A Three-Dimensional Representation of Orbitals in Glass Blocks

Nakako TOKITA, Sumio TOKITA*,
Akira IKUO, and Haruo Ogawa****
Saitama University (Emeritus) 255 Shimo-Ohkubo, Sakura-ku, Saitama, Saitama, 338-8570 Japan
***** Department of Chemistry, Tokyo Gakugei University, Tokyo 184-8501, Japan***
***studionebula@gmail.com**

In order to understand the characteristic features of atomic orbitals, electron clouds are recorded in glass blocks by the use of three – dimensional (3-D) laser technique.

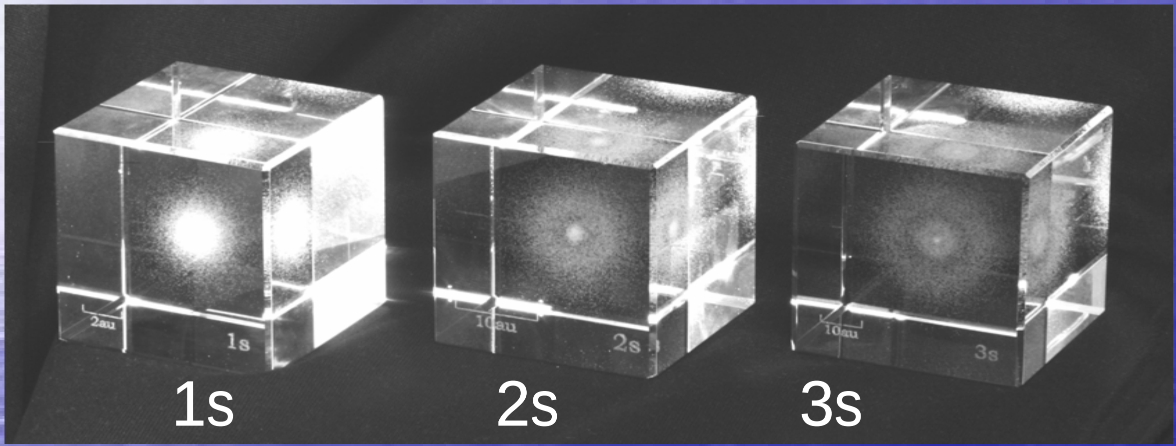
It is difficult for us to imagine the 3-D appearance of orbitals and the physical meaning from the solution χ of Schroedinger equation. χ^2 gives the probability density of finding an electron, namely electron clouds.

Methods

- Calculate the probability densities of hydrogen atomic orbitals in a 3-D space by the rejection method.

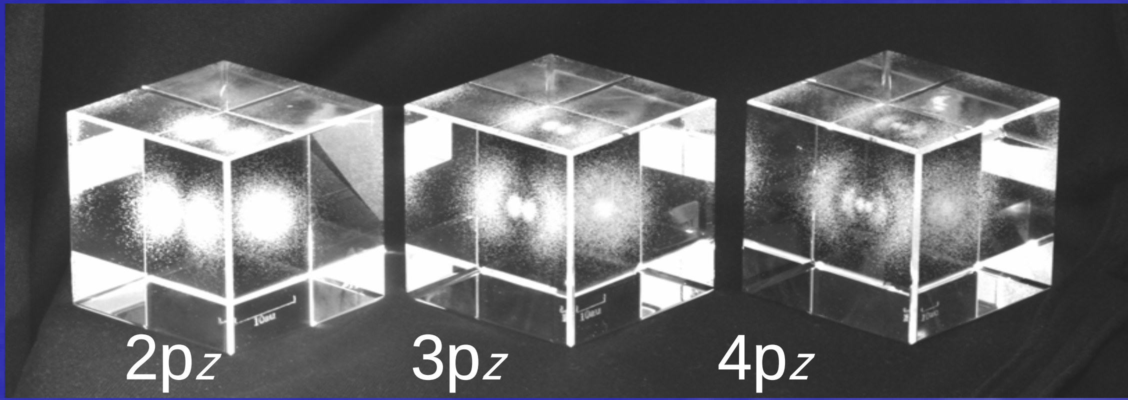
Sculpture the collected data in a glass block by using laser equipment (LeLee Laser Mini Type YF-YAG-200).

