

Table 1: Wyckoff site: 1o, site symmetry: $-42m$

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

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

No.	position	mapping
1	[0, 0, z]	[1, 2, 7, 8]
2	[0, 0, $-z$]	[3, 4, 5, 6]

Table 3: Wyckoff site: 4b, site symmetry: $.2.$

No.	position	mapping
1	[x , 0, 0]	[1, 6]
2	[$-x$, 0, 0]	[2, 5]
3	[0, $-x$, 0]	[3, 7]
4	[0, x , 0]	[4, 8]

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

No.	position	mapping
1	[x , x , z]	[1, 8]
2	[$-x$, $-x$, z]	[2, 7]
3	[x , $-x$, $-z$]	[3, 6]
4	[$-x$, x , $-z$]	[4, 5]

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

No.	position	mapping
1	[x , y , z]	[1]
2	[$-x$, $-y$, z]	[2]
3	[y , $-x$, $-z$]	[3]
4	[$-y$, x , $-z$]	[4]
5	[$-x$, y , $-z$]	[5]
6	[x , $-y$, $-z$]	[6]
7	[$-y$, $-x$, z]	[7]

continued ...

Table 5

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