

MSG No. 54.344  $Pc'ca'$  [ Type III, orthorhombic ]

Table 1: Wyckoff site: 4a, site symmetry: -1

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

Table 2: Wyckoff site: 4b, site symmetry: -1

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

Table 3: Wyckoff site: 4c, site symmetry: .2.

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

Table 4: Wyckoff site: 4d, site symmetry: ..2'

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

Table 5: Wyckoff site: 4e, site symmetry: ..2'

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

*continued ...*

Table 5

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

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

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