Visualizing Three-Dimensional Hybrid Atomic Orbitals Using Winplot: An Application for Student Self Instruction

By Noor Fadiawati

VISUALIZING THREE DIMENSIONAL HYBRID ATOMIC ORBITALS USING WINPLOT: AN APPLICATION FOR STUDENT SELF INSTRUCTION

Andrian Saputra[1,*], Lorentz R. Canaval[2], Sunyono[1], Noor Fadiawati[1], Chansyanah Diawati[1], M. Setyorini[1], Nina Kadaritna[1], [3]Budi Kadaryanto

[1)]Department of Chemical Education, Faculty of Teacher Training and Education, University of Lampung, Bandar Lampung 35145, Indonesia
[2)]Theoretical Chemistry Division, Institute of General, Inorganic and Theoretical Chemistry, University of Innsbruck, Innrain 80–82, A–6020 Innsbruck, Austria
[3)]Department of English Education, Faculty of Teacher Training and Education, University of Lampung, Bandar Lampung 35145, Indonesia

The angular wave function, $|Y(\theta,\phi)|$, for the individual atomic orbital and the square of the angular wave function, $|Y(\theta,\phi)|^2$, for the hybrid atomic orbital is written in the ready form to input in Winplot.

i. Individual atomic orbital

Orbital	Angular function	|Y(θ, ϕ)| in Winplot format[‡] f(t,u)
s	$Y_s = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2\pi}}$	((1/sqrt(2))(1/(sqrt(2pi))))
p_x	$Y_{p_x} = \frac{\sqrt{3}\sin\theta}{2}\frac{\cos\varphi}{\sqrt{\pi}}$	((sqrt(3)sin(u)/2)(cos(t)/sqrt(pi)))
p_y	$Y_{p_y} = \frac{\sqrt{3}\sin\theta}{2}\frac{\sin\varphi}{\sqrt{\pi}}$	((sqrt(3)sin(u)/2)(sin(t)/sqrt(pi)))
p_z	$Y_{p_z} = \frac{\sqrt{6}\cos\theta}{2}\frac{1}{\sqrt{2\pi}}$	((sqrt(6)cos(u)/2)(1/(sqrt(2pi))))
d_{xz}	$Y_{d_{xz}} = \frac{\sqrt{15}\sin\theta\cos\theta}{2}\frac{\cos\varphi}{\sqrt{\pi}}$	((sqrt(15)sin(u)cos(u)/2)(cos(t)/sqrt(pi)))
d_{yz}	$Y_{d_{yz}} = \frac{\sqrt{15}\sin\theta\cos\theta}{2}\frac{\sin\varphi}{\sqrt{\pi}}$	((sqrt(15)sin(u)cos(u)/2)(sin(t)/sqrt(pi)))
d_{xy}	$Y_{d_{xy}} = \frac{\sqrt{15}\sin^2\theta}{4}\frac{\sin 2\varphi}{\sqrt{\pi}}$	((sqrt(15)(sin(u))^2/4)(sin(2t)/sqrt(pi)))
$d_{x^2-y^2}$	$Y_{d_{x^2-y^2}} = \frac{\sqrt{15}\sin^2\theta}{4}\frac{\cos 2\varphi}{\sqrt{\pi}}$	((sqrt(15)(sin(u))^2/4)(cos(2t)/sqrt(pi)))

d_{z^2}	$Y_{d_{z^2}} = \frac{\sqrt{10}\,(3\cos^2\theta - 1)}{4}\frac{1}{\sqrt{2\pi}}$	((sqrt(10)((3(cos(u))^2)-1)/4)(1/sqrt(2pi)))