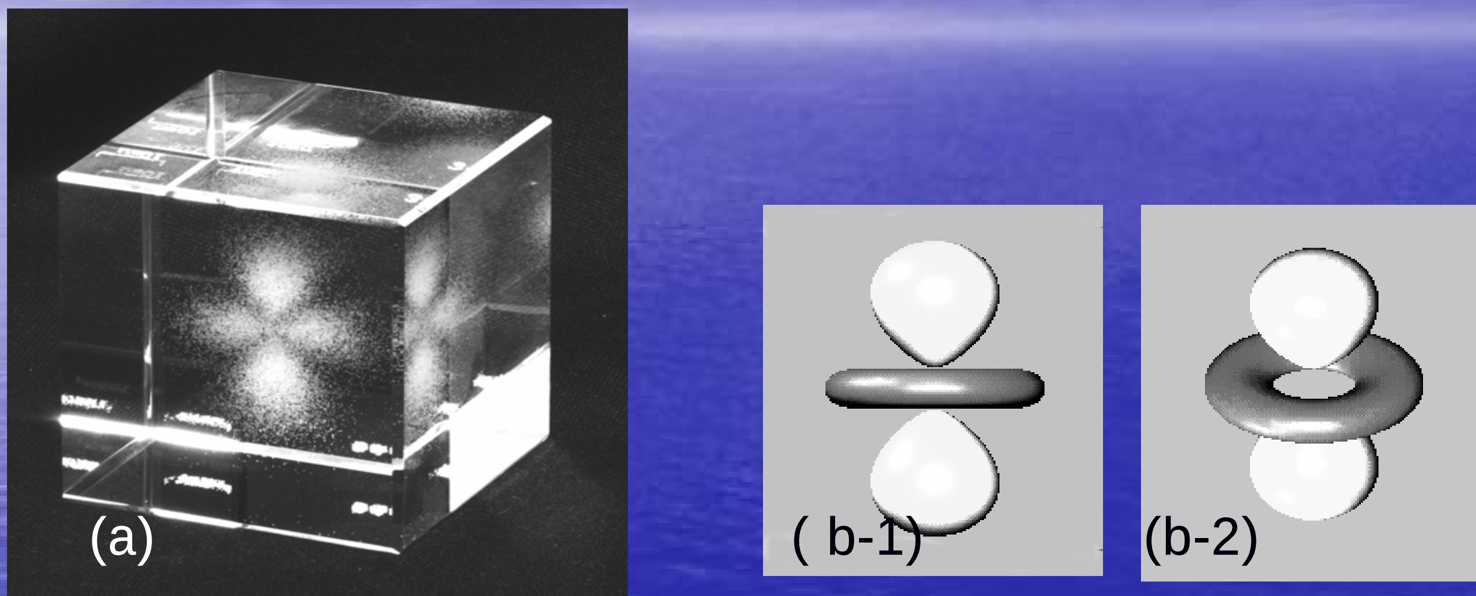
Images of the 3-D probability densities of hydrogen atomic orbitals



The spherical shape of the orbitals together with the inner nodes are shown.

There are existence of planar or planar and spherical nodes.





Comparison of (a) probability density in this work with (b) conventional isosurface representations of 3d($3z^2 - r^2$) orbital.

Please see glass block models !!!

What can be seen in these models ?

What becomes of the shape
of atomic orbital by
the quantum number ?

Why can be seen similar pattern of atomic orbitals having the same magnetic quantum number |*m*| ?

Nodes in atomic orbitals

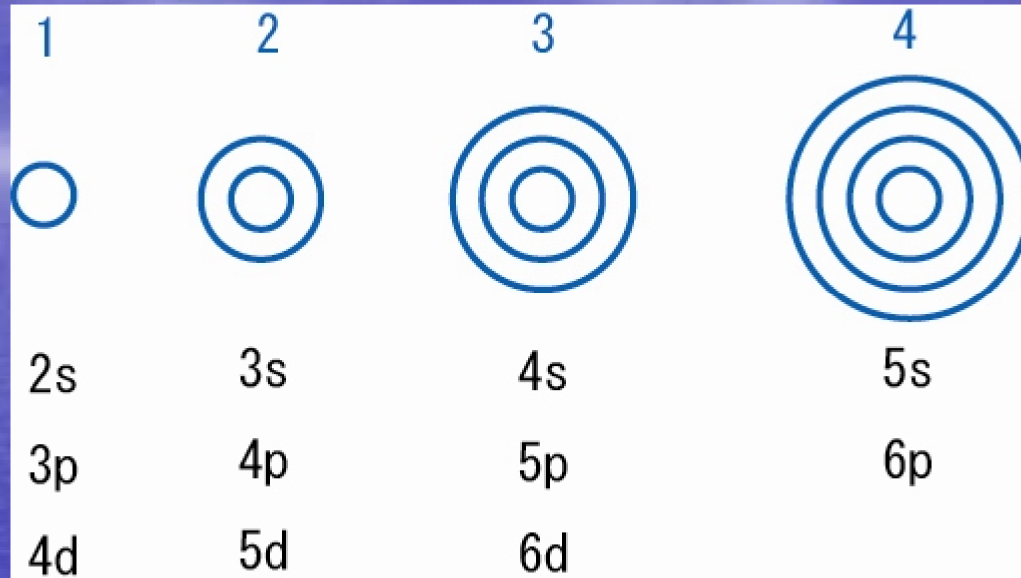
	number of nodes
[A] Spherical nodes	$n - l - 1$
[B] Planar nodes containing *z* axis	$\mid m \mid$
[C] Planar and conical nodes symmetrical about *z* axis	$l - \mid m \mid$

