

The k-vector types of space group *Fm-3m* (225)

(Table for arithmetic crystal class *m -3 mF*)

*Fm-3m-O_h*⁵ (225) to *Fd-3c-O_h*⁸(228)

Reciprocal-space group (*Im-3m*)^{*}, No.229

Brillouin zone

k-vector description			ITA description			
CDML ¹		Conventional basis	Wyckoff Position		Coordinates	
Label	Primitive basis					
GM	0,0,0	0,0,0	2	a	m-3m	0,0,0
X	1/2,0,1/2	0,1,0	6	b	4/mm.m	0,1/2,0
L	1/2,1/2,1/2	1/2,1/2,1/2	8	c	.-3m	1/4,1/4,1/4
W	1/2,1/4,3/4	1/2,1,0	12	d	-4m.2	1/4,1/2,0
DT	u,0,u	0,2u,0	12	e	4m.m	0,y,0 : 0 < y < 1/2
LD	u,u,u	u,u,u	16	f	.3m	x,x,x : 0 < x < 1/4
V	1/2,u,1/2+u	2u,1,0	24	g	mm2..	x,1/2,0 : 0 < x < 1/4
SM	u,u,2u ex	2u,2u,0	24	h	m.m2	x,x,0 : 0 < x <= 3/8
S	1/2+u,2u,1/2+u ex	2u,1,2u	24	h	m.m2	x,1/2,x : 0 < x < 1/8
S~SM ₁ =[K M]			24	h	m.m2	x,x,0 : 3/8 < x < 1/2
SM SM ₁ =[GM M]			24	h	m.m2	x,x,0 : 0 < x < 1/2
Q	1/2,1/4+u,3/4-u	1/2,1-2u,2u	48	i	..2	1/4,1/2-y,y : 0 < y < 1/4
A	u,-u+v,v ex	-2u+2v,2u,0	48	j	m..	x,y,0 : 0 < x < y <= 3/8 U U x,y,0 : 0 < x < 3/4-y < y < 1/2
B	1/2+u,u+v,1/2+v	2v,1,2u	48	j	m..	x,1/2,z : 0 <

	ex					$z < x \leq 1/4 - z$
$B \sim B_1 = [K \ M \ W]$			48	j	m..	$x, y, 0 : 3/4 - y \leq x < y < 1/2$
$A \ B_1 = [GM \ M \ X]$			48	j	m..	$x, y, 0 : 0 < x < y < 1/2$
C	u,u,v ex	v,v,-v+2u	48	k	..m	$x, x, z : 0 < z < x \leq 3/8 - z/2$
J	u,v,u[GMXUL] ex	v,-v+2u,v	48	k	..m	$x, y, x : 0 < x < y \leq 1/2 - x \cup$ $\cup x, y, x : 1/4 < y < 1/2,$ $1/2 - y < x < 3/8 - y/2$
$J \sim J_1 = [GM \ L \ X_3] + [L \ K \ M]$			48	k	..m	$x, x, z : 0 < x < z \leq 1/2 - x \cup$ $\cup x, x, z : 0 < z < 1/4, 3/8 - z/2 < x < 1/2 - z$
$C + J_1 = [GM \ M \ X_3] \setminus [GM \ L]$			48	k	..m	$x, x, z : 0 < z < 1/2 - x < 1/2, x \neq z$
GP	u,v,w	-u+w+v, u+w-v, u-w+v	96	l	1	$x, y, z : 0 < z < x < y < 1/2 - x \cup$ $\cup x, y, z : 0 < z < 1/2 - y < x < y < 1/2 \cup$ $\cup x, y, 1/2 - y : 1/4 < y < 1/2;$ $1/2 - y < x < 1/4.$

The asymmetric unit of ITA is obtained from that used in these tables by
reflection through the plane x, x, z .

The asymmetric unit is obtained from the representation domain of CDML by the equivalence

$[L \ K \ W \ M] \sim [L \ U \ W \ X]$ through the two-fold rotation around the axis Q.

Wing: $[GM \ L \ X_3] \ x, x, z : 0 < x < z < 1/2 - x$

¹ Cracknell, A. P., Davies, B.L., Miller, S. C., and Love, W. F. (1979). Kronecker Product Tables. Vol. 1. General Introduction and Tables of Irreducible Representations of Space Groups. New York: IFI/Plenum.

If you want to identify a **k**-vector you have to introduce:

1. The reciprocal bases:

2. The

k-vector: k_x k_y k_z

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