

PG No. 13 C_{4v} $4mm$ [tetragonal]

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

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

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

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

Table 4: 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	$[-y, -x, z]$	$[7]$
8	$[y, x, z]$	$[8]$