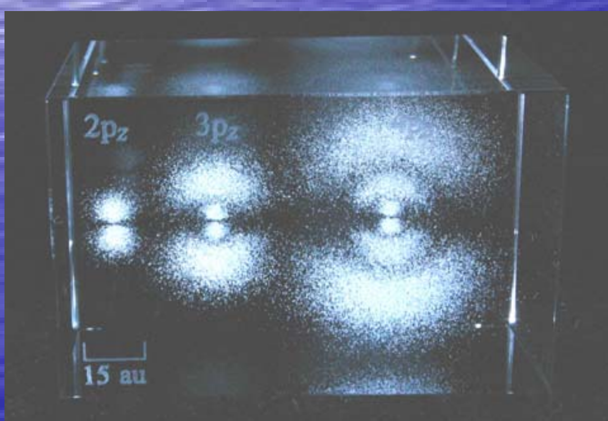
n : principal quantum number

l : azimuthal quantum number

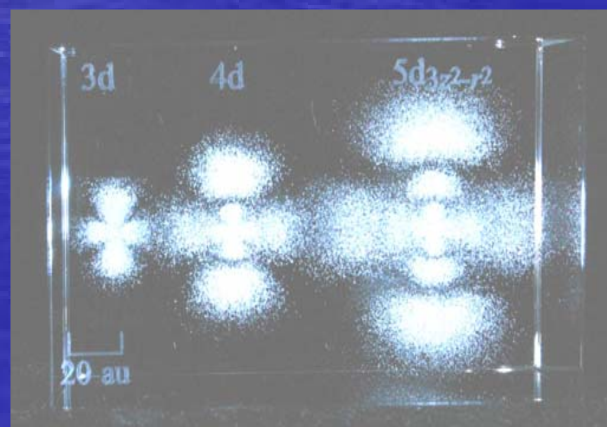
m : magnetic quantum number

[A] Spherical nodes

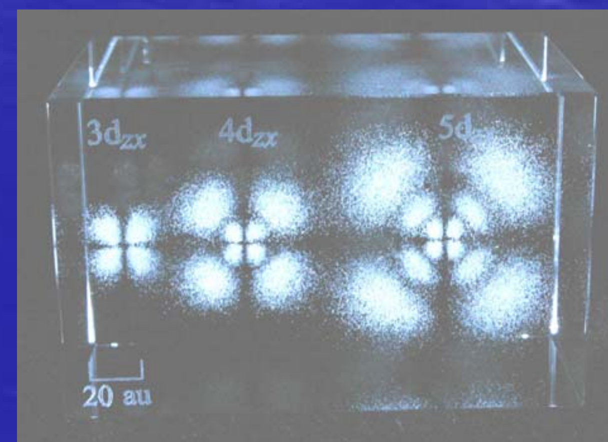




2p 3p 4p



3d 4d 5d

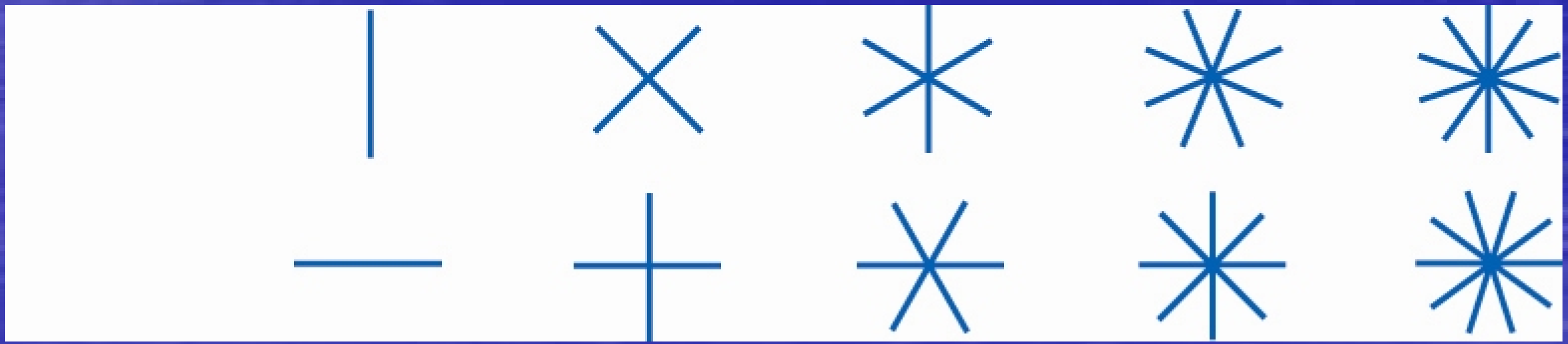


3d 4d 5d

[B] Planar nodes containing z axis

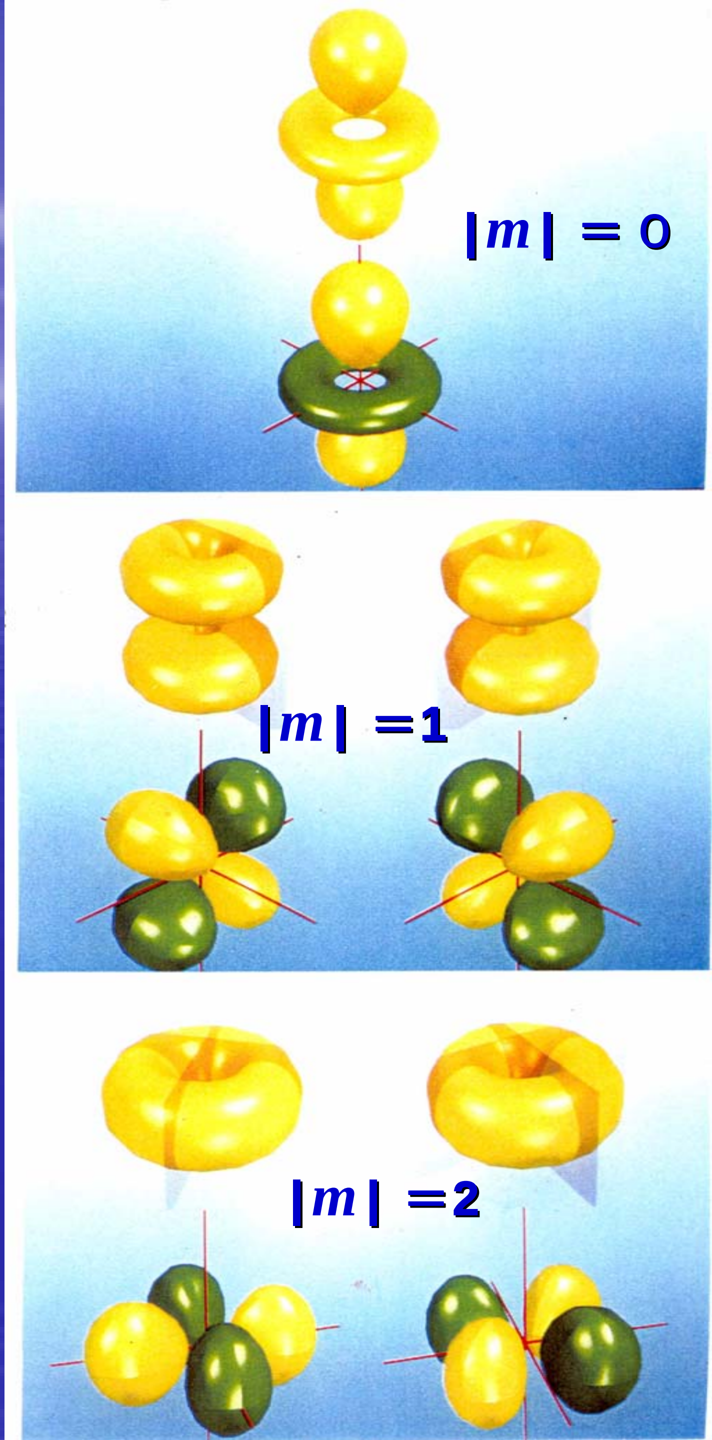
When $|m|$ is not equal to 0, the orbitals have vertical nodes equal to the $|m|$ value. The square of imaginary wave function $\left|\chi_{nlm}\right|^2$ is sliced by these nodal planes as below.

