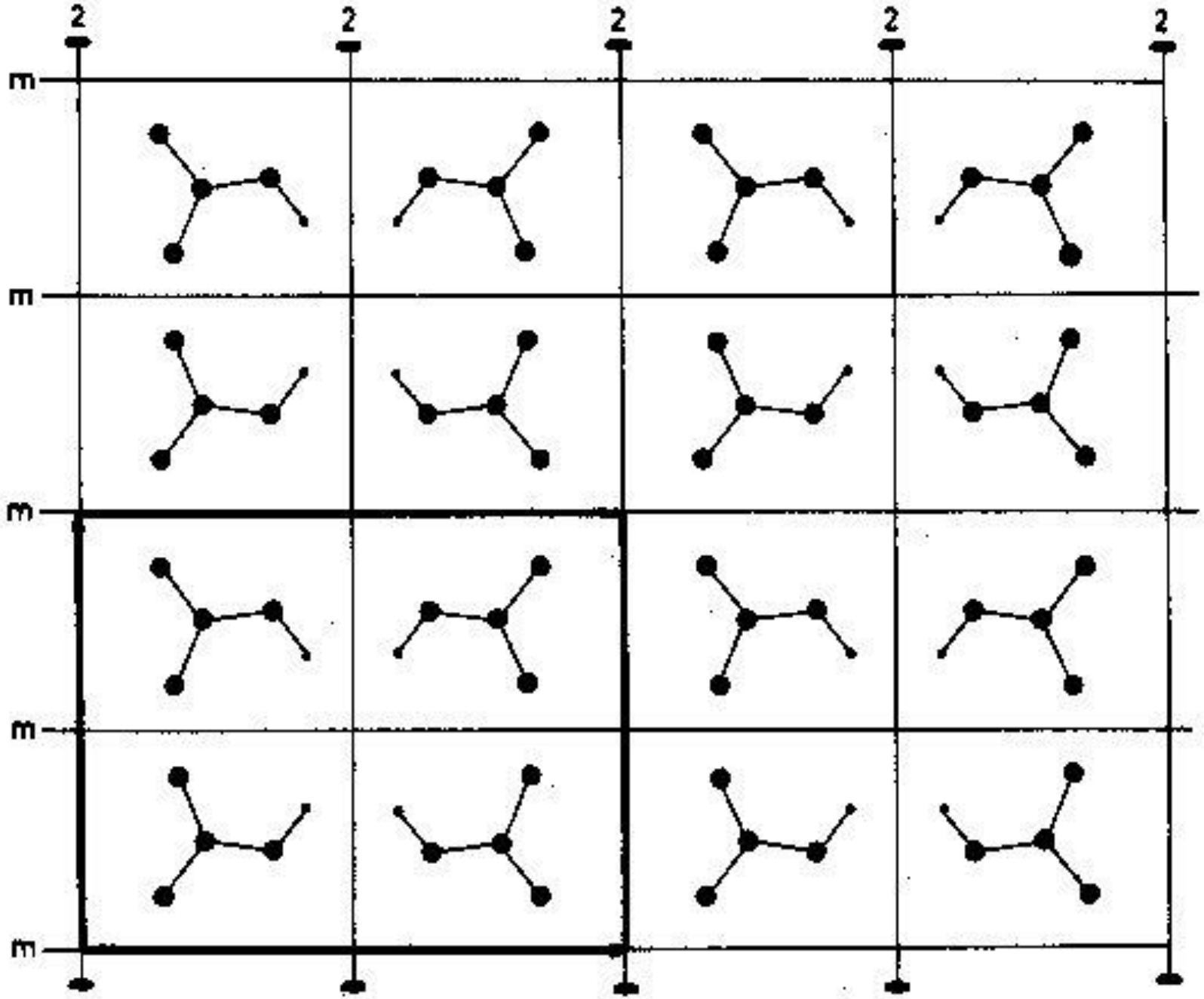
cP

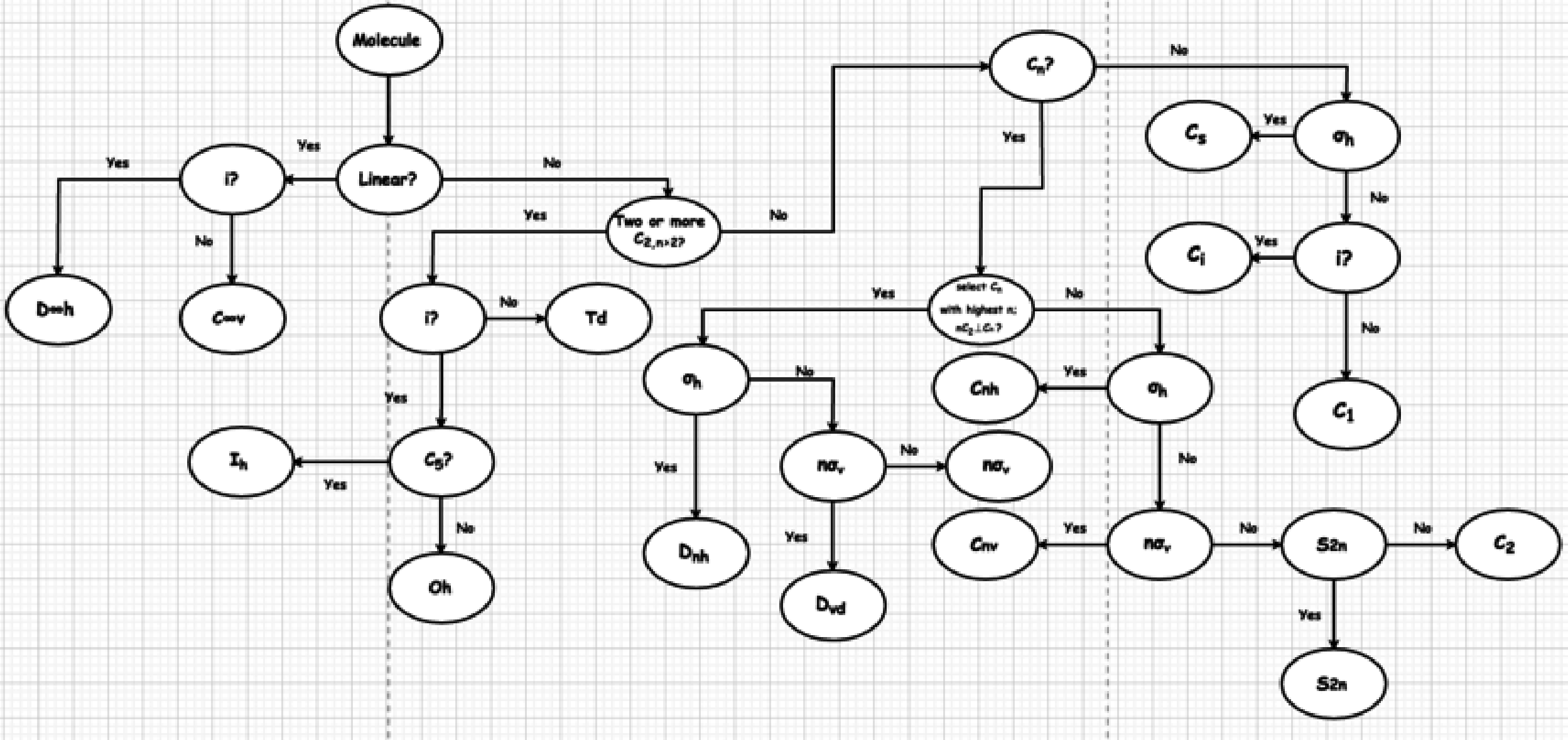


cI

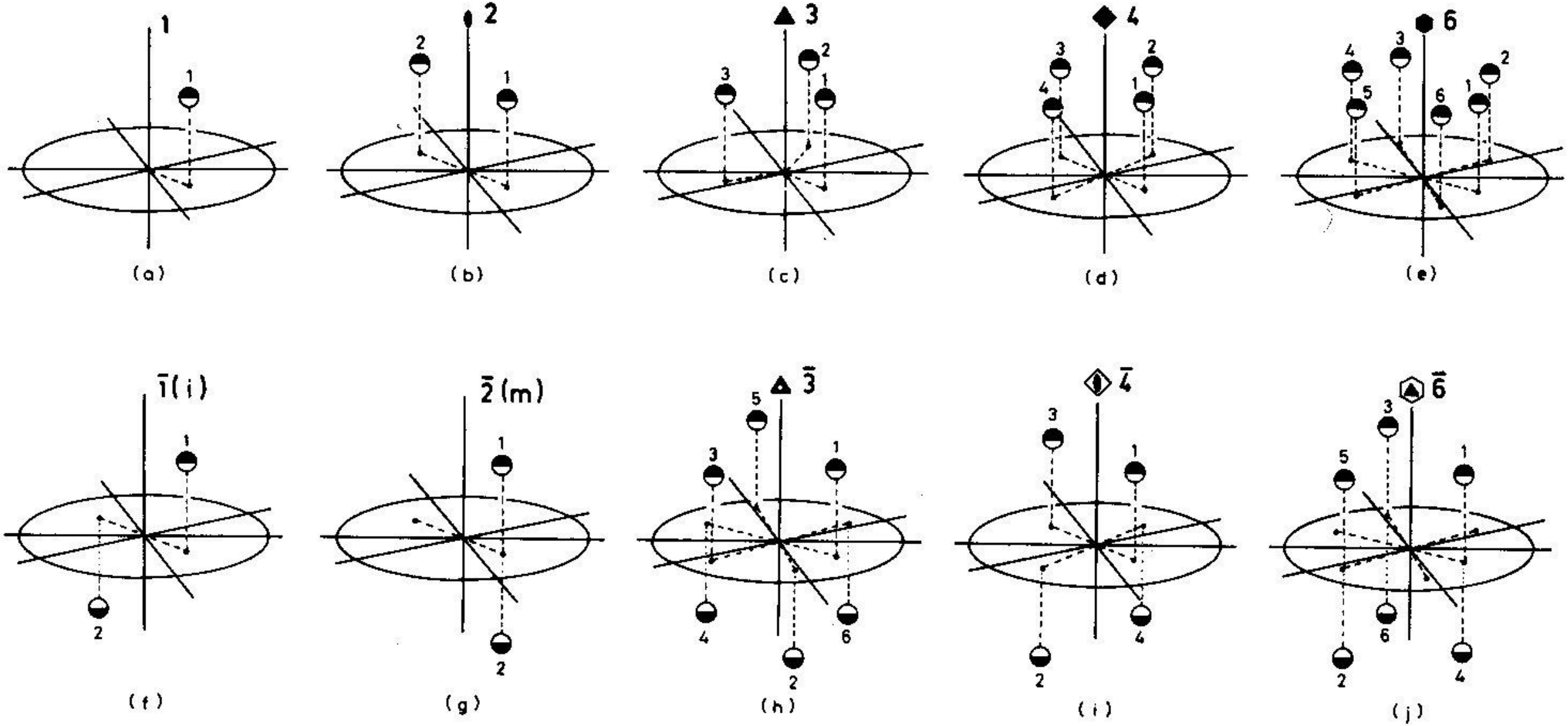


cF


2
2
2
2
2
m
m
m
m
m


Molecule
Linear?
Yes
No
i?
Yes
No
D∞h
C∞v
Two or more C2,n>2?
Yes
No
i?
No
Td
Yes
Ih
Yes
Cn?
Yes
No
Cs
Yes
σh
No
Ci
Yes
i?
No
C1
select Cn with highest n: nC2 ⊥ Cn?
Yes
No
σh
No
Yes
Dnh
nσv
No
nσv
Yes
Dnd
Cnh
Yes
σh
No
Cnv
Yes
nσv
No
S2n
No
C2
Yes
S2n
Oh

Hermann-Mauguin



Screw axis and Glide Planes