PG No. 12 D_4 422   [tetragonal]

Table 1: Wyckoff site: 1o, site symmetry: 422

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

Table 2: Wyckoff site: 2a, site symmetry: 4..

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

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

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

Table 4: Wyckoff site: 4c, 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 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 ...

1

Table 5

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