ii. Hybrid Atomic Orbitals

Orbital	Angular function	$\lvert Y(\theta, \phi)\rvert^2$ in Winplot format‡ f(t,u)
sp (linear)	$Y_{sp}(1) = \frac{1}{\sqrt{2}}Y_s + \frac{1}{\sqrt{2}}Y_{p_x}$ $Y_{sp}(2) = \frac{1}{\sqrt{2}}Y_s - \frac{1}{\sqrt{2}}Y_{p_x}$	• ((sqrt(1/2))(1/sqrt(2))(1/sqrt(2pi))+(sqrt(1/2))(sqrt(3)sin(u)/2)(cos(t)/sqrt(pi)))^2 • ((sqrt(1/2))(1/sqrt(2))(1/sqrt(2pi))-(sqrt(1/2))(sqrt(3)sin(u)/2)(cos(t)/sqrt(pi)))^2
sp^2 (trigonal planar)	$Y_{sp^2}(1) = \frac{1}{\sqrt{3}}Y_s + \frac{1}{\sqrt{6}}Y_{p_x} + \frac{1}{\sqrt{2}}Y_{p_y}$ $Y_{sp^2}(2) = \frac{1}{\sqrt{3}}Y_s + \frac{1}{\sqrt{6}}Y_{p_x} - \frac{1}{\sqrt{2}}Y_{p_y}$ $Y_{sp^2}(3) = \frac{1}{\sqrt{3}}Y_s - \frac{2}{\sqrt{6}}Y_{p_x}$	• ((1/sqrt(3))(1/sqrt(2))(1/sqrt(2pi))+(1/sqrt(6))((sqrt(3)sin(u)/2)(cos(t)/sqrt(pi)))+(1/sqrt(2))((sqrt(3)sin(u)/2)(sin(t)/sqrt(pi))))^2 • ((1/sqrt(3))(1/sqrt(2))(1/sqrt(2pi))+(1/sqrt(6))((sqrt(3)sin(u)/2)(cos(t)/sqrt(pi)))-(1/sqrt(2))((sqrt(3)sin(u)/2)(sin(t)/sqrt(pi))))^2 • ((1/sqrt(3))(1/sqrt(2))(1/sqrt(2pi))-(2/sqrt(6))((sqrt(3)sin(u)/2)(cos(t)/sqrt(pi))))^2
sp^3 (tetrahedral)	$Y_{sp^3}(1) = \frac{1}{2}\left(Y_s + Y_{p_x} + Y_{p_y} + Y_{p_z}\right)$ $Y_{sp^3}(2) = \frac{1}{2}\left(Y_s + Y_{p_x} - Y_{p_y} - Y_{p_z}\right)$ $Y_{sp^3}(3) = \frac{1}{2}\left(Y_s - Y_{p_x} - Y_{p_y} + Y_{p_z}\right)$ $Y_{sp^3}(4) = \frac{1}{2}\left(Y_s - Y_{p_x} + Y_{p_y} - Y_{p_z}\right)$	• ((1/2)(1/sqrt(2))(1/sqrt(2pi))+(1/2)((sqrt(3)sin(u)/2)(cos(t)/sqrt(pi)))+(1/2)((sqrt(3)sin(u)/2)(sin(t)/sqrt(pi)))+(1/2)(sqrt(6)cos(u)/2)(1/(sqrt(2pi))))^2 • ((1/2)(1/sqrt(2))(1/sqrt(2pi))+(1/2)((sqrt(3)sin(u)/2)(cos(t)/sqrt(pi)))-(1/2)((sqrt(3)sin(u)/2)(sin(t)/sqrt(pi)))-(1/2)(sqrt(6)cos(u)/2)(1/(sqrt(2pi))))^2 • ((1/2)(1/sqrt(2))(1/sqrt(2pi))-(1/2)((sqrt(3)sin(u)/2)(cos(t)/sqrt(pi)))-(1/2)((sqrt(3)sin(u)/2)(sin(t)/sqrt(pi)))+(1/2)(sqrt(6)cos(u)/2)(1/(sqrt(2pi))))^2 • ((1/2)(1/sqrt(2))(1/sqrt(2pi))-(1/2)((sqrt(3)sin(u)/2)(cos(t)/sqrt(pi)))+(1/2)((sqrt(3)sin(u)/2)(sin(t)/sqrt(pi)))-(1/2)(sqrt(6)cos(u)/2)(1/(sqrt(2pi))))^2
sp^2d (square planar)	$Y_{sp^2d}(1) = \frac{1}{2}Y_s + \frac{1}{\sqrt{2}}Y_{p_x} + \frac{1}{2}Y_{d_{x^2-y^2}}$ $Y_{sp^2d}(2) = \frac{1}{2}Y_s - \frac{1}{\sqrt{2}}Y_{p_x} + \frac{1}{2}Y_{d_{x^2-y^2}}$ $Y_{sp^2d}(3) = \frac{1}{2}Y_s + \frac{1}{\sqrt{2}}Y_{p_y} - \frac{1}{2}Y_{d_{x^2-y^2}}$ $Y_{sp^2d}(4) = \frac{1}{2}Y_s - \frac{1}{\sqrt{2}}Y_{p_y} - \frac{1}{2}Y_{d_{x^2-y^2}}$	• ((1/2)(1/sqrt(2))(1/sqrt(2pi))+(sqrt(1/2))(sqrt(3)sin(u)/2)(cos(t)/sqrt(pi))+(1/2)(sqrt(15) (sin(u))^2/4)(cos(2t)/sqrt(pi)))^2 • ((1/2)(1/sqrt(2))(1/sqrt(2pi))-(sqrt(1/2))(sqrt(3)sin(u)/2)(cos(t)/sqrt(pi))+(1/2)(sqrt(15)(sin(u))^2/4)(cos(2t)/sqrt(pi)))^2 • ((1/2)(1/sqrt(2))(1/sqrt(2pi))+(sqrt(1/2))(sqrt(3)sin(u)/2)(sin(t)/sqrt(pi))-(1/2)(sqrt(15)(sin(u))^2/4)(cos(2t)/sqrt(pi)))^2 • ((1/2)(1/sqrt(2))(1/sqrt(2pi))-(sqrt(1/2))(sqrt(3)sin(u)/2)(sin(t)/sqrt(pi))-(1/2)(sqrt(15)(sin(u))^2/4)(cos(2t)/sqrt(pi)))^2

