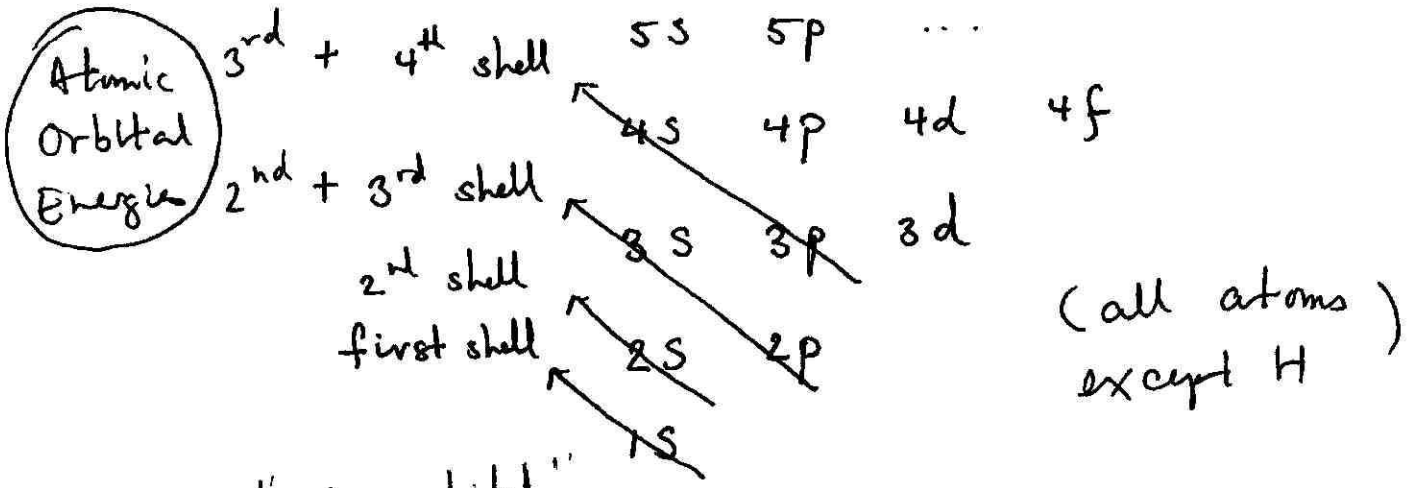
Lecture II

① Aufbau Principle and the Shape of Orbitals



These are "spin-orbitals"

- ns : Two ns (eg. 1s) orbitals $m_\ell = 0$; $m_s = \pm 1/2$
- np : Six np (eg 2p) " $m_\ell = 1, 0, -1$; $m_s = \pm 1/2$
- nd : Ten nd (eg 3d) " $m_\ell = 2, 1, 0, -1, -2$; $m_s = \pm 1/2$

② Filled shells are stable

first shell	1s	$2e^-$	He $2e^-$
2nd shell	2s 2p	$2 + 6\ e^- = 8e^-$	Ne $10e^-$ (2+8)
3rd shell	3s 3p	$8\ e^-$	Ar (2+8+8 $=18e^-$)
4th shell	4s 3d 4p	$18\ e^-$	Kr

Ar is the third most common molecule in air. At 1% in air Ar is much more abundant than CO_2 (.04%) At atomic wt 40 it is heavier than O_2 (wt 32 AU).

- demonstration -

Note: Performing your original search, ***argon and carbon dioxide in air***, in PubMed will retrieve *84* citations.

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All: 1 Review: 0

1: Vet Rec. 1996 Jun 15;138(24):592-3. Related Articles, Links

Aversive reactions of turkeys to argon, carbon dioxide and a mixture of carbon dioxide and argon.

Raj AB.

Department of Clinical Veterinary Science, University of Bristol. Langford.

