

1.2. REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

Table 1.2.6.11. Special points in the Brillouin zones in three dimensions

(a) Triclinic

k	$K_{\mathbf{k}}$	Kovalev
$a\ 000$	$\bar{1}$	k_8
$b\ 00\frac{1}{2}$	$\bar{1}$	k_7
$c\ 0\frac{1}{2}0$	$\bar{1}$	k_6
$d\ \frac{1}{2}00$	$\bar{1}$	k_5
$e\ \frac{1}{2}\frac{1}{2}0$	$\bar{1}$	k_4
$f\ \frac{1}{2}0\frac{1}{2}$	$\bar{1}$	k_3
$g\ 0\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_2
$h\ \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_1

k	$K_{\mathbf{k}}$	Kovalev
$u\ 0\beta\gamma$	m	k_1
$v\ \frac{1}{2}\beta\gamma$	$m11$	k_2
$w\ \alpha0\gamma$	$1m1$	k_3
$x\ \alpha\frac{1}{2}\gamma$	$1m1$	k_4
$y\ \alpha\beta0$	$11m$	k_5
$z\ \alpha\beta\frac{1}{2}$	$11m$	k_6

k	$K_{\mathbf{k}}$	Kovalev
$-\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{11}
$\frac{1}{2}-\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{12}
$\frac{1}{2}\frac{1}{2}-\frac{1}{2}$	$\bar{1}$	k_{13}
$l\ 0\beta\gamma$	$m11$	k_1
$m\ \alpha0\gamma$	$1m1$	k_2
$n\ \alpha\beta0$	$11m$	k_3

(b) Monoclinic P

k	$K_{\mathbf{k}}$	Kovalev
$a\ 000$	$2/m$	k_7
$b\ 00\frac{1}{2}$	$2/m$	k_{11}
$c\ \frac{1}{2}00$	$2/m$	k_{12}
$d\ 0\frac{1}{2}0$	$2/m$	k_{13}
$e\ 0\frac{1}{2}\frac{1}{2}$	$2/m$	k_9
$f\ \frac{1}{2}0\frac{1}{2}$	$2/m$	k_8
$g\ \frac{1}{2}\frac{1}{2}0$	$2/m$	k_{14}
$h\ \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$2/m$	k_{10}
$i\ 00\gamma$	2	k_3
$j\ 0\frac{1}{2}\gamma$	2	k_5
$k\ \frac{1}{2}0\gamma$	2	k_4
$l\ \frac{1}{2}\frac{1}{2}\gamma$	2	k_6
$m\ \alpha\beta0$	m	k_1
$n\ \alpha\beta\frac{1}{2}$	m	k_2

(e) Orthorhombic C

k	$K_{\mathbf{k}}$	Kovalev
$a\ 000$	mmm	k_{14}
$b\ 010$	mmm	k_{15}
$c\ 01\frac{1}{2}$	mmm	k_{17}
$d\ 00\frac{1}{2}$	mmm	k_{16}
$e\ \frac{1}{2}\frac{1}{2}0$	$2/m$	k_{12}
$f\ \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$2/m$	k_{13}
$g\ \alpha00$	$2mm$	k_8
$h\ \alpha0\frac{1}{2}$	$2mm$	k_9
$i\ 0\beta0$	$m2m$	k_{10}
$j\ 0\beta\frac{1}{2}$	$m2m$	k_{11}
$k\ 00\gamma$	$mm2$	k_6
$l\ 01\gamma$	$mm2$	k_7
$m\ \frac{1}{2}\frac{1}{2}\gamma$	112	k_5
$n\ 0\beta\gamma$	$m11$	k_1
$o\ \alpha0\gamma$	$1m1$	k_2
$p\ \alpha\beta0$	$11m$	k_3
$q\ \alpha\beta\frac{1}{2}$	$11m$	k_4

