

11 Tabela Internacional de Cristalografia

1. As tabelas internacionais de cristalografia mostram as seguintes informações para o grupo $Fm\bar{3}m$:

CONTINUED		No. 225				$Fm\bar{3}m$	
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)							
Positions							
Multiplicity, Wyckoff letter, Site symmetry	(0,0,0)+	(0, $\frac{1}{2}$, $\frac{1}{2}$)+	($\frac{1}{2}$,0, $\frac{1}{2}$)+	($\frac{1}{2}$, $\frac{1}{2}$,0)+	Reflection conditions		
192 <i>l</i> 1	(1) x,y,z (5) z,x,y (9) y,z,x (13) y,x,z (17) x,z,\bar{y} (21) z,y,\bar{x} (25) \bar{x},\bar{y},\bar{z} (29) \bar{z},\bar{x},\bar{y} (33) \bar{y},\bar{x},z (37) \bar{y},\bar{x},z (41) \bar{x},\bar{z},y (45) \bar{z},\bar{y},x	(2) \bar{x},\bar{y},z (6) z,\bar{x},\bar{y} (10) \bar{y},z,\bar{x} (14) \bar{y},\bar{x},z (18) \bar{x},z,y (22) z,\bar{y},x (26) x,y,z (30) z,x,y (34) y,z,x (38) y,x,z (42) x,\bar{z},\bar{y} (46) z,y,\bar{x}	(3) \bar{x},y,\bar{z} (7) \bar{z},\bar{x},y (11) y,\bar{x},\bar{z} (15) y,\bar{x},z (19) \bar{x},z,\bar{y} (23) \bar{z},y,x (27) x,\bar{y},z (31) z,x,\bar{y} (35) \bar{y},z,x (39) \bar{y},x,\bar{z} (43) x,z,y (47) z,\bar{y},\bar{x}	(4) x,\bar{y},\bar{z} (8) \bar{z},x,\bar{y} (12) \bar{y},z,x (16) \bar{y},x,z (20) x,\bar{z},y (24) \bar{z},\bar{y},\bar{x} (28) \bar{x},y,z (32) z,\bar{x},y (36) y,z,\bar{x} (40) y,\bar{x},\bar{z} (44) \bar{x},z,\bar{y} (48) z,y,x	h,k,l permutable General: $hkl : h+k, h+l, k+l = 2n$ $OkI : k, l = 2n$ $hhl : h+l = 2n$ $h00 : h = 2n$		
Special: as above, plus							
96 <i>k</i> . . <i>m</i>	x,x,z \bar{z},\bar{x},x x,x,\bar{z} \bar{x},\bar{z},\bar{x}	\bar{x},\bar{x},z \bar{z},x,\bar{x} \bar{x},\bar{x},z x,\bar{z},\bar{x}	\bar{x},x,\bar{z} x,z,x \bar{x},x,z z,x,\bar{x}	x,\bar{x},\bar{z} \bar{x},z,\bar{x} \bar{x},x,z z,\bar{x},x	z,x,x x,\bar{z},\bar{x} \bar{x},z,x \bar{z},x,x	no extra conditions	
96 <i>j</i> <i>m</i> . .	$0,y,z$ $z,0,y$ $y,0,z$ $0,\bar{z},\bar{y}$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$ $\bar{y},0,\bar{z}$ $0,z,y$	$0,y,\bar{z}$ $y,z,0$ $y,0,z$ $z,\bar{y},0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$ $\bar{y},0,z$ $z,\bar{y},0$	$z,0,y$ $y,\bar{z},0$ $0,z,\bar{y}$ $\bar{z},y,0$	no extra conditions	
48 <i>i</i> <i>m</i> . <i>m</i> 2	$\frac{1}{2},y,y$ $\bar{y},\frac{1}{2},y$	$\frac{1}{2},\bar{y},y$ $\bar{y},\frac{1}{2},\bar{y}$	$\frac{1}{2},y,\bar{y}$ $y,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{y}$ $\bar{y},y,\frac{1}{2}$	$y,\frac{1}{2},y$ $y,\bar{y},\frac{1}{2}$	no extra conditions	
48 <i>h</i> <i>m</i> . <i>m</i> 2	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,\bar{y},0$	no extra conditions	
48 <i>g</i> 2 <i>m</i> <i>m</i>	$x,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},x,\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$ $x,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$ $\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$ $\frac{1}{2},\frac{1}{2},\bar{x}$	$hkl : h = 2n$	
32 <i>f</i> . 3 <i>m</i>	x,x,x x,x,\bar{x}	\bar{x},\bar{x},x \bar{x},\bar{x},\bar{x}	\bar{x},x,\bar{x} x,\bar{x},x	x,\bar{x},\bar{x} \bar{x},x,x	no extra conditions		
24 <i>e</i> 4 <i>m</i> . <i>m</i>	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
24 <i>d</i> <i>m</i> . <i>m</i> <i>m</i>	$0,\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$hkl : h = 2n$
8 <i>c</i> $\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					$hkl : h = 2n$
4 <i>b</i> $m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	no extra conditions					
4 <i>a</i> $m\bar{3}m$	$0,0,0$	no extra conditions					
Symmetry of special projections							
Along [001] $p4mm$ $a' = \frac{1}{2}a$ $b' = \frac{1}{2}b$ Origin at $0,0,z$	Along [111] $p6mm$ $a' = \frac{1}{3}(2a-b-c)$ $b' = \frac{1}{3}(-a+2b-c)$ Origin at x,x,x		Along [110] $c2mm$ $a' = \frac{1}{2}(-a+b)$ $b' = c$ Origin at $x,x,0$				

Colocamos dentro de uma malha um átomo A na posição de Wyckoff *c* e um átomo B na posição *a*.

- Qual o sistema cristalino desta estrutura?
- O que podemos dizer sobre os parâmetros de rede desta malha?
- Esquematize a estrutura ao longo do eixo *c*.
- Qual a fórmula estequiométrica do composto.
- Qual o número de vizinhos próximos do átomo A.
- Qual o número de vizinhos próximos do átomo B.
- Qual é a simetria (figura geométrica formada pelos vizinhos) em torno de cada átomo?
- Calcule a distância A-B em função dos parâmetros de rede.