

Table 1: Wyckoff site: 2a, site symmetry: $-4..1'$

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

Table 2: Wyckoff site: 2b, site symmetry: $-4..1'$

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

Table 3: Wyckoff site: 4c, site symmetry: $2..1'$

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

Table 4: Wyckoff site: 4d, site symmetry: $2..1'$

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

Table 5: Wyckoff site: 8e, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 9]$
2	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	$[2, 10]$
3	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	$[3, 11]$
4	$[-x, -y, z]$	$[4, 12]$
5	$[y, -x, -z]$	$[5, 13]$
6	$[-y, x, -z]$	$[6, 14]$

continued ...

Table 5

No.	position	mapping
7	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[7,15]
8	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[8,16]