MPG No. 12.2.41 4221′ [Type II, tetragonal]

Table 1: Wyckoff site: 1o, site symmetry: 4221'

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: 4..

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

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

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

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]