

MSG No. 54.341 $Pcc\alpha'$ [Type III, orthorhombic]

Table 1: Wyckoff site: **4a**, site symmetry: $-1'$

No.	position	mapping
1	[0, 0, 0]	[1, 7]
2	[\frac{1}{2}, 0, 0]	[2, 8]
3	[\frac{1}{2}, 0, \frac{1}{2}]	[3, 5]
4	[0, 0, \frac{1}{2}]	[4, 6]

Table 2: Wyckoff site: **4b**, site symmetry: $-1'$

No.	position	mapping
1	[0, \frac{1}{2}, 0]	[1, 7]
2	[\frac{1}{2}, \frac{1}{2}, 0]	[2, 8]
3	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[3, 5]
4	[0, \frac{1}{2}, \frac{1}{2}]	[4, 6]

Table 3: Wyckoff site: **4c**, site symmetry: $.2'$.

No.	position	mapping
1	[0, y, \frac{1}{4}]	[1, 6]
2	[\frac{1}{2}, -y, \frac{1}{4}]	[2, 5]
3	[\frac{1}{2}, y, \frac{3}{4}]	[3, 8]
4	[0, -y, \frac{3}{4}]	[4, 7]

Table 4: Wyckoff site: **4d**, site symmetry: $\dots 2$

No.	position	mapping
1	[\frac{1}{4}, 0, z]	[1, 2]
2	[\frac{1}{4}, 0, z + \frac{1}{2}]	[3, 4]
3	[\frac{3}{4}, 0, \frac{1}{2} - z]	[5, 6]
4	[\frac{3}{4}, 0, -z]	[7, 8]

Table 5: Wyckoff site: **4e**, site symmetry: $\dots 2$

No.	position	mapping
1	[\frac{1}{4}, \frac{1}{2}, z]	[1, 2]
2	[\frac{1}{4}, \frac{1}{2}, z + \frac{1}{2}]	[3, 4]

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{2} - z\right]$	[5,6]
4	$\left[\frac{3}{4}, \frac{1}{2}, -z\right]$	[7,8]

Table 6: Wyckoff site: 8f, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$\left[\frac{1}{2} - x, -y, z\right]$	[2]
3	$\left[\frac{1}{2} - x, y, z + \frac{1}{2}\right]$	[3]
4	$\left[x, -y, z + \frac{1}{2}\right]$	[4]
5	$\left[x + \frac{1}{2}, -y, \frac{1}{2} - z\right]$	[5]
6	$\left[-x, y, \frac{1}{2} - z\right]$	[6]
7	$\left[-x, -y, -z\right]$	[7]
8	$\left[x + \frac{1}{2}, y, -z\right]$	[8]