

## BASIS FUNCTIONS

Irreducible representations and their basis functions which transform like components of polar vectors  $(x, y, z)$ , axial vectors  $(S_x, S_y, S_z)$  and second-rank tensors  $(x^2, y^2, z^2, yz, xz, xy)$ . An orthogonal coordinate system is used for *all* crystal classes. For hexagonal crystal classes, the  $x$  axis is chosen to be in the direction of the hexagonal  $a$  axis.

Class	Irreducible Representations and Basis Functions
1	$\Gamma_1(x; y; z; S_x; S_y; S_z; x^2; y^2; z^2; yz; xz; xy)$
$\bar{1}$	$\Gamma_1^+(S_x; S_y; S_z; x^2; y^2; z^2; yz; xz; xy), \Gamma_1^-(x; y; z)$
2	$\Gamma_1(y; S_y; x^2; y^2; z^2; xz), \Gamma_2(x; z; S_x; S_z; yz; xy)$
$m$	$\Gamma_1(x; z; S_y; x^2; y^2; z^2; xz), \Gamma_2(y; S_x; S_z; yz; xy)$
$2/m$	$\Gamma_1^+(S_y; x^2; y^2; z^2; xz), \Gamma_2^+(S_x; S_z; yz; xy), \Gamma_1^-(y), \Gamma_2^-(x; z)$
222	$\Gamma_1(x^2; y^2; z^2), \Gamma_2(z; S_z; xy), \Gamma_3(x; S_x; yz), \Gamma_4(y; S_y; xz)$
$mm2$	$\Gamma_1(z; x^2; y^2; z^2), \Gamma_2(S_z; xy), \Gamma_3(y; S_x; yz), \Gamma_4(x; S_y; xz)$
$Amm2$	$\Gamma_1(z; x^2; y^2; z^2), \Gamma_2(S_z; xy), \Gamma_3(x; S_y; xz), \Gamma_4(y; S_x; yz)$
$mmm$	$\Gamma_1^+(x^2; y^2; z^2), \Gamma_2^+(S_z; xy), \Gamma_3^+(S_x; yz), \Gamma_4^+(S_y; xz), \Gamma_2^-(z), \Gamma_3^-(x), \Gamma_4^-(y)$
4	$\Gamma_1(z; S_z; x^2 + y^2; z^2), \Gamma_2(x^2 - y^2; xy), \Gamma_3\Gamma_4(y, x; S_y, S_x; yz, xz)$
$\bar{4}$	$\Gamma_1(S_z; x^2 + y^2; z^2), \Gamma_2(z; x^2 - y^2; xy), \Gamma_3\Gamma_4(x, y; S_y, S_x; yz, xz)$
$4/m$	$\Gamma_1^+(S_z; x^2 + y^2; z^2), \Gamma_2^+(x^2 - y^2; xy), \Gamma_3^+\Gamma_4^+(S_y, S_x; yz, xz), \Gamma_1^-(z), \Gamma_3^-\Gamma_4^-(y, x)$
422	$\Gamma_1(x^2 + y^2; z^2), \Gamma_2(x^2 - y^2), \Gamma_3(z; S_z), \Gamma_4(xy), \Gamma_5(x, y; S_x, S_y; yz, -xz)$
$4mm$	$\Gamma_1(z; x^2 + y^2; z^2), \Gamma_2(x^2 - y^2), \Gamma_3(xy), \Gamma_4(S_z), \Gamma_5(x, y; S_y, -S_x; xz, yz)$
$\bar{4}2m$	$\Gamma_1(x^2 + y^2; z^2), \Gamma_2(x^2 - y^2), \Gamma_3(z; xy), \Gamma_4(S_z), \Gamma_5(x, y; S_x, -S_y; yz, xz)$
$\bar{4}m2$	$\Gamma_1(x^2 + y^2; z^2), \Gamma_2(z; x^2 - y^2), \Gamma_3(S_z), \Gamma_4(xy), \Gamma_5(x, y; S_y, S_x; xz, -yz)$
$4/mmm$	$\Gamma_1^+(x^2 + y^2; z^2), \Gamma_2^+(x^2 - y^2), \Gamma_3^+(S_z), \Gamma_4^+(xy), \Gamma_5^+(S_x, S_y; yz, -xz), \Gamma_3^-(z), \Gamma_5^-(x, y)$
3	$\Gamma_1(z; S_z; x^2 + y^2; z^2), \Gamma_2\Gamma_3(y, x; S_y, S_x; x^2 - y^2, 2xy; yz, xz)$
$\bar{3}$	$\Gamma_1^+(S_z; x^2 + y^2; z^2), \Gamma_2^+\Gamma_3^+(S_y, S_x; x^2 - y^2, 2xy; yz, xz), \Gamma_1^-(z), \Gamma_2^-\Gamma_3^-(y, x)$