The reactions of turkeys to the presence of either 90 per cent argon in air (anoxia), 72 per cent carbon dioxide in air or a mixture of 30 per cent carbon dioxide and 60 per cent argon in air with 3 per cent residual oxygen were tested. The majority of the turkeys did not avoid a feeding chamber containing either argon or the mixture of carbon dioxide and argon, but 50 per cent of the turkeys avoided a feeding chamber containing 72 per cent carbon dioxide in air. It is concluded that from the point of view of welfare, either 90 per cent argon in air or a mixture of 30 per cent carbon dioxide and 60 per cent argon in air, would be preferable to a high concentration of carbon dioxide for stunning/killing turkeys.

Publication Types:
- Clinical Trial

PMID: 8799986 [PubMed - indexed for MEDLINE]

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③ Fe element 26

$\underbrace{2 + 8 + 8}_{Ar\ (18e^-)} + 8$ ← 8 valence e^- $\quad = 26$

(roughly 2 in 4S & 6 in 3d)

Rb element 37

$\underbrace{2 + 8 + 8 + 18}_{Kr\ (36e^-)} + 1$ ← 1 valence e^-

Rb "feels" how close it is to a filled shell & readily loses a single electron.

O $2 + 6 = 8$ ← 6 valence e^-. Needs to gain $2e^-$ to reach filled shell

↝ He

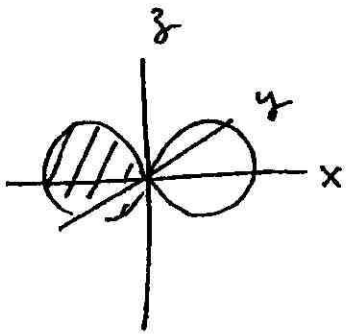
– movie –

④ The filling of the orbitals corresponds to the properties of the elements. We may not understand (yet) why there are s, p & d orbitals but they certainly play a role in chemistry.

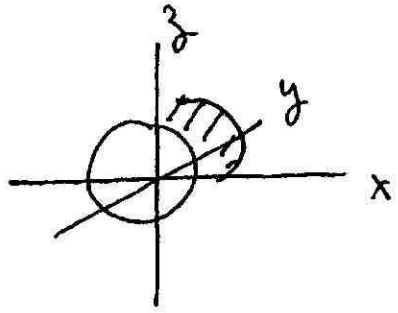
⑤ For H

$$\text{Energy}(2S) = \text{Energy}(2p)$$
$$E(3S) = E(3p) = E(3d)$$
$$E(4S) = E(4p) = E(4d) = E(4f)$$

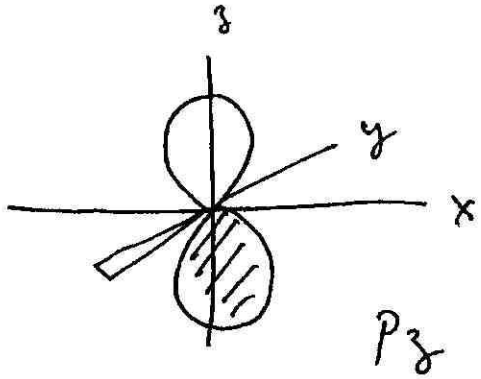
⑥ What do orbitals look like?