$|m|$: 0 1 2 3 4 5

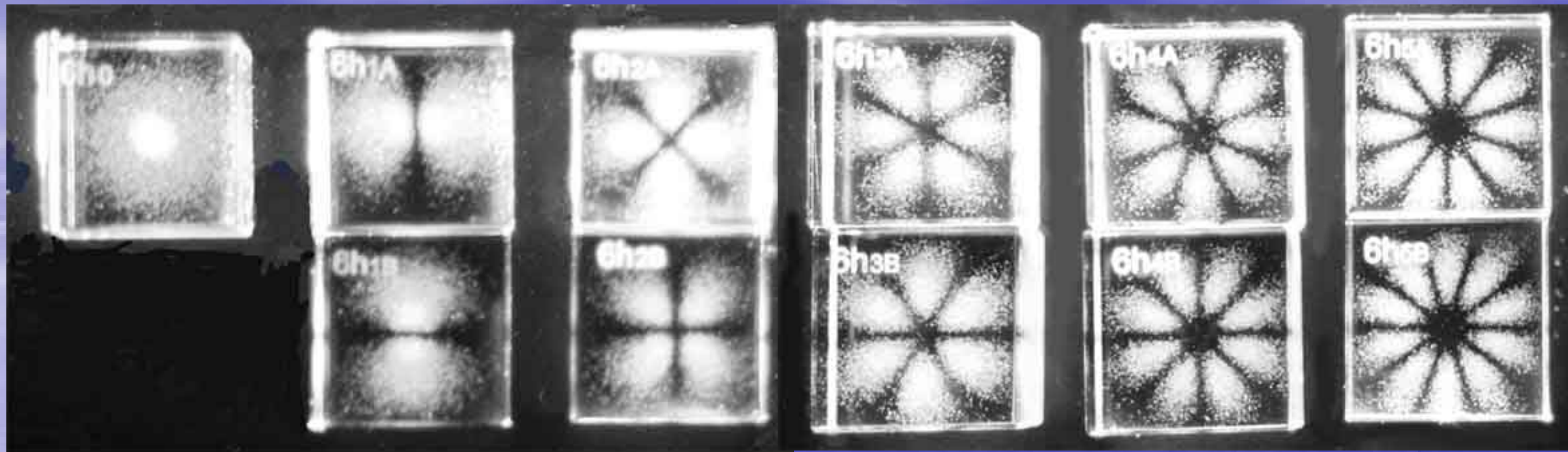


The process of making the real function from $\left|\chi_{nlm}\right|^2$

- $|m| = 0$: yellow: plus sign
  green: minus sign
- When $|m| = 1$, $\left|\chi_{nlm}\right|^2$ is sliced by one node
- When $|m| = 2$, $\left|\chi_{nlm}\right|^2$ is sliced by two nodes



Patterns in eleven 6h orbitals



| m | = 0 | m | = 1 | m | = 2 | m | = 3 | m | = 4 | m | = 5

The orbital patterns in the view from *z* axis are classified by the magnetic quantum number, *m* , as follows.

s orbital pattern | *m* | = 0

p orbital pattern | *m* | = 1

d orbital pattern | *m* | = 2

f orbital pattern | *m* | = 3

g orbital pattern | *m* | = 4

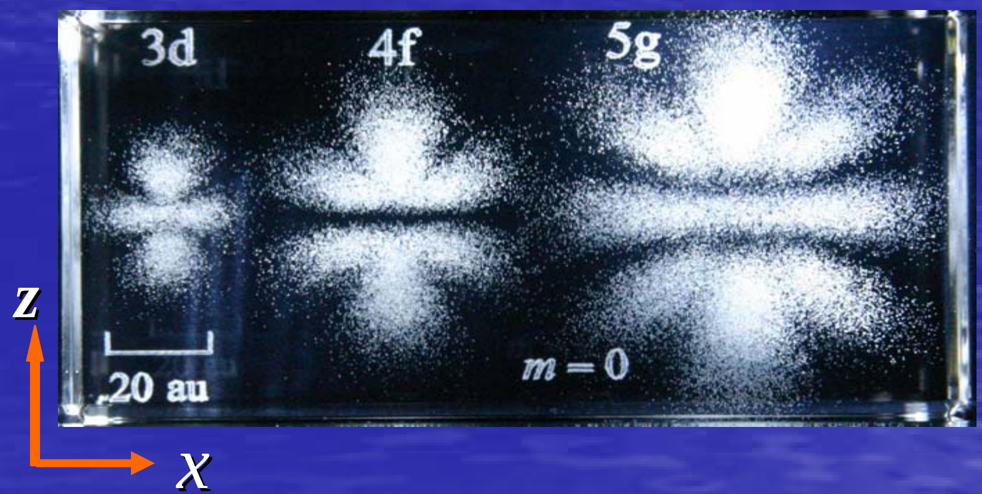
h orbital pattern | *m* | = 5 …

$|m| = 0$: for example,

3d($3z^2$-r^2), 4f($5z^3$-$3zr^2$), and 5g($35z^4$-$30z^2r^2$+$3r^4$)

