

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	$[y, x, z]$	$[7, 15]$