p_x



p_y



p_z

In all cases $\ell = 1$

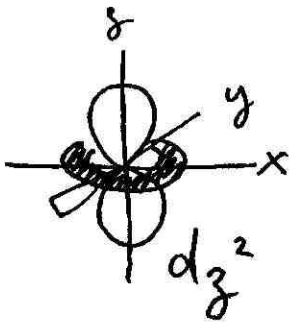
p_z is $m_\ell = 0$ state

$p_x + ip_y$ is $m_\ell = +1$ state

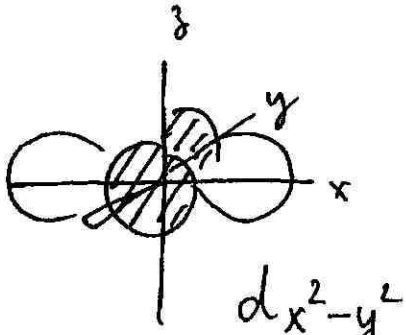
$p_x - ip_y$ " " $= -1$ state

where $i^2 = -1$

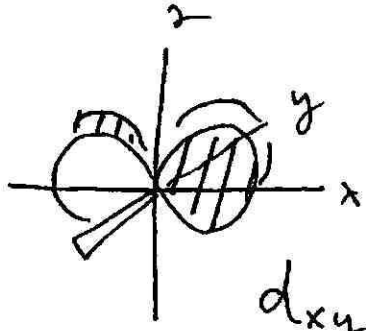
⑦ 5 d · orbitals ($l = 2$ orbitals)



d_{z^2}

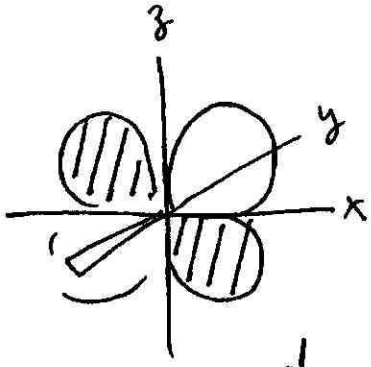


$d_{x^2-y^2}$

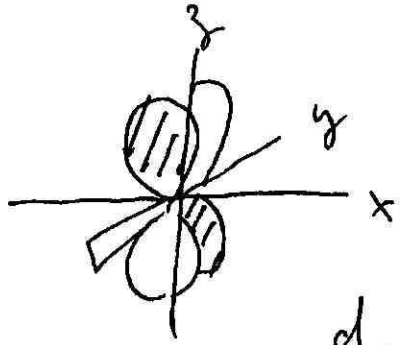


d_{xy}

$m_l = 0$



d_{xz}

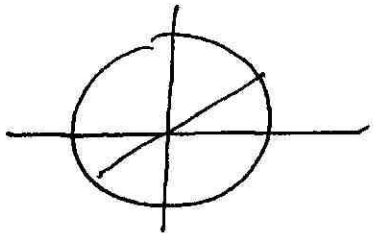


d_{yz}

correspond to the 5 $m_l = -2, -1, 0, 1, 2$ states.

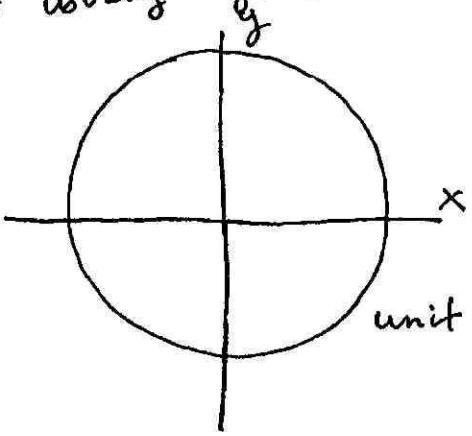
⑧ For chemistry (to a good approximation) we do not need to know what f orbitals look like.

⑨



s · orbitals are spherical.

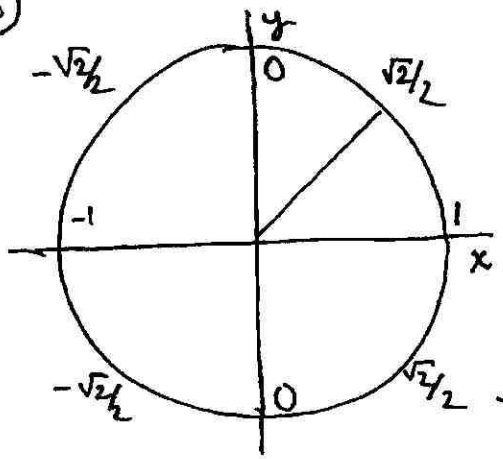
(10) The shapes of the orbitals have to do with the names of the orbitals. [Information not usually given in textbooks]



