

Table 1: Wyckoff site: $1a$, site symmetry: $6'm'm$

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

Table 2: Wyckoff site: $6b$, site symmetry: $.m$

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

Table 3: Wyckoff site: $6c$, site symmetry: $.m.$

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

Table 4: Wyckoff site: $12d$, site symmetry: 1

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

12	$[-x, -x + y, z]$	[10]
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