- The view from the *z* axis gives "s" orbital pattern.

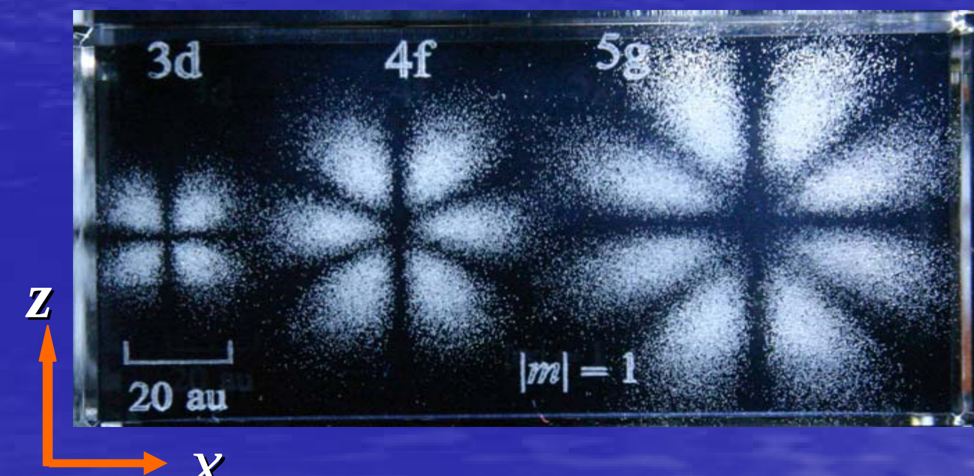
- The view of *xz* plane from the *y* axis.



$|m| = 1$: for example, 3d(zx), 4f($5xz^2$-xr^2), and 5g($7xz^3$-$3xzr^2$)

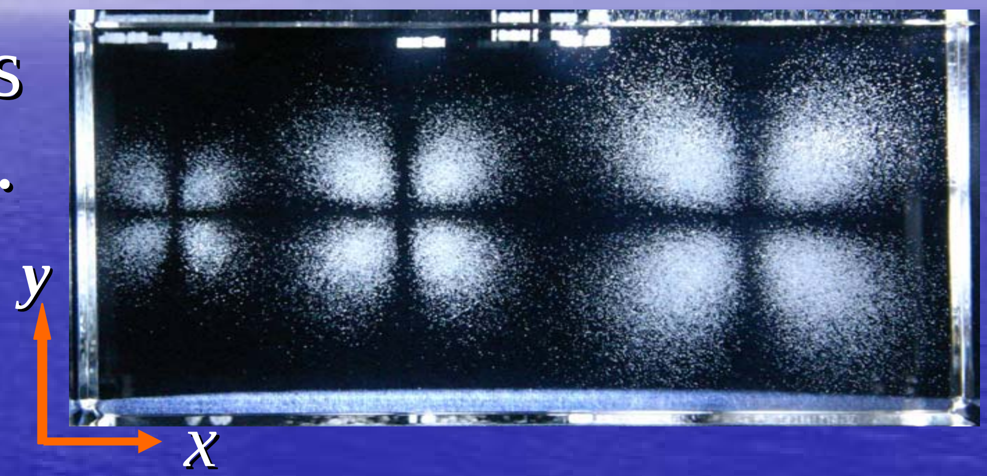
- The view from the *z* axis gives “p” orbital pattern.

- The view of *xz* plane from the *y* axis.

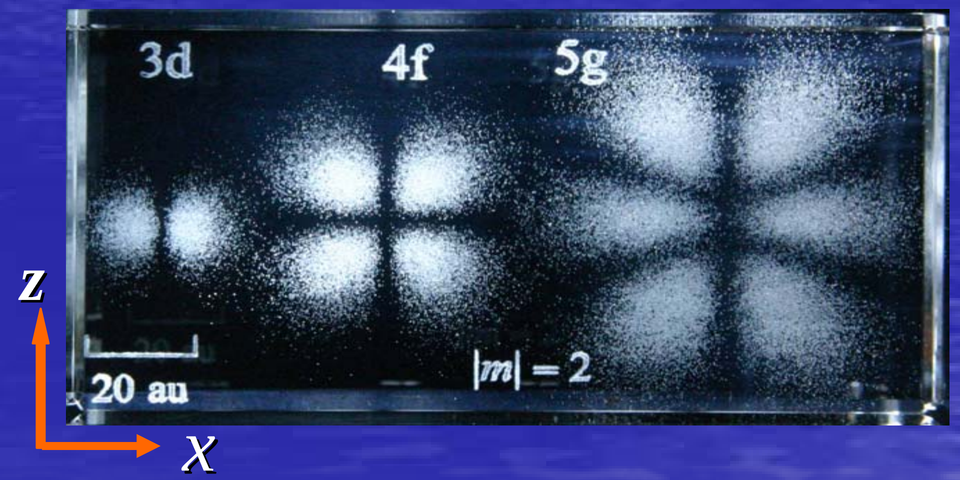


$|m| = 2$: for example, 3d(xy), 4f(xyz), and 5g($7xyz^2$-xyr^2)