312	$\Gamma_1(x^2 + y^2; z^2), \Gamma_2(z; S_z), \Gamma_3(y, -x; S_y, -S_x; x^2 - y^2, -2xy; xz, yz)$
321	$\Gamma_1(x^2 + y^2; z^2), \Gamma_2(z; S_z), \Gamma_3(x, y; S_x, S_y; x^2 - y^2, -2xy; yz, -xz)$
$3m1$	$\Gamma_1(z; x^2 + y^2; z^2), \Gamma_2(S_z), \Gamma_3(y, -x; S_x, S_y; x^2 - y^2, -2xy; yz, -xz)$
$31m$	$\Gamma_1(z; x^2 + y^2; z^2), \Gamma_2(S_z), \Gamma_3(x, y; S_y, -S_x; x^2 - y^2, -2xy; xz, yz)$
$\bar{3}1m$	$\Gamma_1^+(x^2 + y^2; z^2), \Gamma_2^+(S_z), \Gamma_3^+(S_y, -S_x; x^2 - y^2, -2xy; xz, yz), \Gamma_2^-(z), \Gamma_3^-(y, -x)$
$\bar{3}m1$	$\Gamma_1^+(x^2 + y^2; z^2), \Gamma_2^+(S_z), \Gamma_3^+(S_x, S_y; x^2 - y^2, -2xy; yz, -xz), \Gamma_2^-(z), \Gamma_3^-(y, -x)$
6	$\Gamma_1(z; S_z; x^2 + y^2; z^2), \Gamma_3\Gamma_5(x^2 - y^2, 2xy), \Gamma_4\Gamma_6(y, x; S_y, S_x; yz, xz)$
$\bar{6}$	$\Gamma_1(S_z; x^2 + y^2; z^2), \Gamma_2(z), \Gamma_3\Gamma_5(y, x; x^2 - y^2, 2xy), \Gamma_4\Gamma_6(S_y, S_x; yz, xz)$
$6/m$	$\Gamma_1^+(S_z; x^2 + y^2; z^2), \Gamma_3^+\Gamma_5^+(x^2 - y^2, 2xy), \Gamma_4^+\Gamma_6^+(S_y, S_x; yz, xz), \Gamma_1^-(z), \Gamma_4^-\Gamma_6^-(y, x)$
622	$\Gamma_1(x^2 + y^2; z^2), \Gamma_2(z; S_z), \Gamma_5(x^2 - y^2, -2xy), \Gamma_6(y, -x; S_y, -S_x; xz, yz)$
$6mm$	$\Gamma_1(z; x^2 + y^2; z^2), \Gamma_2(S_z), \Gamma_5(x^2 - y^2, -2xy), \Gamma_6(y, -x; S_x, S_y; yz, -xz)$
$\bar{6}m2$	$\Gamma_1(x^2 + y^2; z^2), \Gamma_2(S_z), \Gamma_3(z), \Gamma_5(y, -x; x^2 - y^2, -2xy), \Gamma_6(S_y, -S_x; xz, yz)$
$\bar{6}2m$	$\Gamma_1(x^2 + y^2; z^2), \Gamma_3(z), \Gamma_4(S_z), \Gamma_5(x, y; x^2 - y^2, -2xy), \Gamma_6(S_y, -S_x; xz, yz)$
$6/mmm$	$\Gamma_1^+(x^2 + y^2; z^2), \Gamma_2^+(S_z), \Gamma_5^+(x^2 - y^2, -2xy), \Gamma_6^+(S_y, -S_x; xz, yz), \Gamma_2^-(z), \Gamma_6^-(y, -x)$
23	$\Gamma_1(x^2 + y^2 + z^2), \Gamma_2\Gamma_3(x^2 + y^2 - 2z^2, \sqrt{3}x^2 - \sqrt{3}y^2), \Gamma_4(x, y, z; S_x, S_y, S_z; yz, xz, xy)$
$m\bar{3}$	$\Gamma_1^+(x^2 + y^2 + z^2), \Gamma_2^+\Gamma_3^+(x^2 + y^2 - 2z^2, \sqrt{3}x^2 - \sqrt{3}y^2), \Gamma_4^+(S_x, S_y, S_z; yz, xz, xy), \Gamma_4^-(x, y, z)$
432	$\Gamma_1(x^2 + y^2 + z^2), \Gamma_3(x^2 + y^2 - 2z^2, \sqrt{3}x^2 - \sqrt{3}y^2), \Gamma_4(x, y, z; S_x, S_y, S_z), \Gamma_5(xy, yz, xz)$
$\bar{4}3m$	$\Gamma_1(x^2 + y^2 + z^2), \Gamma_3(x^2 + y^2 - 2z^2, \sqrt{3}x^2 - \sqrt{3}y^2), \Gamma_4(x, y, z; yz, xz, xy), \Gamma_5(S_x, S_y, S_z)$
$m\bar{3}m$	$\Gamma_1^+(x^2 + y^2 + z^2), \Gamma_3^+(x^2 + y^2 - 2z^2, \sqrt{3}x^2 - \sqrt{3}y^2), \Gamma_4^+(S_x, S_y, S_z), \Gamma_5^+(xy, yz, xz), \Gamma_4^-(x, y, z)$