

Table 1: Wyckoff site: **2a**, site symmetry: $2.mm1'$

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry: $..m1'$

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

Table 4: Wyckoff site: **8d**, site symmetry: $11'$

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