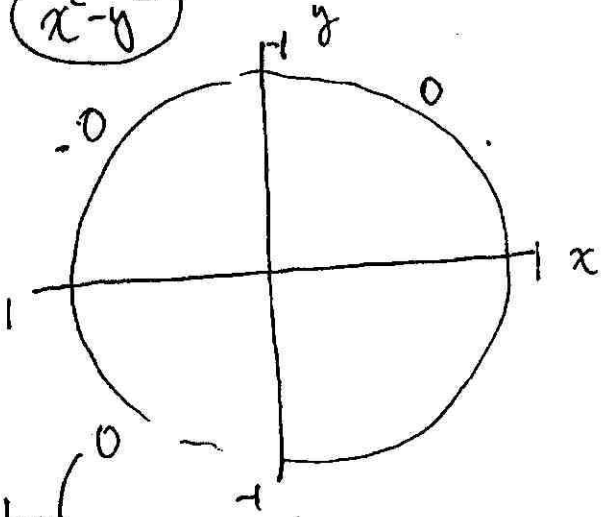
unit circle.

Plot the value of functions such as x or x^2-y^2 on the unit circle

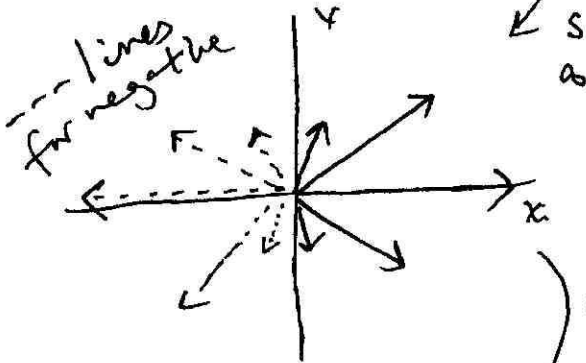
(x)