(h) Tetragonal P

k	$K_{\mathbf{k}}$	Kovalev
$a\ 000$	$4/mmm$	k_{17}
$b\ 00\frac{1}{2}$	$4/mmm$	k_{19}
$c\ \frac{1}{2}\frac{1}{2}0$	$4/mmm$	k_{18}
$d\ \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$4/mmm$	k_{20}
$e\ 0\frac{1}{2}\frac{1}{2}$	mmm	k_{16}
$f\ 0\frac{1}{2}0$	mmm	k_{15}
$g\ 00\gamma$	$4mm$	k_{13}
$h\ \frac{1}{2}\frac{1}{2}\gamma$	$4mm$	k_{14}
$i\ 0\frac{1}{2}\gamma$	$mm2$	k_{12}
$j\ \alpha\alpha0$	$2mm$	k_{10}
$k\ \alpha\alpha\frac{1}{2}$	$2mm$	k_{11}
$l\ 0\beta0$	$m2m$	k_8
$m\ 0\beta\frac{1}{2}$	$m2m$	k_9
$n\ \alpha\frac{1}{2}0$	$2mm$	k_6
$o\ \alpha\frac{1}{2}\frac{1}{2}$	$2mm$	k_7
$p\ \alpha\beta0$	$11m$	k_1
$q\ \alpha\beta\frac{1}{2}$	$11m$	k_2
$r\ \alpha\alpha\gamma$	m	k_5
$s\ 0\beta\gamma$	$m11$	k_3
$t\ \alpha\frac{1}{2}\gamma$	$1m1$	k_4

(c) Monoclinic A

k	$K_{\mathbf{k}}$	Kovalev
$a\ 000$	$2/m$	k_6
$b\ 010$	$2/m$	k_8
$c\ \frac{1}{2}00$	$2/m$	k_7
$d\ \frac{1}{2}10$	$2/m$	k_9
$e\ 0\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_4
$f\ \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_5
$g\ 00\gamma$	2	k_2
$h\ \frac{1}{2}0\gamma$	2	k_3
$i\ \alpha\beta0$	m	k_1

(f) Orthorhombic I

k	$K_{\mathbf{k}}$	Kovalev
$a\ 000$	mmm	k_{17}
$b\ 001$	mmm	k_{18}
$c\ 0\frac{1}{2}\frac{1}{2}$	$2/m11$	k_{13}
$1\ \frac{1}{2}\frac{1}{2}$	$2/m11$	k_{10}
$d\ \frac{1}{2}0\frac{1}{2}$	$12/m1$	k_{14}
$\frac{1}{2}\frac{1}{2}$	$12/m1$	k_{11}
$e\ \frac{1}{2}\frac{1}{2}0$	$112/m$	k_{15}
$\frac{1}{2}\frac{1}{2}1$	$112/m$	k_{12}
$f\ \frac{1}{2}\frac{1}{2}\frac{1}{2}$	222	k_{16}
$g\ \alpha00$	$2mm$	k_7
$h\ 0\beta0$	$m2m$	k_8
$i\ 00\gamma$	$mm2$	k_9
$j\ \frac{1}{2}\frac{1}{2}\gamma$	112	k_6
$k\ \frac{1}{2}\beta\frac{1}{2}$	121	k_5
$l\ \alpha\frac{1}{2}\frac{1}{2}$	211	k_4
$m\ 0\beta\gamma$	$m11$	k_1
$n\ \alpha0\gamma$	$1m1$	k_2
$o\ \alpha\beta0$	$11m$	k_3

(i) Tetragonal I

k	$K_{\mathbf{k}}$	Kovalev
$a\ 000$	$4/mmm$	k_{14}
$b\ 001$	$4/mmm$	k_{15}
$c\ \frac{1}{2}\frac{1}{2}0$	mmm	k_{13}
$d\ \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{4}m2$	k_{12}
$e\ 00\gamma$	$4mm$	k_{10}
$f\ \frac{1}{2}0\frac{1}{2}$	$12/m1$	k_{11}
$g\ \frac{1}{2}\frac{1}{2}\gamma$	$2mm$	k_9
$h\ \alpha\alpha0$	$2mm$	k_7
$i\ \alpha00$	$2mm$	k_7
$j\ \alpha(1-\alpha)0$	$2mm$	k_8
$k\ \frac{1}{2}\beta\frac{1}{2}$	121	k_5
$l\ \alpha\beta0$	$11m$	k_2
$m\ \alpha\alpha\gamma$	m	k_3
$\alpha(1-\alpha)\gamma$	m	k_4
$n\ \alpha0\gamma$	$1m1$	k_1