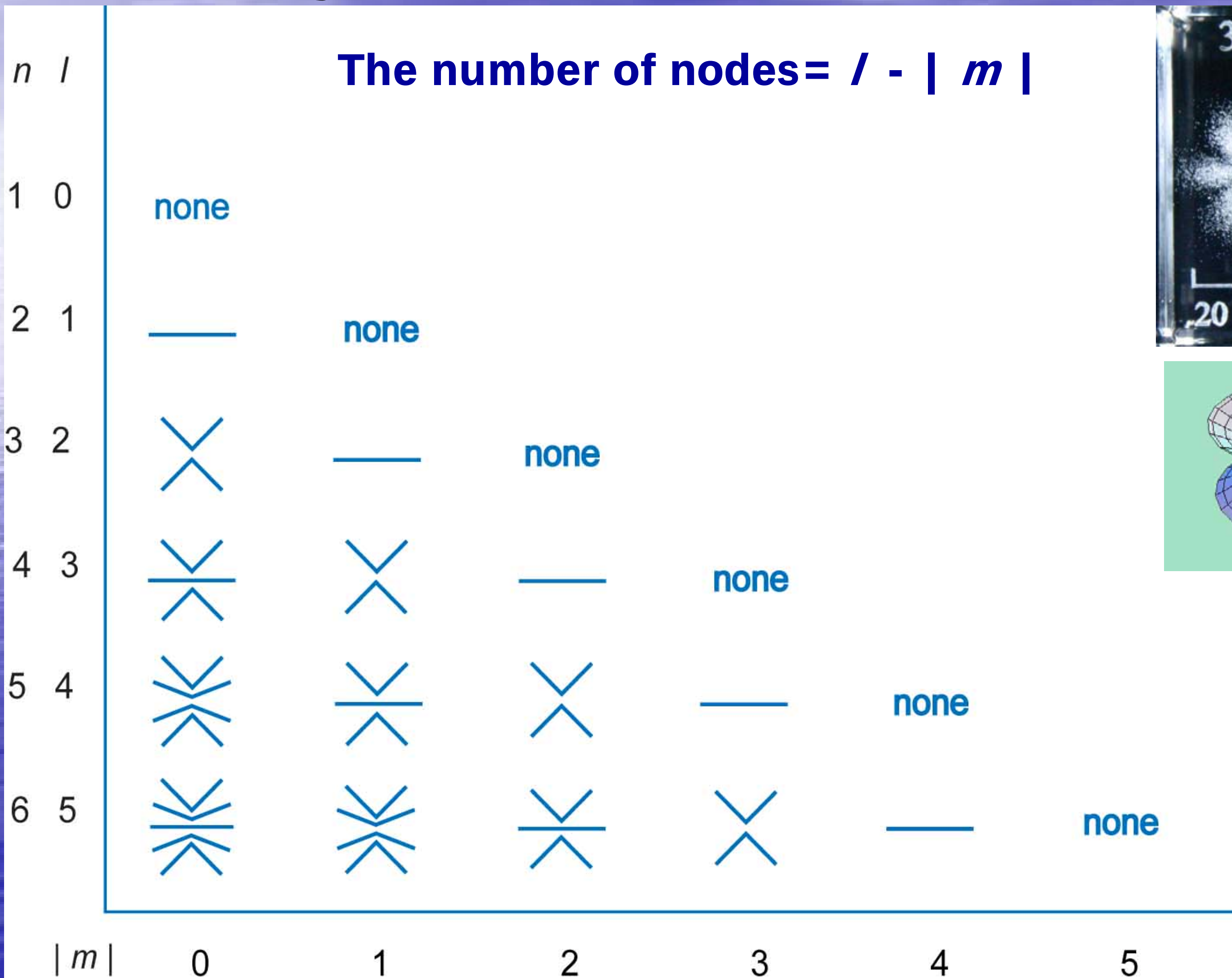
- The view from the z axis gives “d” orbital pattern.