sp^3d (trigonal bipyramidal)	$Y_{sp^3d}(1) = \frac{1}{\sqrt{3}}Y_s + \frac{1}{\sqrt{6}}Y_{p_x} + \frac{1}{\sqrt{2}}Y_{p_y}$ $Y_{sp^3d}(2) = \frac{1}{\sqrt{3}}Y_s + \frac{1}{\sqrt{6}}Y_{p_x} - \frac{1}{\sqrt{2}}Y_{p_y}$ $Y_{sp^3d}(3) = \frac{1}{\sqrt{3}}Y_s - \sqrt{\frac{2}{3}}Y_{p_x}$ $Y_{sp^3d}(4) = \frac{1}{\sqrt{2}}Y_{d_{z^2}} + \frac{1}{\sqrt{2}}Y_{p_z}$ $Y_{sp^3d}(5) = \frac{1}{\sqrt{2}}Y_{d_{z^2}} - \frac{1}{\sqrt{2}}Y_{p_z}$	• ((sqrt(1/3))(1/sqrt(2))(1/sqrt(2pi))+(sqrt(1/3))(sqrt(3)sin(u)/2)(cos(t)/sqrt(pi))+(sqrt(1/2))(sqrt(3)sin(u)/2)(sin(t)/sqrt(pi)))^2 • ((sqrt(1/3))(1/sqrt(2))(1/sqrt(2pi))+(sqrt(1/3))(sqrt(3)sin(u)/2)(cos(t)/sqrt(pi))-(sqrt(1/2))(sqrt(3)sin(u)/2)(sin(t)/sqrt(pi)))^2 • ((sqrt(1/3))(1/sqrt(2))(1/sqrt(2pi))-(sqrt(2/3))(sqrt(3)sin(u)/2)(cos(t)/sqrt(pi)))^2 • ((sqrt(1/2))(sqrt(10)((3(cos(u))^2)-1)/4)(1/sqrt(2pi))+(sqrt(1/2))(sqrt(6)cos(u)/2)(1/(sqrt(2pi))))^2 • ((sqrt(1/2))(sqrt(10)((3(cos(u))^2)-1)/4)(1/sqrt(2pi))-(sqrt(1/2))(sqrt(6)cos(u)/2)(1/(sqrt(2pi))))^2
sp^3d^2 (octahedral)	$Y_{sp^3d^2}(1) = \frac{1}{\sqrt{6}}Y_s - \frac{1}{\sqrt{2}}Y_{p_x} - \frac{1}{\sqrt{12}}Y_{d_{z^2}} + \frac{1}{2}Y_{d_{x^2-y^2}}$ $Y_{sp^3d^2}(2) = \frac{1}{\sqrt{6}}Y_s + \frac{1}{\sqrt{2}}Y_{p_x} - \frac{1}{\sqrt{12}}Y_{d_{z^2}} + \frac{1}{2}Y_{d_{x^2-y^2}}$ $Y_{sp^3d^2}(3) = \frac{1}{\sqrt{6}}Y_s - \frac{1}{\sqrt{2}}Y_{p_y} - \frac{1}{\sqrt{12}}Y_{d_{z^2}} - \frac{1}{2}Y_{d_{x^2-y^2}}$ $Y_{sp^3d^2}(4) = \frac{1}{\sqrt{6}}Y_s + \frac{1}{\sqrt{2}}Y_{p_y} - \frac{1}{\sqrt{12}}Y_{d_{z^2}} - \frac{1}{2}Y_{d_{x^2-y^2}}$ $Y_{sp^3d^2}(4) = \frac{1}{\sqrt{6}}Y_s - \frac{1}{\sqrt{2}}Y_{p_z} + \frac{1}{\sqrt{3}}Y_{d_{z^2}}$ $Y_{sp^3d^2}(4) = \frac{1}{\sqrt{6}}Y_s + \frac{1}{\sqrt{2}}Y_{p_z} + \frac{1}{\sqrt{3}}Y_{d_{z^2}}$	• ((1/sqrt(6))(1/sqrt(2))(1/sqrt(2pi))-(1/sqrt(2))(sqrt(3)sin(u)/2)(cos(t)/sqrt(pi))-(1/sqrt(12))(sqrt(10)((3(cos(u))^2)-1)/4)(1/sqrt(2pi))+(1/sqrt(4))(sqrt(15)(sin(u))^2/4) (cos(2t)/sqrt(pi)))^2 • ((1/sqrt(6))(1/sqrt(2))(1/sqrt(2pi))+(1/sqrt(2))(sqrt(3)sin(u)/2)(cos(t)/sqrt(pi))-(1/sqrt(12))(sqrt(10)((3(cos(u))^2)-1)/4)(1/sqrt(2pi))+(1/sqrt(4))(sqrt(15)(sin(u))^2/4) (cos(2t)/sqrt(pi)))^2 • ((1/sqrt(6))(1/sqrt(2))(1/sqrt(2pi))-(1/sqrt(2))(sqrt(3)sin(u)/2)(sin(t)/sqrt(pi))-(1/sqrt(12))(sqrt(10)((3(cos(u))^2)-1)/4)(1/sqrt(2pi))-(1/sqrt(4))(sqrt(15)(sin(u))^2/4) (cos(2t)/sqrt(pi)))^2 • ((1/sqrt(6))(1/sqrt(2))(1/sqrt(2pi))+(1/sqrt(2))(sqrt(3)sin(u)/2)(sin(t)/sqrt(pi))-(1/sqrt(12))(sqrt(10)((3(cos(u))^2)-1)/4)(1/sqrt(2pi))-(1/sqrt(4))(sqrt(15)(sin(u))^2/4)(cos(2t)/sqrt(pi)))^2 • ((1/sqrt(6))(1/sqrt(2))(1/sqrt(2pi))-(1/sqrt(2))(sqrt(6)cos(u)/2)(1/(sqrt(2pi)))+(1/sqrt(3))(sqrt(10)((3(cos(u))^2)-1)/4)(1/sqrt(2pi)))^2 • ((1/sqrt(6))(1/sqrt(2))(1/sqrt(2pi))+(1/sqrt(2))(sqrt(6)cos(u)/2)(1/(sqrt(2pi)))+(1/sqrt(3))(sqrt(10)((3(cos(u))^2)-1)/4)(1/sqrt(2pi)))^2