(d) Orthorhombic P

k	$K_{\mathbf{k}}$	Kovalev
$a\ 000$	mmm	k_{19}
$b\ \frac{1}{2}00$	mmm	k_{20}
$c\ 00\frac{1}{2}$	mmm	k_{22}
$d\ \frac{1}{2}0\frac{1}{2}$	mmm	k_{24}
$e\ 0\frac{1}{2}0$	mmm	k_{21}
$f\ \frac{1}{2}\frac{1}{2}0$	mmm	k_{25}
$g\ 0\frac{1}{2}\frac{1}{2}$	mmm	k_{23}
$h\ \frac{1}{2}\frac{1}{2}\frac{1}{2}$	mmm	k_{26}
$i\ \alpha00$	$2mm$	k_7
$j\ \alpha0\frac{1}{2}$	$2mm$	k_{12}
$k\ \alpha\frac{1}{2}0$	$2mm$	k_{10}
$l\ \alpha\frac{1}{2}\frac{1}{2}$	$2mm$	k_{11}
$m\ 0\beta0$	$m2m$	k_8
$n\ 0\beta\frac{1}{2}$	$m2m$	k_{15}
$o\ \frac{1}{2}\beta0$	$m2m$	k_{13}
$p\ \frac{1}{2}\beta\frac{1}{2}$	$m2m$	k_{14}
$q\ 00\gamma$	$mm2$	k_9
$r\ 0\frac{1}{2}\gamma$	$mm2$	k_{18}
$s\ \frac{1}{2}0\gamma$	$mm2$	k_{16}
$t\ \frac{1}{2}\frac{1}{2}\gamma$	$mm2$	k_{17}

(g) Orthorhombic F

k	$K_{\mathbf{k}}$	Kovalev
$a\ 000$	mmm	k_{14}
$b\ 100$	mmm	k_{15}
$c\ 010$	mmm	k_{16}
$d\ 001$	mmm	k_{17}
$e\ \alpha00$	$2mm$	k_4
$f\ \alpha10$	$2mm$	k_5
$g\ 0\beta0$	$m2m$	k_6
$h\ 1\beta0$	$m2m$	k_7
$i\ 00\gamma$	$mm2$	k_8
$j\ 01\gamma$	$mm2$	k_9
$k\ \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{10}

(j) Trigonal R (rhombohedral axes)

k	$K_{\mathbf{k}}$	Kovalev
$a\ 000$	$\bar{3}m$	k_7
$b\ \frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{3}m$	k_8
$c\ \alpha\alpha\alpha$	$3m$	k_6
$d\ 00\frac{1}{2}$	$2/m$	k_4
$e\ \frac{1}{2}\frac{1}{2}0$	$2/m$	k_5
$f\ \alpha(-\alpha)0$	2	k_2
$g\ \alpha(-\alpha)\frac{1}{2}$	2	k_2
$h\ \alpha\beta\beta$	m	k_1

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

Table 1.2.6.11 (cont.)

(k) Hexagonal *P*

k	$K_{\mathbf{k}}$	Kovalev
<i>a</i> 000	6/ <i>mmm</i>	k_{16}
<i>b</i> 00 $\frac{1}{2}$	6/ <i>mmm</i>	k_{17}
<i>c</i> $\frac{1}{3}\frac{1}{3}0$	$\bar{6}m2$	k_{13}
<i>d</i> $\frac{1}{3}\frac{1}{3}\frac{1}{2}$	$\bar{6}m2$	k_{15}
<i>e</i> 00 γ	6 <i>mm</i>	k_{11}
<i>f</i> $\frac{1}{2}00$	<i>mmm</i>	k_{12}
<i>g</i> $\frac{1}{2}0\frac{1}{2}$	<i>mmm</i>	k_{14}
<i>h</i> $\frac{1}{3}\frac{1}{3}\gamma$	3 <i>m</i>	k_{10}
<i>i</i> $\frac{1}{2}0\gamma$	2 <i>mm</i>	k_9
<i>j</i> $\alpha 00$	2 <i>mm</i>	k_5
<i>k</i> $\alpha 0\frac{1}{2}$	2 <i>mm</i>	k_7
<i>l</i> $\alpha\alpha 0$	2 <i>mm</i>	k_6
<i>m</i> $\alpha\alpha\frac{1}{2}$	2 <i>mm</i>	k_8
<i>n</i> $\alpha 0\gamma$	<i>m</i>	k_3
<i>o</i> $\alpha\alpha\gamma$	<i>m</i>	k_4
<i>p</i> $\alpha\beta 0$	<i>m</i>	k_1
<i>q</i> $\alpha\beta\frac{1}{2}$	<i>m</i>	k_2

