

Table 1: Wyckoff site: 1o, site symmetry: $-4m21'$

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

 Table 2: Wyckoff site: 2a, site symmetry: $2mm$.

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

 Table 3: Wyckoff site: 4b, site symmetry: $\dots 2$

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

 Table 4: Wyckoff site: 4c, site symmetry: $\dots m$.

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

Table 5: Wyckoff site: 8d, site symmetry: 1

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

continued ...

Table 5

No.	position	mapping
8	$[-y, -x, -z]$	[5,13]