

MPG No. 13.2.45 $4mm1'$ [Type II, tetragonal]

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

No.	position	mapping
1	[0, 0, z]	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]

Table 2: Wyckoff site: **4b**, site symmetry: **..m**

No.	position	mapping
1	[x, x, z]	[1,7,9,15]
2	[-x, -x, z]	[2,8,10,16]
3	[-x, x, z]	[3,5,11,13]
4	[x, -x, z]	[4,6,12,14]

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

No.	position	mapping
1	[x, 0, z]	[1,6,9,14]
2	[-x, 0, z]	[2,5,10,13]
3	[0, x, z]	[3,7,11,15]
4	[0, -x, z]	[4,8,12,16]

Table 4: Wyckoff site: **8d**, site symmetry: **1**

No.	position	mapping
1	[x, y, z]	[1,9]
2	[-x, -y, z]	[2,10]
3	[-y, x, z]	[3,11]
4	[y, -x, z]	[4,12]
5	[x, -y, z]	[6,14]
6	[-x, y, z]	[5,13]
7	[-y, -x, z]	[8,16]
8	[y, x, z]	[7,15]