‡The symbols *u* and *t* in Winplot format are θ and φ for the polar and azimuthal angles respectively.

Visualizing Three-Dimensional Hybrid Atomic Orbitals Using Winplot: An Application for Student Self Instruction

ORIGINALITY REPORT

8%

SIMILARITY INDEX

PRIMARY SOURCES

1	Andrian Saputra, Lorentz R. Canaval, Sunyono, Noor Fadiawati et al. "Visualizing Three-Dimensional Hybrid Atomic Orbitals Using Winplot: An Application for Student Self Instruction", Journal of Chemical Education, 2015 Crossref	61 words — 4%
2	Meghna A. Manae, Anirban Hazra. "Graphical Representation of Hydrogenic Orbitals: Incorporating Both Radial and Angular Parts of the Wave Function", Journal of Chemical Education, 2018 Crossref	20 words — 1%
3	Wilfredo Credo Chung. "Three-Dimensional Atomic Orbital Plots in the Classroom Using Winplot", Journal of Chemical Education, 2013 Crossref	10 words — 1%
4	edoc.pub Internet	9 words — 1%
5	Walter Strampp, Victor Ganzha, Evgenij Vorozhtsov. "Höhere Mathematik mit Mathematica", Springer Science and Business Media LLC, 1997 Crossref	9 words — 1%
6	www.grahamkendall.net Internet	8 words — 1%

EXCLUDE QUOTES	OFF	EXCLUDE MATCHES	OFF
EXCLUDE BIBLIOGRAPHY	OFF		