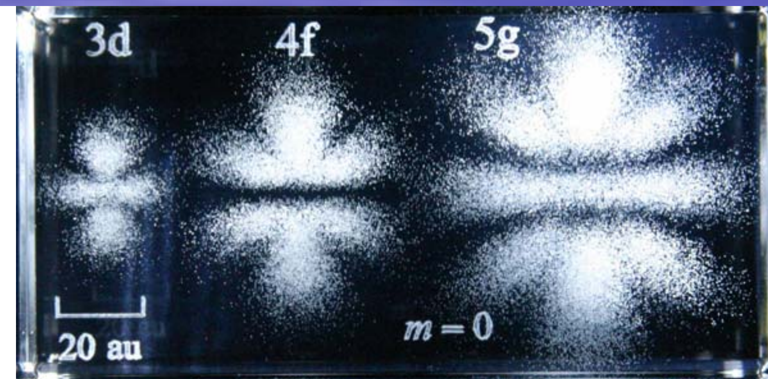


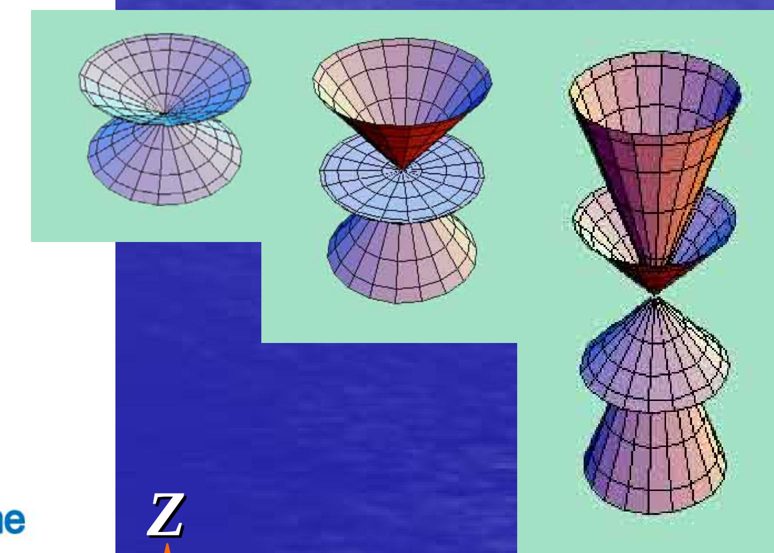
- The view of xz plane from the y axis.

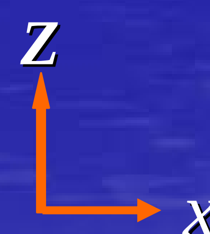


[C] Planar and conical nodes symmetrical about *z* axis







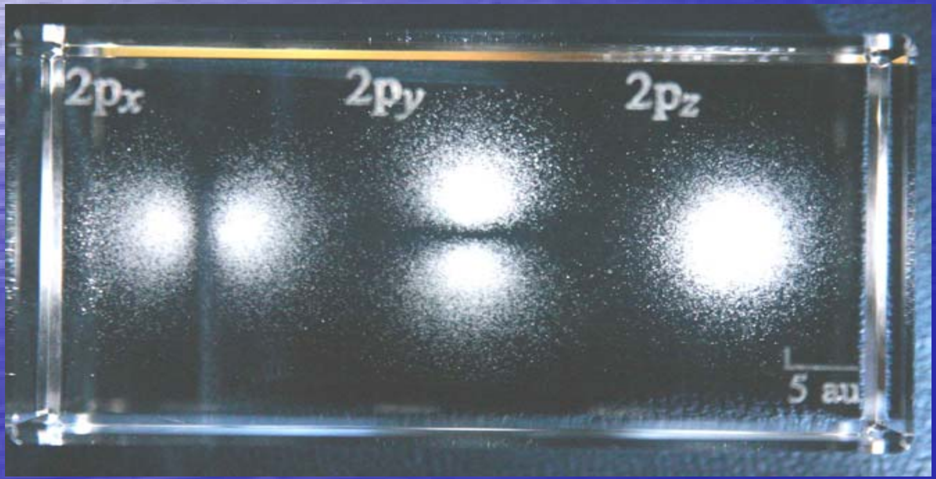


Advantageous representation seeing through one side of a glass block

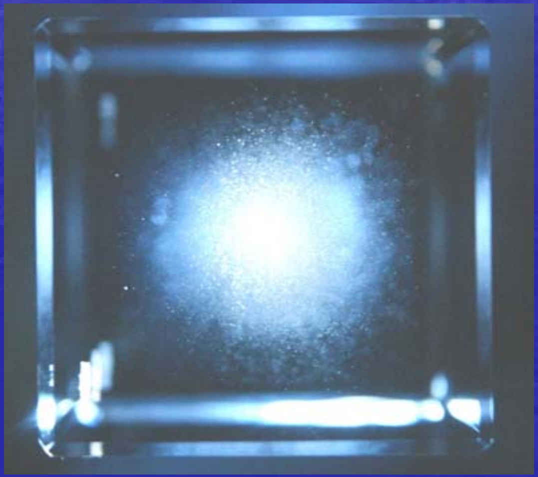
This can be made possible only in the method to sculpture electron clouds in a glass block.

Superposition of three 2p orbitals gives a sphere.

$$\chi_{2px}{}^2 + \chi_{2py}{}^2 + \chi_{2pz}{}^2 = 1/(32\pi)\exp(-r)\{x^2 + y^2 + z^2\}$$



Hydrogen 2p*x*, 2p*y*, and 2pz orbitals
(a) The view from the *z* axis

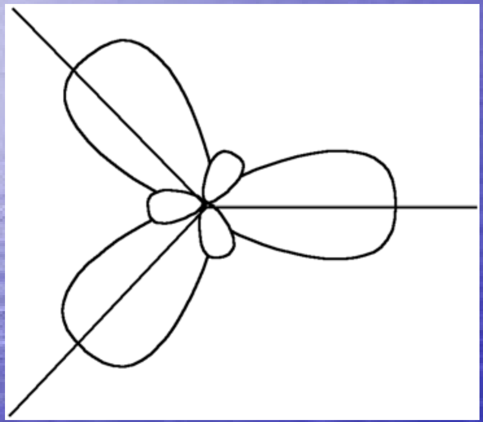


(b) The view from the *x* axis gives image of a sphere.

Superposition of three sp^2 orbitals

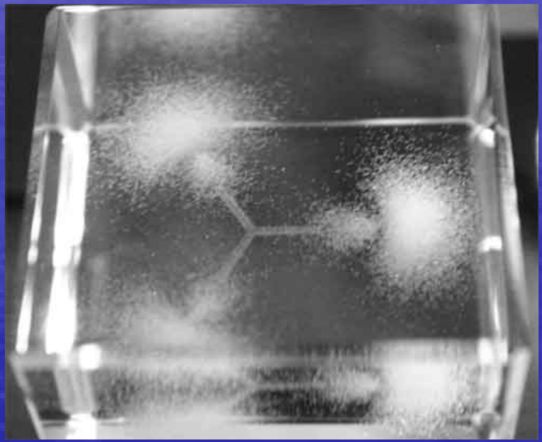
$$\chi_{2s}^2 + \chi_{2px}^2 + \chi_{2py}^2 = 1/(32\pi)\exp(-r)\{(2-r)^2 + x^2 + y^2\}$$

Picture of three sp^2 orbitals in many textbooks is shown. Orbitals have common origin. Is that right ?



