

MSG No. 61.435 *Pb'ca* [Type III, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: **8c**, site symmetry: **1**

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