(l) Cubic *P*

k	$K_{\mathbf{k}}$	Kovalev
<i>a</i> 000	$m\bar{3}m$	k_{12}
<i>b</i> $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$m\bar{3}m$	k_{13}
<i>c</i> $\frac{1}{2}\frac{1}{2}0$	4/ <i>mmm</i>	k_{11}
<i>d</i> 00 $\frac{1}{2}$	4/ <i>mmm</i>	k_{10}
<i>e</i> 00 γ	4 <i>mm</i>	k_8
<i>f</i> $\frac{1}{2}\frac{1}{2}\gamma$	4 <i>mm</i>	k_7
<i>g</i> $\alpha\alpha\alpha$	3 <i>m</i>	k_9
<i>h</i> $\frac{1}{2}0\gamma$	<i>mm</i> 2	k_6
<i>i</i> $\alpha\alpha 0$	2 <i>mm</i>	k_4
<i>j</i> $\alpha\alpha\frac{1}{2}$	2 <i>mm</i>	k_5
<i>k</i> $\alpha\beta 0$	11 <i>m</i>	k_1
<i>l</i> $\alpha\beta\frac{1}{2}$	11 <i>m</i>	k_2
<i>m</i> $\alpha\alpha\gamma$	<i>m</i>	k_3

(m) Cubic *F*

k	$K_{\mathbf{k}}$	Kovalev
<i>a</i> 000	$m\bar{3}m$	k_{11}
<i>b</i> 001	4/ <i>mmm</i>	k_{10}
<i>c</i> $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{3}m$	k_9
<i>d</i> 10 $\frac{1}{2}$	4 <i>m</i> 2	k_8
<i>e</i> $\alpha 00$	4 <i>mm</i>	k_6
<i>f</i> $\alpha\alpha\alpha$	3 <i>m</i>	k_5
<i>g</i> $\alpha 01$	2 <i>mm</i>	k_7
<i>h</i> $\alpha\alpha 0$	2 <i>mm</i>	k_4
<i>i</i> $\alpha(1-\alpha)\frac{1}{2}$	2	k_3
<i>j</i> $\alpha\beta$	11 <i>m</i>	k_1
<i>k</i> $\alpha\alpha\gamma$	<i>m</i>	k_2

(n) Cubic *I*

k	$K_{\mathbf{k}}$	Kovalev
<i>a</i> 000	$m\bar{3}m$	k_{11}
<i>b</i> 001	$m\bar{3}m$	k_{10}
<i>c</i> $\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{4}3m$	k_{10}
<i>d</i> $\frac{1}{2}\frac{1}{2}0$	<i>mmm</i>	k_9
<i>e</i> $\alpha 00$	4 <i>mm</i>	k_8
<i>f</i> $\alpha\alpha\alpha$	3 <i>m</i>	k_7
<i>g</i> $\alpha\frac{1}{2}\frac{1}{2}$	2 <i>mm</i>	k_6
<i>h</i> $\alpha\alpha 0$	2 <i>mm</i>	k_4
<i>i</i> $\alpha(1-\alpha)0$	2 <i>mm</i>	k_9
<i>j</i> $\alpha\beta$	11 <i>m</i>	k_1
<i>k</i> $\alpha\alpha\gamma$	<i>m</i>	k_2
$\alpha(1-\alpha)\gamma$	<i>m</i>	k_3