Right answer can be seen in a glass block.

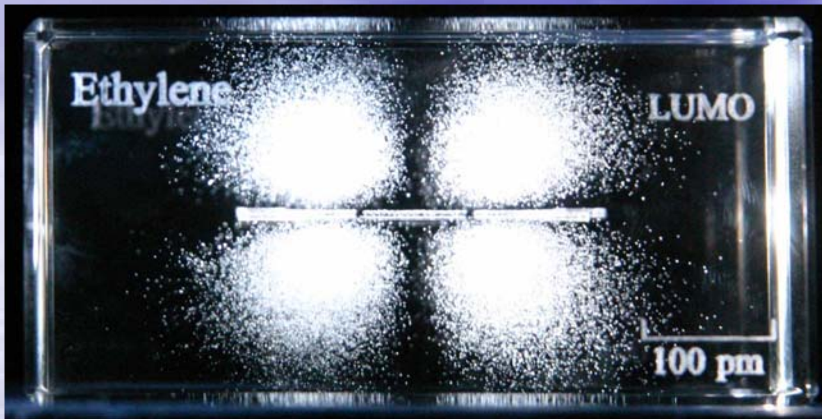
Centers of these orbitals are moved on the vertices of a regular triangle, because common origin gives a cylindrical pattern.



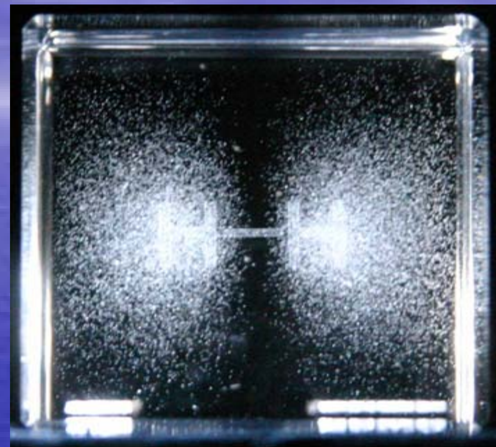
The superposition of 2p*x* and 2p*y* orbitals gives cylindrical pattern.

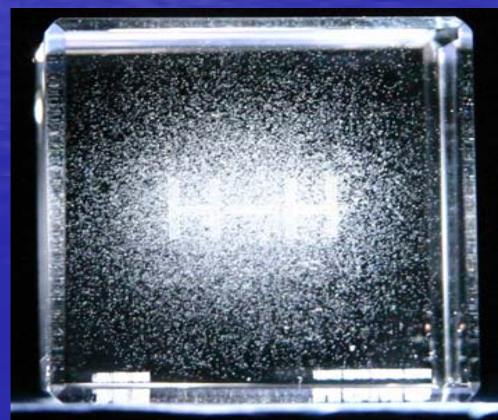
$$\chi_{2px}^2 + \chi_{2py}^2 = 1/(32\pi)\exp(-r)\{x^2 + y^2\}$$

Representations for molecular orbitals

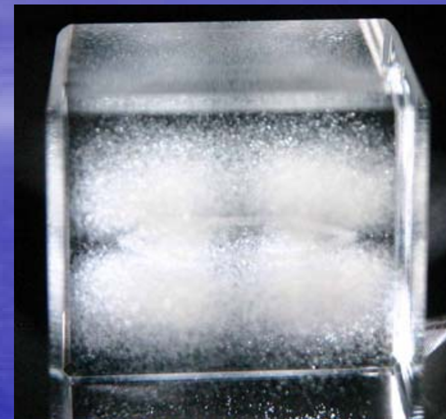


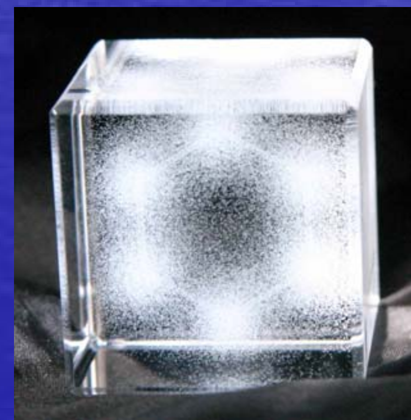
Ethylene π orbitals
HOMO and LUMO





H_2 molecular
orbitals





Benzene
π occ. orbitals

These designs are registered on the Registers of the Japan Patent Office.

Design Registration Number :
1280636, 129427, 1298894, 1298428,
1298429, 1298430, 1298431, 1298895

References

[1] M. Born, *Z. Phys.*, **37**, 863-867 (1926).

[2] S. Tokita, T. Watanabe, F. Kido, H. Maekawa, and T. Shimozawa, *J. Chem. Software*, **3**, 37 (1996).

[3] N. Tokita, S. Tokita, and T. Nagao, *J. Comput. Chem. Jpn.*, **5**, 153 (2006).
http://www.sccj.net/publications/JCCJ/v5n3/a12/document.pdf

Studio Nebula

http://winmostar.com/nebula
http://www.ecosci.jp/sa07/NEBULA01.pdf
http://www.ecosci.jp/sa07/NEBULA02.pdf
e-mail: studionebula@gmail.com