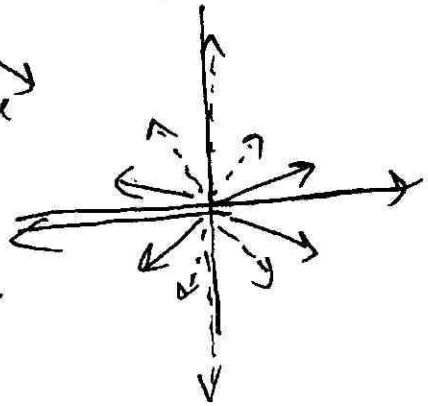


x^2-y^2

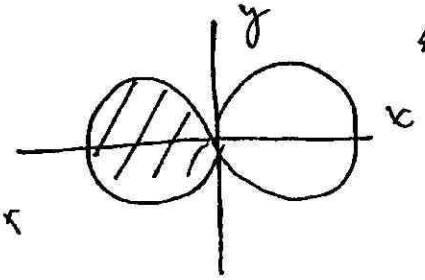


draw vectors same length as unit circle values



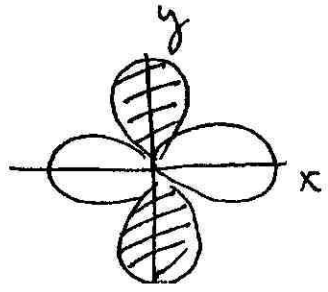


connect the vector arrows

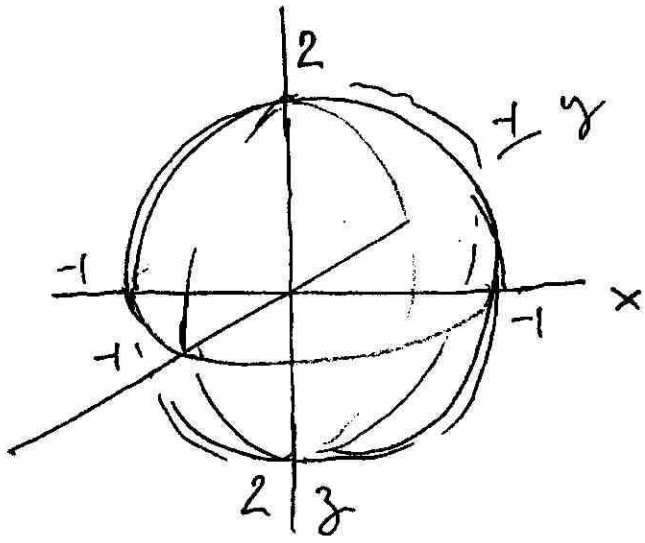


p_x

$d_{x^2-y^2}$

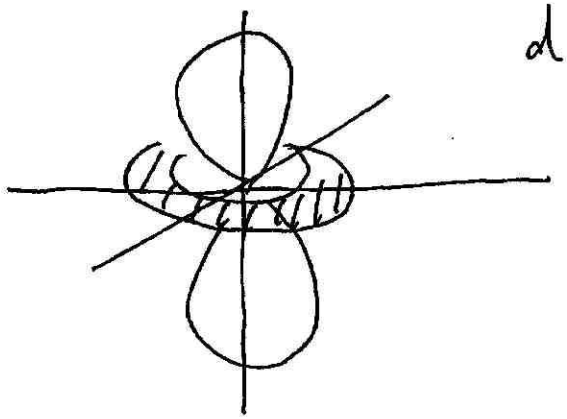


(11) In 3-dimensions, draw the values on a unit sphere



z^2 is short for $2z^2 - x^2 - y^2$

leads to



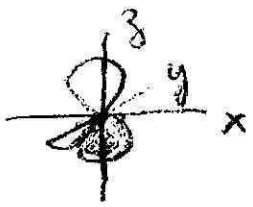
- ask for a violin for next class -

Lecture I & II Summary

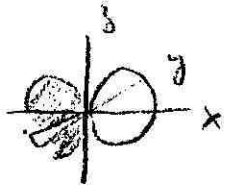
① n, l, m_l & m_s : we don't know where these come from but the rules fit in with the periodic table and the Aufbau (build-up) principle.

② The letters n, l, m_l correspond to particular orbitals d_{z^2}, d_{xy} etc... We don't know why these are orbitals but we know they have something to do with the names z^2, xy, x^2-y^2, x, etc...

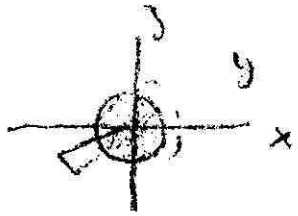
③ Three p-orbitals ($m_l = -1, 0, 1$)



p_z

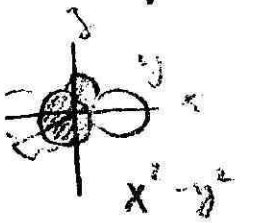


p_x

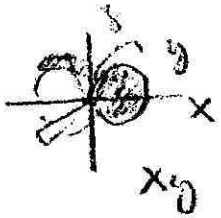


p_y

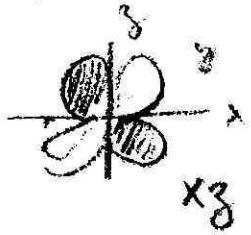
Five d-orbitals ($m_l = -2, -1, 0, 1, 2$)



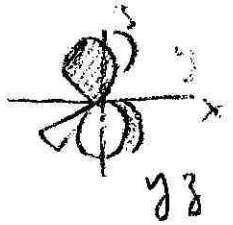
x^2-y^2



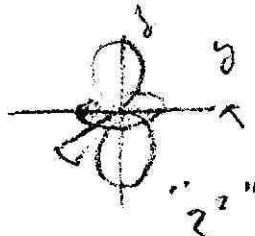
xy



xz



yz



"z^2"

④ Six p-spin orbitals ↑↑↑↓↓↓ $m_s = \pm 1/2$; $m_l = -1, 0, 1$

Ten d-spin orbitals ↑↑↑↑↑↓↓↓↓↓ $m_s = \pm 1/2$; $m_l = -2, -1, 0, 1, 2$