Table 1.2.6.12. Magnetic point groups

Type I	Type II	Type III
1	1'	$\bar{1}'$
$\bar{1}$	$\bar{1}1'$	
2	21'	2'
<i>m</i>	<i>m</i> 1'	<i>m</i> '
2/ <i>m</i>	21'/ <i>m</i>	2'/ <i>m</i> , 2/ <i>m</i> ', 2'/ <i>m</i> '
222	2221'	2'2'
2 <i>mm</i>	2 <i>mm</i> 1'	2' <i>mm</i> ', 2 <i>m</i> ' <i>m</i> '
<i>mmm</i>	<i>mmm</i> 1'	<i>m</i> ' <i>mm</i> ', <i>m</i> ' <i>m</i> ' <i>m</i> ', <i>m</i> ' <i>m</i> ' <i>m</i> '
4	41'	4'
$\bar{4}$	41'	$\bar{4}'$
4/ <i>m</i>	41'/ <i>m</i>	4'/ <i>m</i> , 4/ <i>m</i> ', 4'/ <i>m</i> '
422	4221'	4'22', 42'2'
4 <i>mm</i>	4 <i>mm</i> 1'	4' <i>mm</i> ', 4 <i>m</i> ' <i>m</i> '
42 <i>m</i>	42 <i>m</i> 1'	4'2' <i>m</i> ', 4'2 <i>m</i> '', 42' <i>m</i> '
4/ <i>mmm</i>	4/ <i>mmm</i> 1'	4/ <i>m</i> ' <i>mm</i> ', 4'/ <i>mm</i> ' <i>m</i> ', 4'/ <i>m</i> ' <i>m</i> ' <i>m</i> ', 4/ <i>mm</i> ' <i>m</i> '', 4/ <i>m</i> ' <i>m</i> ' <i>m</i> '
3	31'	$\bar{3}'$
$\bar{3}$	31'	
32	321'	32'
3 <i>m</i>	3 <i>m</i> 1'	3 <i>m</i> '
$\bar{3}m$	3 <i>m</i> 1'	3' <i>m</i> ', 3' <i>m</i> '', 3' <i>m</i> '
6	61'	6'
$\bar{6}$	61'	$\bar{6}'$
6/ <i>m</i>	61'/ <i>m</i>	6'/ <i>m</i> , 6/ <i>m</i> ', 6'/ <i>m</i> '
622	6221'	6'22', 62'2'
6 <i>mm</i>	6 <i>mm</i> 1'	6' <i>mm</i> ', 6 <i>m</i> ' <i>m</i> '
62 <i>m</i>	62 <i>m</i> 1'	6'2' <i>m</i> ', 6'2 <i>m</i> '', 62' <i>m</i> '
6/ <i>mmm</i>	6/ <i>mmm</i> 1'	6/ <i>m</i> ' <i>mm</i> ', 6'/ <i>mm</i> ' <i>m</i> ', 6'/ <i>m</i> ' <i>m</i> ' <i>m</i> ', 6/ <i>mm</i> ' <i>m</i> '', 6/ <i>m</i> ' <i>m</i> ' <i>m</i> '
23	231'	$m\bar{3}$
$m\bar{3}$	$m\bar{3}1'$	
432	4321'	4'32'
43 <i>m</i>	43 <i>m</i> 1'	4'3 <i>m</i> '
$m\bar{3}m$	$m\bar{3}m1'$	$m\bar{3}'m$, $m\bar{3}'m'$, $m\bar{3}'m'$

dimension, the rank, the permutation symmetry and the setting basis transformation, and the calculated data: the number of independent elements (*f*) and the relations of these elements. They are either zero or expressed in terms of the free parameters a_0, \dots, a_{f-1} . The tensor elements are given by sequences x, y, z, \dots . The four elements of a general rank-two tensor in two dimensions are xx, xy, yx, yy , corresponding to T_{11}, T_{12}, T_{21} and T_{22} , respectively.

1.2.7.3. Characters

Calculations with characters of representations of point groups can be done in the character module of the program. It is selected in the main window by clicking 'character'. A selection window opens in which a point group may be selected just as in the tensor module. The point groups are organized according to dimension and geometric crystal class. Selection of a point group leads to the display of the character table if one asks for it by selecting 'view character table'.

The character table consists of a square array of (complex) numbers. The number of rows is the number of nonequivalent irreducible representations and is equal to the number of columns, which is the number of conjugacy classes of the group. For crystallographic groups, the complex numbers that form the entries of the character table are cyclotomic numbers. These are linear combinations with fractions as coefficients of complex numbers of the form $\exp(2\pi i n/m)$. For example, the square root of -1 (*i*) can be written as $\exp(2\pi i/4)$. A real number like $\sqrt{2}$ can be written as

$$\sqrt{2} = \frac{1}{2}\sqrt{2}(1+i+1-i) = \exp(2\pi i/3) + \exp(2\pi i/3).$$

Another example is

$$\sqrt{5} = 1 + 2\exp(2\pi i/5) + 2\exp(2\pi i/5).$$