

MSG No. 54.337 *Pcca* [Type I, orthorhombic]

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

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

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

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

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

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

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

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

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

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

continued ...

Table 5

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

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

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