

MSG No. 35.166 $Cmm21'$ [Type II, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: $mm21'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 9, 10, 11, 12]$
2	$[\frac{1}{2}, \frac{1}{2}, z]$	$[5, 6, 7, 8, 13, 14, 15, 16]$

Table 2: Wyckoff site: 2b, site symmetry: $mm21'$

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 2, 3, 4, 9, 10, 11, 12]$
2	$[\frac{1}{2}, 0, z]$	$[5, 6, 7, 8, 13, 14, 15, 16]$

Table 3: Wyckoff site: 4c, site symmetry: $. . 21'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, z]$	$[1, 6, 9, 14]$
2	$[\frac{3}{4}, \frac{3}{4}, z]$	$[2, 5, 10, 13]$
3	$[\frac{3}{4}, \frac{1}{4}, z]$	$[3, 8, 11, 16]$
4	$[\frac{1}{4}, \frac{3}{4}, z]$	$[4, 7, 12, 15]$

Table 4: Wyckoff site: 4d, site symmetry: $.m.1'$

No.	position	mapping
1	$[x, 0, z]$	$[1, 4, 9, 12]$
2	$[-x, 0, z]$	$[2, 3, 10, 11]$
3	$[x + \frac{1}{2}, \frac{1}{2}, z]$	$[5, 8, 13, 16]$
4	$[\frac{1}{2} - x, \frac{1}{2}, z]$	$[6, 7, 14, 15]$

Table 5: Wyckoff site: 4e, site symmetry: $m. . 1'$

No.	position	mapping
1	$[0, y, z]$	$[1, 3, 9, 11]$
2	$[0, -y, z]$	$[2, 4, 10, 12]$
3	$[\frac{1}{2}, y + \frac{1}{2}, z]$	$[5, 7, 13, 15]$
4	$[\frac{1}{2}, \frac{1}{2} - y, z]$	$[6, 8, 14, 16]$

Table 6: Wyckoff site: **8f**, site symmetry: **11'**

No.	position	mapping
1	$[x, y, z]$	[1,9]
2	$[-x, -y, z]$	[2,10]
3	$[-x, y, z]$	[3,11]
4	$[x, -y, z]$	[4,12]
5	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[5,13]
6	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[6,14]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[7,15]
8	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[8,16]