

Supplementary Material : The Multipoles.

List of the spherical harmonics functions y_{lm} in real form defining the multipoles P_{lm} (Hansen & Coppens, 1978) with the normalization factors.

x , y and z are direction cosines. The normalization factors of the density function are based on $\int |y_{lm}| dV = 2$ except for the case $l=0$ where $\int |y_{lm}| dV = 1$.

(l,m)	y_{lm}	Normalization factor
$(0, 0)$	1	Monopole $1/4\pi$
$(1, 0)$	z	Dipoles $\left. \right\} 1/\pi$
$(1, 1)$	x	
$(1, -1)$	y	
Quadripoles		
$(2, 0)$	$2z^2 - (x^2 + y^2)$	$3\sqrt{3}/8\pi$
$(2, 1)$	zx	$\left. \right\} 3/4$
$(2, -1)$	zy	
$(2, 2)$	xy	
$(2, -2)$	$(x^2 - y^2)/2$	
Octapoles		
$(3, 0)$	$2z^3 - 3z(x^2 + y^2)$	$10/13\pi$
$(3, 1)$	$x [4z^2 - (x^2 + y^2)]$	$\left. \right\} 1/(\arctan(2) + 14/5 - \pi/4)$
$(3, -1)$	$y [4z^2 - (x^2 + y^2)]$	
$(3, 2)$	$z(x - y)(x + y)$	
$(3, -2)$	$2xyz$	$\left. \right\} 1$
$(3, 3)$	$x^3 - 3xy^2$	
$(3, -3)$	$y^3 - 3yx^2$	
Hexadecapoles		
$(4, 0)$	$8z^4 - 24z^2(x^2 + y^2) + 3(x^2 + y^2)^2$	$1/[14(A_-^5 - A_+^5) + 20(A_+^3 - A_-^3) + 6(A_- - A_+)]2\pi$ where $A_{\pm} = [(30 \pm 4\sqrt{30})/70]^{1/2}$
$(4, 1)$	$x [4z^3 - 3z(x^2 + y^2)]$	$\left. \right\} 735 / (512\sqrt{7} - 196)$
$(4, -1)$	$y [4z^3 - 3z(x^2 + y^2)]$	
$(4, 2)$	$(x^2 - y^2)[6z^2 - (x^2 + y^2)]$	
$(4, -2)$	$2xy [6z^2 - (x^2 + y^2)]$	$\left. \right\} 105\sqrt{7} / [4(136 + 28\sqrt{7})]$
$(4, 3)$	$z(x^3 - 3xy^2)$	
$(4, -3)$	$z(y^3 - 3yx^2)$	
$(4, 4)$	$x^4 - 6x^2y^2 + y^4$	$\left. \right\} 15/32$
$(4, -4)$	$4x^3y - 4xy^3$	