

MSG No. 56.365 *Pccn* [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, \frac{1}{2}, \frac{1}{2}]	[3, 7]
4	[\frac{1}{2}, \frac{1}{2}, 0]	[4, 8]

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

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

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

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

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

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

Table 5: Wyckoff site: **8e**, site symmetry: **1**

No.	position	mapping
1	[x, y, z]	[1]
2	[x + \frac{1}{2}, -y, \frac{1}{2} - z]	[2]

continued ...

Table 5

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